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Asymmetric Transfer Hydrogenation of Ketones Using New Iron(II) (P-NH-N-P') Catalysts: Changing the Steric and Electronic Properties at Phosphorus P'

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Abstract. The asymmetric transfer hydrogenation (ATH) of ketones is an efficient method for producing enantio-enriched alcohols which are used as intermediates in a variety of industrial processes. Here we report the synthesis of new iron ATH precatalysts (S,S) -[FeBr(CO)(Ph₂PCH₂CH₂NHCHPh-CHPhN=CHCH₂PR'₂)] [BPh₄] (R' = Et, and *ortho*-tolyl) where one of the phosphine groups is modified with a small alkyl and a large aryl substituent to probe the effect of this change on the activity and selectivity of the catalytic system. A simple reversible equilibrium kinetic model is used to obtain the initial TOF and the inherent enantioselectivity $S = k_R/k_S$ of these catalysts along with those for the previously reported catalysts with R' = Ph and Cy for the ATH of acetophenone. With an increase in the size of the PR'₂ group, the TOF goes through a maximum at PPh₂ while the S value goes through a maximum of 510 at R' = Cy. The complex with R' = *o*-Tol starts with a high S value of 200 but is rapidly changed to a second catalyst with an S value of 28. For the reduction of acetophenone to (*R*)-1-phenylethanol, turnover numbers of up to 5200 and ee up to 98% were achieved. The chemotherapeutic pharmaceutical precursor (*R*)-(3',5'-bis(trifluoromethyl))-1-phenylethanol is synthesized in up to 95% ee. Several other alcohols can be prepared in greater than 90% ee by choosing the precatalyst with the correctly matched steric properties. A hydride complex derived from the catalyst with R' = Cy is characterized by NMR spectroscopy. It is proposed that low concentration *trans*-hydride carbonyl complexes with the FeH parallel to the NH of the ligand are the active catalysts in all of these systems.

Keywords: homogeneous catalysis, iron catalysis, asymmetric transfer hydrogenation

Biographies

Samantha Smith studied Honours Chemistry and Mathematics as a double major at Wilfrid Laurier University where she was first exposed to research. She continued on to the University of Toronto's Department of Chemistry where she is currently working on a Ph. D.

Demyan Prokopchuk was born in Saskatoon, Canada. He received his undergraduate degree from the University of Saskatchewan in 2009 and his PhD from the University of Toronto in 2015 under the supervision of Prof. Robert Morris. He is currently a postdoctoral fellow at Pacific Northwest National Laboratory in the Center for Molecular Electrocatalysis, directed by R. Morris Bullock. His current research interests include ligand design and electrochemistry for applications in small molecule activation.

Bob Morris is a professor of chemistry at the University of Toronto. He was born in Ottawa in 1952. He received his PhD from the University of British Columbia in 1978. After postdoctoral work at the Nitrogen Fixation Laboratory, University of Sussex and the Pennsylvania State University he joined the faculty of the University of Toronto in 1980. He was appointed full Professor there in 1989 and served as Acting Chair and Chair of the Chemistry Department from 2008-2013. His research interests include inorganic, organic and catalytic chemistry with applications in the fine chemical industry. He is a Fellow of the Royal Society of Canada and of the Chemical Institute of Canada and Killam Research Fellow (2015-2017).

1. Introduction

The asymmetric reduction of ketones is a challenging process that is useful for many industries including pharmaceutical and fine chemical. Usually precious-metal-based catalysts are employed.^[1] The use of abundant metals such as iron for this transformation is attractive due to their lower cost and toxicity, and this has been a topic of much interest in the last decade.^[2] Recently discovered iron catalysts stand out for their high enantioselectivity and activity in the asymmetric transfer hydrogenation of ketones.^[2b, 2c, 2m, 3]

The activity and selectivity of our iron-based ATH catalysts (Figure 1) has steadily improved using the reduction of acetophenone by isopropanol as a test case. Our first generation ATH precatalyst (*R,R*)-**A** in isopropanol produced, after activation by isopropoxide, (*S*)-1-phenylethanol in 63% ee (TOF 400, TON 1630 h⁻¹ at 24 °C)^[2h, 4] although this ATH system likely involves iron nanoparticles.^[5] Kinetic and mechanistic studies uncovered a high energy barrier for the activation of our more active second generation ATH precatalysts **B** that involved the reduction of one of the imine groups of the **B**^[2i, 2l, 3a] Our group conducted a stereo-electronic study of complexes **B** that involved varying the substituents R of the phosphine moieties of the P-N-N-P ligand and found that only the use of aryl groups led to very active

catalysts for the ATH of ketones.^[6] It was unclear from these studies whether some of the complexes with R = alkyl were inactive due to a high energy barrier to the reduction of the imine of the ligand that is needed for activation or due to a higher barrier for catalysis after imine reduction. The work described below helps to answer this question.

The design of the third generation precatalysts **C** (Figure 1) eliminates this activation barrier by providing the amine(imine ligand) in the structure. This dramatically increases the ATH activity of the catalyst systems in basic isopropanol when aryl groups are on the phosphine donors. The ATH of acetophenone catalyzed by **C1** (R = R' = Ph) produces (*R*)-1-phenylethanol in 78% ee (*R*) with a turnover number (TON) of 5000 and turnover frequency (TOF) 100,000 h⁻¹ at 28 °C while that by **C2** gives 90% ee (*R*).^[3b] The use of other aryl ketones yielded alcohols with ee greater than 90% (*R*) in certain cases.^[3b, 7] The initial work showed that a complex could be prepared with phosphorus donors with different groups on each side, namely **C3** with R = Ph, R' = 4-MeC₆H₃. The **C3** system reduced acetophenone with comparable activity to **C1** but with lower enantioselectivity, 70% ee (*R*).^[3b]

Figure 1. Three generations of ATH Precatalysts.

Complex **C4** with R = Ph and R' = Cy (Figure 2) was found to be more stereoselective but much less active for ketone reduction than **C1-C3**.^[3c] For example the **C4** system catalyzed the reduction of acetophenone to (*R*)-1-phenylethanol in 98% ee.^[3c] The complex was assumed to have a *trans* configuration shown on the left of Figure 2. Recently, **C4** was crystallized, and was found to adopt an unexpected *cis*- β geometry (Figure 2, right).^[8] An objective of the current work is to investigate whether this *cis*- β geometry is of relevance to the activity and selectivity of **C4** relative to **C1**.

Proposed structures

Recent Findings

Figure 2. Previously proposed and recently discovered geometries of **C4** with a *cis*- β stereochemistry

Herein we explore the introduction into the Fe(II) complexes $trans\text{-}[\text{FeBr}(\text{CO})(\text{P-NH-N-P}')]\text{+}$ of two other substituents PR'_2 , the small, basic PEt_2 donor and the large, less basic $\text{P}(o\text{-Tol})_2$ donor while keeping PR_2 group constant as PPh_2 . This work explores a wider range of stereochemical and electronic properties in order to better understand the relationship between the structures and the resulting activity and enantioselectivity of the catalysts for the reduction of a variety of ketone structures. Simulating the reaction progress of the reductions also sheds light on the factors that determine how quickly the ee of the product alcohol is lost after the reaction reaches equilibrium. We also investigate the properties of the active hydride-containing species.

2. Results and Discussion

2.1 Preparation and characterization of complexes

The syntheses of the new iron(II) precatalysts were carried out using routes developed in our lab previously.^[3b, 6b, 9] Complexes **(*S,S*)-1** with $\text{R}' = \text{Et}$ and **(*S,S*)-2** with $\text{R}' = o\text{-Tol}$ were synthesized using the enantiopure (*S,S*)- $\text{PPh}_2\text{CH}_2\text{CH}_2\text{NHCHPhCHPhNH}_2$ compound and the phosphonium dimers **D1** or **D2**,^[10] respectively, in two main steps (Scheme 1).

Scheme 1. The two-step synthesis of complexes **(S,S)-1** and **(S,S)-2**

First an intermediate complex is made *in situ* by the reaction of the appropriate phosphonium dimer with base, Fe(II), and an enantiopure (S,S)-PNN ligand in acetonitrile. On the basis of previous work^[3b, 6b, 9] this is assumed to be a *trans-bis*(acetonitrile) complex. This is then treated with 1 atm CO and excess KBr. The complexes **(S,S)-1** and **(S,S)-2** were precipitated as the BPh₄⁻ salts in 35 and 56% yield, respectively, with respect to the starting (S,S)-P-NH-NH₂ compound. Complex **(S,S)-1** was produced as a mixture of two *trans* diastereomers with structures **E** and **E'** (Figure 3) with NMR properties very similar to **C1** and **C4** in addition to a small fraction (17%) of two other isomers with poorly resolved doublet resonances at 62, 59 and 55 ppm (Table 1). These minor isomers might have the *cis-β* geometries shown in Figure 2 but this could not be definitively established. Similarly **(S,S)-2** appears to have two *trans* isomers (75% of mixture) and at least one additional isomer at 58 and 63 ppm. Each diastereomer has a characteristic set of doublets in the ³¹P{¹H} NMR spectrum (see Table 1).

Figure 3. Geometries of the *trans* tetradentate complexes.

Table 1. $^{31}\text{P}\{^1\text{H}\}$ NMR resonances of the *trans* isomers of **C1**, **C4**, (*S,S*)-**1** and (*S,S*)-**2** with structures **E** or **E'** of Figure 3.

Complex	PR'_2	isomer fraction (%)	PR'_2 (ppm)	PPh_2 (ppm)	$^2J_{\text{PP}}$ (Hz)	Struct.
C1	PPh_2	100	62.6	58.0	40	E
C4	PCy_2	75	78.4	47.3	33	E or E'
(<i>S,S</i>)- 1-1	PEt_2	38	65.1	59.3	38	E' or E
(<i>S,S</i>)- 1-2	PEt_2	45	67.1	53.7	36	E or E'
(<i>S,S</i>)- 2-1	Po-Tol_2	41	61.6	55.4	41	E or E'
(<i>S,S</i>)- 2-2	Po-Tol_2	34	63.7	54.1	39	E' or E

One relatively broad ($w_{1/2}$ 20 cm^{-1}) CO absorption (ν_{CO}) is observed in the IR spectrum for the iron(II) complexes as mixtures of isomers as listed in Table 2 for the two complexes as well as the complexes **C1** and **C4** for comparison (Table 2). Only one peak maximum representing an averaged electronic property of the various isomers present is reported because separate peak maxima were not resolved. There is no clear trend in the ν_{CO} values. The steric parameters of the $\text{PR}'_2\text{CH}_2$ - group can be expressed in terms of Tolman's cone angles θ of the corresponding $\text{PR}'_2\text{Et}$ ligands as also listed in Table 2.^[11]

Table 2. Stereoelectronic effects represented by Tolman's cone angle and IR wavenumbers of the CO ligand.

Complex	PR'_2	IR ν_{CO} (cm^{-1})	Tolman's Cone Angle (θ) ^[a]
(<i>S,S</i>)- 1	PEt_2	1956	132
C1-Br ^[b]	PPh_2	1979 ^[b]	141

C4	PCy ₂	1960	157
(S,S)-2	P <i>o</i> -Tol ₂	1963	173
[a] Cone angle of R' ₂ P ^{Et} representing the PR' ₂ CH ₂ fragment of the complex. [b] Like C1 from Figure 1, but synthesized with a bromo instead of a chloro ligand for better comparison.			

2.2 Analysis of the structures of the isomers in solution.

Complex **C3** has been characterized crystallographically in the *trans* configuration with the NH locked anti with respect to the hydrogen of the adjacent CHPh group with (*S*) chirality as shown in Figure 1. All 43 racemic or enantiopure open metal derivatives in the Cambridge Crystallographic Databank have the NH and CH locked anti (see the Supporting information). The similarity of the NMR spectra of complexes **C1** to **C3** suggest that the major isomers all have this *trans* structure as do a wide variety of more symmetrical *trans*-[Fe(CO)Br(PR₂-N-N-PR₂)]⁺ complexes reported by our group with a wide range of substituents (Et, Cy, aryl).^[21, 6]

The *cis-β* structure of **C4** in the solid state introduces another possibility for structural assignments and it has been observed in related iron and ruthenium complexes with tetradentate phosphorus and nitrogen ligands^[2b, 12]. However in solution the main isomer of **C4** (75%) has the *trans* configuration with either the NH next to the CO ligand (structure **E**) or the Br ligand (**E'**) as in Figure 3. This is determined by assigning all of the protons around the backbone of the ligand using 2D NMR experiments and spin simulations and demonstrating the similarity to the proton spectra of *trans* complex **C1** (see the Supporting Information). In particular the ³J_{HH} coupling constants of the PPh₂CH₂CH₂NH part of the ligand backbone should be sensitive to the differences in dihedral angles between the *trans* and the *cis-β* configurations where this part of the tetradentate ligand that folds away from the PNN plane. The simulated ³J_{HH} couplings are similar for the **C1**, **(S,S)-1** and **C4** isomers in the assigned *trans*-configuration. The large ³J_{HH} coupling (12-14 Hz) indicative of *anti*-vicinal CH groups in the *trans* structure is present in the ¹H spectra of all of these compounds. The minor isomer of **C4** with ³¹P{¹H} NMR signals at 76.0 and 75.5 ppm probably has a *cis-β*-**C4** structure, but it is in too low a concentration to provide definitive proton assignments. In another sample prepared for HMBC NMR analysis, another *trans*-isomer, (**E** or **E'**) with ³¹P{¹H} NMR resonances at 73.0 (d, ²J_{PP} 35 Hz) and 51.8 ppm (d, ²J_{PP} 35 Hz) were also observed. Thus the PPh₂CH₂CH₂ arm of **C4** is mobile and allows a switch that is slow on the NMR timescale between the structures shown in Figure 2.

A ^1H - ^{31}P HMBC experiment and spin simulations were used to assign the structures of the *trans* isomers of complex **(S,S)-1**, although it was not possible to distinguish which of the two diastereomers was **E** vs **E'** of Figure 3 ($\text{PR}'_2 = \text{PEt}_2$). Table 1 lists the $^{31}\text{P}\{^1\text{H}\}$ chemical shifts and coupling constants of these isomers. Obtaining good NMR spectra for **(S,S)-2** was challenging but its $^{31}\text{P}\{^1\text{H}\}$ NMR spectra appear to be similar to those of **(S,S)-1**.

2.2 Catalytic results

2.2.1 Acetophenone reduction and reaction progress modelling

The ATH of acetophenone (Figure 4) was carefully examined for catalysts **(S,S)-1**, **(S,S)-2** as well as **C1** and **C4** for comparison under a range of conditions (Figure 4).

Figure 4. Conditions for the ATH of acetophenone.

Initial catalytic reactions were done with acetophenone (**K1**) with a precatalyst/KOtBu/substrate ratio (C/B/S) of 1/2/500 with [**K1**] 0.70 M in iPrOH at 28 °C. Figure 5 shows that complexes **(S,S)-1** with the small PEt_2 group reduces acetophenone to 1-phenylethanol to the equilibrium point of 86% conversion with a high initial TOF of approx. 12 s^{-1} as determined by reaction profile fitting (see below). The conversion can be increased to over 90% by using a lower concentration of ketone (e.g. 0.1 M). The complexes **C4** and **(S,S)-2** with bulkier PCy_2 and $\text{P}o\text{-Tol}_2$ groups have lower initial TOF and lose activity before reaching equilibrium. On the other hand the last two complexes maintain a high ee in the product while **(S,S)-1** has significant losses in ee over time because of its poor selectivity. There is less ee degradation over the course of the reaction when using a lower catalyst loading^[3b] with the C/B/S ratio 1/8/6121 with [ketone] 0.63 M (Figure 6). **C4** and **(S,S)-2** were again slower at reducing acetophenone; however the ee for **C4** was much higher (98% *R*) at maximum conversion. The reaction slows after 40% conversion and attains only 80% of the possible conversion at 120 min. This is also true for **(S,S)-2**. **(S,S)-2** produces the alcohol in 89% ee (*R*) after 120 minutes. **(S,S)-1** has the higher activity to a maximum conversion

of 87% after 50 min, but also a lower ee of 85%. For comparison **C1** with PPh₂ groups produces 1-phenethanol at 82% ee at the time of maximum conversion.^[3b]

Figure 5. ATH of acetophenone (**K1**) with **(S,S)-1**, **(S,S)-2** and **C4**. Reaction conditions: 28 °C, 1.4×10^{-3} M precatalyst, 2.8×10^{-3} M KOTBu, 0.70 M acetophenone, 6 mL iPrOH, C/B/S=1/2/500; % conversion and % ee determined by chiral GC.

Figure 6. ATH of **K1** with **(S,S)-1**, **(S,S)-2** and **C4**. Reaction conditions: 28 °C, 1.0×10^{-4} M precatalyst, 8×10^{-4} M KOtBu, 0.63 M acetophenone, 6 mL iPrOH, C/B/S=1/8/6121; % conversion and % ee determined by chiral GC.

The reaction progress and changes in ee for the ATH of acetophenone (AP) were semi-quantitatively fit for the first time to a simple kinetic model^[13] for a reversible equilibrium using the program Dynafit^[14] (Figures 7-10). The progress of the reactions catalyzed by **(S,S)-1**, **(S,S)-2**, **C1** and **C4** were fit to only three parameters: two rate constants k_R and k_S for pseudo first order reactions producing (R)- and (S)-1-phenylethanol (abbreviated RPE and SPE, respectively) and one equilibrium constant ($K_{rac} = 2k_R/k_{-R} = 2k_S/k_{-S}$) for the reversible reaction of acetophenone with isopropanol to give 1-phenylethanol and acetone. The same $K_{rac} = 12$ applies to all of the reactions of Figures 5 and 6. From the rate constants the intrinsic enantioselectivity of the catalyst is obtained ($S = k_R/k_S$).^[13] The value of S determines the initial ee of the system. The initial TOF is given by $(k_R+k_S)[AP]/[Cat]$ and the initial e.e. is given by $(k_R-k_S)/(k_R+k_S)$.

This simple approach makes the following assumptions:

1. The forward reaction to produce RPE is first order in AP with a steady-state catalyst concentration included in the rate constant k_R .
2. The forward reaction to produce SPE is first order in AP with a steady-state catalyst concentration included in the rate constant k_S .
3. At equilibrium, the concentrations of RPE and SPE will be equal (0 ee) and the equilibrium constant will be $K_{rac} = 2K_R = 2K_S = 12.0$ for the conditions described here.
4. The backward reaction to produce AP from RPE is first order in RPE with a steady-state catalyst concentration included in the rate constant $k_{-R} = k_R/K_R = 2k_R/K_{rac}$.
5. The backward reaction to produce AP from SPE is first order in SPE with a steady-state catalyst concentration included in the rate constant $k_{-S} = k_S/K_S = 2k_S/K_{rac}$.

Assumptions 4 and 5 explain why the ee of the product degrades with the progress of the reaction if k_S is non-negligible.

The model was validated using data from the well-defined catalyst **C1** (Figure 7). The parameters obtained are listed in Table 3. Catalyst **C1** with two moderately sized PPh_2 groups has an extremely high TOF of 250 s^{-1} as documented elsewhere^[3b] and an inherent selectivity S of 12, resulting in a starting ee of 85% which degrades to 78% at maximum conversion at 120 s. The experimental ee have larger uncertainties early in the reaction because of the low concentration of the (*S*)-1-phenylethanol in the sample but the model fits the general trends in the ee.

Figure 7. (Left) Kinetic fit to the changes in concentration in the ATH of acetophenone catalyzed by **C1**. (Right) Fit to the changes in ee for the reaction.

Table 3. Results of fitting the reaction profiles.¹

Catalyst	k_R (s ⁻¹)	k_S (s ⁻¹)	TOF (s ⁻¹)	S	ee initial (R %)	ee (at time, min)	TON
C1²	3.6e-2	3.2e-3	235	12	85	78 (2)	5900
(S,S)-1	2.1e-3	1.1e-4	14	19	90	80 (40)	5000
(S,S)-2³	4.0e-4	2.0e-6	6	200	99	93 (4)	500
(S,S)-2³	4.1e-4	1.7e-5	3	28	92	90 (90)	3700
C4	4.5e-4	1e-6	3	510	99.6	98.5 (120)	4400

¹ [FeBr(CO)(PR'₂CH₂CHNCHPhCPhNHCH₂CH₂PPh₂)]BPh₄: [Cat]= 1.05e-4 M, [KOtBu]=8e-4 M, [AP]=0.63 M, 28°C in isopropanol, K_{rac} =12.0. ² [FeCl(CO)(PPh₂CH₂CHN-CHPhCPhNHCH₂CH₂PPh₂)]BF₄: [Cat]=6.8e-5 M, [KOtBu]=5.4e-4 M, [AP]=0.41 M, 28°C in

isopropanol, $K_{rac}=12.0$.³ There is a change in catalyst structure over the course of the first 250 seconds.

The fits to the reaction progress for **(S,S)-1** (Figure 8) show that this system is slower (TOF 14 s^{-1}) than **C1** but more enantioselective ($S\ 20$). Thus there are dramatic effects in changing one PPh_2 (on **C1**) with one PEt_2 group.

Figure 8. Simulation of the reaction progress of **(S,S)-1** of Figure 6.

(S,S)-2 and **C4** do not fit the simple model (Figures 9 and 10). The reactions slow more than expected with conversion and this indicates that the catalyst concentration is being reduced over the course of the catalytic run. This may be due to inhibition due to binding of the product alcohol. It is interesting that for **(S,S)-2**, the ee drops rapidly from a high value of 99% R over the course of the first 250 seconds. This is modelled by a more enantioselective catalyst ($S = 200$) being completely replaced by a less selective one (with $S = 28$) over this time period. This is likely to be caused by the dissociation and repositioning of the bulky $\text{CH}_2\text{CH}_2\text{P}(o\text{-Tol})_2$ arm of the ligand in an as-of-yet, undefined way. Complex **C4** with the slightly smaller PCy_2 group is more stable and produces the alcohol in exceptionally high ee up to maximum conversion.

Figure 9. Simulation of the reaction progress of **(S,S)-2** of Figure 6. The catalyst is converted over 250 s from one that is very enantioselective ($S=200$) to one that is less ($S=28$).

Figure 10. Simulation of the reaction progress of **C4** of Figure 6.

The TOF and S values obtained from fitting the reaction profiles are plotted as a function of the cone angle of the $\text{PR}'_2\text{CH}_2$ group in the complex Figures 11 and 12. Variations in the electronic environment as reflected in the $\nu(\text{CO})$ of the complexes are too small to show a meaningful

variation with TOF or *S*. As far as activity (TOF) is concerned there is a region in the plot around the size of the PPh_2 group where the TOF is high (Figure 11). The PPh_2 complex **C1** is an order of magnitude more active than the PEt_2 and PiPr_2 complexes. The use of bulky PCy_2 and Po-Tol_2 groups result in lower TOF. This is consistent with our earlier stereoelectronic study of precatalysts **B** (Figure 1) indicating that both studies reflect the actual activity of the catalyst and not the activation of the precatalyst; an induction period was observed for catalysis with **B** because an imine in **B** has to be reduced to an amine^[3a] while no induction period is observed for the catalyst systems discussed here.

Figure 11. TOF (s^{-1}) for the ATH of acetophenone catalyzed by complexes as a function of cone angle (°) of the PR'_2 group (see Tables 2 and 3). Reaction conditions are as in Figure 6.

However as far as the intrinsic enantioselectivity *S* is concerned, it rises from less than 20 for the smaller substituents (PEt_2 , PPh_2) to a maximum of 510 for bulky PCy_2 (98% ee) and then falls again to 200 and then to 28 for the very bulky Po-Tol_2 as discussed above (Figure 12).

Figure 12. The intrinsic enantioselectivity $S = k_R/k_S$ for the ATH of acetophenone catalyzed by **(S,S)-1** to **(S,S)-2** and **C1** and **C4** as a function of cone angle (°) of the PR'_2CH_2 group. Reaction conditions are as in Figure 6. The selectivity of **(S,S)-2** drops over the first 250 s of the reaction.

2.2.2 Other substrates

The ATH of a range of ketones shown in Figure 13 were tested for the complexes, **(S,S)-1** and **(S,S)-2** (Figure). All of the catalytic results from this study were compared to those of **C4**, and those of **C1**, retested under the conditions of the present study for ease of comparison.

Figure 13. Substrate scope for ATH using complexes **(S,S)-1**, **(S,S)-2**, **C1** and **C4**.

Figure 14. Conditions of ATH catalysis.

The best results are summarized in Table 4; a more complete Table can be found in the SI. Included are results for **C4** as reported elsewhere.^[3c] All of the chiral alcohol products are enriched in the *R*-enantiomer which is consistent with our previous findings.^[3b, 3c, 15]

First the series of substrates with one phenyl group and one R group of increasing size (H to Me to Et to iPr) are considered. All of the complexes quantitatively convert benzaldehyde (**A1**) to benzyl alcohol within a few minutes. The reduction of propiophenone, **K2**, is achieved with around 80% conversion for each complex. Complexes **C4** and **(S,S)-2** with the bulky substituents make product with ee greater than 90% ee while **(S,S)-1** is less enantioselective (86% ee) but much more active; **C1** produces a low ee product. The bulkier **K3**, i-butyrophenone, is only

reduced by **(S,S)**-1 and **C1** with the smaller PR'₂ substituents ($\theta < 142^\circ$) but the enantioselectivity is poor; this suggests that the active sites of the other catalysts are too restricted in size.

Table 4. Results for the ATH of ketones in Figure 13 using complexes **C1**, **(S,S)**-1 to **(S,S)**-2, and previously reported results using **C4** ^[a]

Entry	Substrate ^[b]	Precatalyst	Conv. (%) ^[c]	Time (min)	ee (%) ^[c]	TON
1	K2	(S,S) -2	82	30	90	410
2		C4	80	60	94	400
3		(S,S) -1	79	3	86	395
4	K3	(S,S) -1	52	60	12	260
5		C1	88	40	40	440
6	K4	C4	92	10	52	460
7		(S,S) -2	92	10	58	460
8	K5	(S,S) -1	>99	1	90	500
9		C4	>99	10	94	500
10		C1	>99	1	94	500
11	K6	(S,S) -2	>99	30	93	500
12		C1	>99	1	91	500
13	K7	(S,S) -2	60	40	63	300
14		C4	60	20	65	300
15	K8	(S,S) -1	>99	3	N/A	500
16		(S,S) -2	>99	5	N/A	500
17		C1	>99	2	N/A	500
18	K9	(S,S) -1	0	60	N/A	0
19	K10	C4	44	60	43	220
20		(S,S) -2	75	40	55	375
21		C1	90	20	23	450
22	K11	(S,S) -1	33	60	N/A	165
23		(S,S) -2	>99	2	N/A	500
24		C1	>99	50	N/A	500
25	K12	(S,S) -1	81	30	23	405
26		C4	88	40	82	440
27		(S,S) -2	84	40	59	420
28	K13	C4	11	60	53	55
29	K14	(S,S) -1	90	20	N/A	450
30		C4	89	20	N/A	445
31		(S,S) -2	91	20	N/A	455
32		C1	89	1	N/A	445
33	K15	(S,S) -2	22	30	46	110

[a] Reaction conditions: 28 C, 8.9×10^{-3} mmol catalyst, 0.18 mmol KOtBu, 44.3 mmol substrate, 6 mL iPrOH. [b] C/B/S=1/2/500. [c] % conversion and % ee determined by chiral GC.

The series of methylketones MeCOAr (**K4** to **K9**) provide a range of functional groups to test the catalysts. The reduction of **K4** and **K5** with chloro substituents on the phenyl ring is achieved with

high conversions, with the *ortho*-chloro substituent in **K5** producing much higher ee (84-94% depending on the catalyst) than with the *para*-chloro group in **K4** (6-58% ee). High enantiopurity is beneficial for the production of (*R*)-2'-chloro-1-phenylethanol as it is a key intermediate for a chemotherapeutic drug.^[16] The bis-CF₃-substituted arylketone **K6** is fully reduced to the alcohol in >90% ee by **C1** and (**S,S**)-**2** that contain PAR₂ groups while (**S,S**)-**1** with a more basic PEt₂ group appears to be deactivated by the acidic alcohol product after 40-60% conversion. The enantiopure alcohol is valuable as it is a key intermediate for the synthesis of Aprepitant.^[17] *Para*-methylacetophenone (**K7**) was more difficult to reduce than the chloro analogue, and relatively low ee are achieved. The presence of a potentially coordinating pyridyl group in **K8** is conducive, not detrimental, to the complete reduction of the ketone. However, the furan in **K9** deactivates all of the complexes except **C1**.^[3b] 3-Methyl-2-butanone (**K10**) is reduced to 90% conversion but with low ee by **C1**, while both **C4** and (**S,S**)-**2** are less active but give higher ee at 43% and 55%, respectively. The complete reduction of cyclohexanone (**K11**) is achieved with (**S,S**)-**2** and **C1**, while only partial conversion is observed for (**S,S**)-**1**. **C4** is the most enantioselective catalyst for the ATH of the 2-naphthyl ketone **K12** with 82% ee, and it was the only complex that successfully reduced cyclohexylphenyl ketone (**K13**), although with only 11% conversion. All of the catalysts reduce benzophenone (**K14**) efficiently. The presence of a C=C bond in benzylidene acetone (**K15**) proved to be a complicating factor as all of the complexes with the exception of (**S,S**)-**2** are unselective and reduced both the C=O and C=C bonds. For the unselective catalysts, the GC traces show the three possible reduction products of C=O reduction, C=C reduction, and both, even at 1 min, with the fully reduced product growing in over time. (**S,S**)-**2** is selective for the formation of the allyl alcohol product with less than <1% conversion to the doubly saturated product after 60 min. In summary, while **C1** is a very active catalyst with a high TOF, replacing one of its PPh₂ groups with a PCy₂ group results in a more enantioenriched alcohol for all of the ketones except **K5**. The change to a P(*o*-Tol)₂ group gave superior ee for **K2**, **K4**, **K6**, **K7** and **K10**. Surprisingly even the small PEt₂ group of (**S,S**)-**1** provided comparable or greater enantioselectivity to that of the PPh₂ group in complex **C1** for **K2**, **K4**, **K7**, **K10**, **K12** and **K13**.

2.3 Observation of Hydride Species

The precatalyst solution of **C4** was treated with base and iPrOH in order to characterize possible catalytically active species by use of NMR and IR spectroscopy as has been done already for **C1**.^[3b] When **C1** was treated by first the addition of KOtBu in THF, then evaporation, dissolution in C₆D₆, a mixture of amido-enamido complexes was identified.^[3b] Then the addition of iPrOH produced first, a transient hydride isomer **G1-1** (Scheme 2) which rearranged over time to a second isomer **G1-2**. Based on NOE studies, isomer **G1-1** has a *trans* configuration with the Fe-H group parallel to the N-H group while **G1-2** is thought to have the *trans* configuration with Fe-CO moiety parallel to the N-H group.^[3b]

Scheme 2. Generation of Iron(II) Hydride Species Starting with **C1** as Reported Previously

The precatalyst **C4** was mixed with 8 equivalents of KOtBu in THF for 5 min, then dried *in vacuo* and dissolved in C₆D₆. The solution at this stage produce complicated NMR spectra with features reported previously for amido-eneamido complexes generated from **C1** (see the Supporting Material).^[3b, 7, 15] The mixture of complexes was then dissolved and stirred in iPrOH for 1 min, or until the residue was completely dissolved. It was then dried immediately affording the new hydride species *trans*-(**S,S**)-**3** (Scheme 3, Table 5). Its NMR properties are similar to those of hydride **G-1-2** and so we tentatively assign the structure as *trans* with the NH parallel to the FeCO group. The ³¹P{¹H} NMR resonances associated with these hydride complexes have ²J_{PP} 25-27 Hz, consistent with *cis* phosphorus nuclei (Table 5). **G-1-2** and *trans*-(**S,S**)-**3** show a similar doublet of doublet hydride pattern in the region of -9.3 to -10.3 ppm with ²J_{PH} of 59-60 and 80-82 Hz. These coupling constants are typical of *cis* phosphorus and hydride nuclei on Fe(II) and thus the stereochemistry of these hydride complexes is likely to be *trans*. In all cases found so far, the magnitude of ²J_{P-Fe-H}^{trans} is smaller than that of ²J_{P-Fe-H}^{cis} for terminal iron hydride complexes: ²J_{P-}

$_{\text{Fe-H}}^{\text{trans}}$ is in the range 12-35 Hz^[18] whereas $^2J_{\text{P-Fe-H}}^{\text{cis}}$ is in the range 30-85 Hz. ^[18a-e, 18i, 19] In some instances the $^2J_{\text{P-Fe-H}}^{\text{trans}}$ and $^2J_{\text{P-Fe-H}}^{\text{cis}}$ in iron hydride polyphosphine complexes are averaged to a small value due to nuclear exchange caused by molecular fluxionality.^[20]

Treating **(S,S)**-1 and **(S,S)**-2 in similar fashion also produce hydride resonances in this region but the hydrides are very reactive and unstable so that the $^{31}\text{P}\{^1\text{H}\}$ NMR spectra are complex with some unidentified species and signals for uncoordinated phosphorus species.

Thus hydride complex *trans*-**(S,S)**-3, like **G1-2**, is thought to have the NH of the ligand parallel to the Fe-CO group and not in a suitable position for an outersphere hydride and proton attack on the ketone.^[3b]

Scheme 3. Generation of Iron(II) Hydride Species **(S,S)**-3

Table 5. NMR properties of the hydride complexes

Precursor to Hydride Complex	PR' ₂	$\delta^{31}\text{P}$ (ppm)	$^2J_{\text{PP}}$ (Hz)	$\delta^1\text{H}$ (ppm)	$^2J_{\text{HP}}$ (Hz)
C1 hydride G-1-1	PPh ₂	84.9, 70.4	33.2	-2.3	71, 62 ^a
C1 hydride G-1-2	PPh ₂	75.7, 71.4	27.5	-9.2	80, 60 ^b
(S,S) -3	PCy ₂	91.2, 83.0	36.6	-10.3	82.2, 59.8
^a previously reported as 70 Hz ^[3b] ^b previously reported as 79 Hz ^[3b]					

3 Density Functional Theory Calculations

Due to the difficulties in establishing the coordination geometries of the products upon reacting **C4** with base, we employed Density Functional Theory to compare relative ground state energies

of various diastereomers. Details of the calculations and the three dimensional Cartesian coordinates are provided in the Supporting Information. The calculated geometries of *cis*- β complexes **C4-R_{NH}** and **C4-S_{NH}** correspond well with the X-ray structural data reported previously for **C4**,^[8] with **C4-S_{NH}** being only 1.8 kcal/mol higher in energy (SI, Scheme S1). The *cis*- β stereochemistry of the two diastereomers can be further characterized as Δ -*cis*- β -**C4-R_{NH}** and Λ -*cis*- β -**C4-S_{NH}**. Deprotonation of **C4** with at least two equivalents of base could lead to the formation of at least four possible amido-eneamido complexes (**S,S**)-**4** (Scheme 4) and the *trans*-amido structure by analogy to mechanistic studies based on **C1**.^[15, 21] We found that the *trans*-(**S,S**)-**4** isomer is slightly lower in energy (3.2 kcal/mol) relative to the Δ -*cis*- β -(**S,S**)-**4** amido complex (Scheme 4). The *trans* isomer can produce, via the transfer of a proton/hydride equivalent from iPrOH, the high energy, catalytically active, octahedral, FeH-NH complex, *trans*-(**S,S**)-**3'**, with FeH and NH parallel as proposed for the *trans*-amido-eneamido from **C1**. In the absence of substrate, the formation of the hydride Δ -*cis*- β -(**S,S**)-**3** is calculated to be most favorable (-13.3 kcal/mol) among the various *cis*- β structures. Experimentally the hydride *trans*-(**S,S**)-**3** is the isomer observed as noted above. It is calculated to have a relative energy of -10.9 kcal/mol, or 2.4 kcal/mol less stable than this Δ -*cis*- β isomer although this difference may be within the errors of the calculation. The relative energy of the kinetically-formed hydride complex *trans*-(**S,S**)-**3'** is calculated to be -8.9 kcal/mol, 4.4 kcal/mol higher than the Δ -*cis*- β isomer and 2 kcal/mol higher than the observed hydride (**S,S**)-**3**.

Scheme 4. Ground state energy comparison of some isomers of Cy-amido complexes **(S,S)-4** and the hydride isomers **(S,S)-3** derived from them by reaction with 2-PrOH. All energies are given in kcal/mol and relative to Δ -*cis*- β -(**(S,S)-4**) plus relevant small molecules. M06L/TZVP/TZVPfit-IEF-PCM(THF).

4. Proposed mechanism

Thus, we suggest that the activity of the system is determined by the relative stability of a catalytic *trans*-hydride like *trans*-(**(S,S)-3'**) and the off cycle *trans* hydride *trans*-(**(S,S)-3**) or Δ -*cis*- β -(**(S,S)-3**) hydride species and of the catalytic *trans* amido-eneamido species as indicated in Scheme 5. The larger and/or more basic PR'₂ groups favor the off-cycle structures and thus are less reactive. The similarity of the structure of the ketone adduct with the unobserved active hydride (Scheme 5) to that of the one proposed for the PPh₂ catalyst system **C1**^[15, 21] could explain why the (*R*)-aryl alcohols are produced by the *trans*-(*S,S*)-hydride catalysts using a transition state structure similar to that described for **C1**.^[15, 21]

DFT calculations (see SI) indicate that **G-1-2** may have a Δ -*cis*- β geometry for the off cycle structure shown in Scheme 5; this structure is 3 kcal/mol more stable than the *trans*-isomer **G-1-1**. Thus it is

possible that the off-cycle hydride complexes with a Δ -cis- β geometry rearrange to low concentration catalytically active isomers with the NH and FeH parallel as shown in Scheme 5.

Scheme 5. Proposed mechanism for the ATH catalyzed by complexes **(S,S)-1**, **(S,S)-2**, **C1** and **C4**. The observed hydride $trans$ -(S,S)-3 when R' is Cy is proposed to be off cycle.

5. Summary

In conclusion, two new precatalyst complexes have been synthesized with varying steric and electronic properties at one phosphine (PEt_2 vs $PO-Tol_2$) coordination site of our third generation iron(II) ($P-NH-N-P'$) system. These have been tested in the catalytic ATH of ketones and compared to the previously reported complexes **C1** and **C4**. The progress of the catalytic reactions could be fit for the first time to a simple three parameter kinetic model which describes the activity and degradation of ee over the course of the reaction. We found that by increasing the steric bulk at one phosphine, the enantioselectivity increases (to greater than 98% in case of **C4**) with a concomitant decrease in activity.

This work provides evidence for a correct matching of catalyst structure with substrate structure to produce superior activity and selectivity. The bulky isobutyrophenone (**K3**) is only reduced by **(S,S)-1** and **C1** probably because these catalysts have the small PEt_2 or PPh_2 groups. Surprisingly

(S,S)-1 provides (*R*)-1-orthochlorophenylethanol in high ee (90%) from **K5**, despite the small size of the PEt₂ group. Cyclohexanone (**K11**) was only reduced by the **(S,S)**-2 and **C1** catalyst systems. We also found that the steric and electronic properties can be varied to introduce chemoselectivity, as in the case of the selective C=O reduction of benzylidene acetone by complex **(S,S)**-2 and none other.

We provided spectroscopic and computational characterization of hydride complexes that provide an understanding of the mechanism of the catalytic ATH using these iron complexes.

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Asymmetric Transfer Hydrogenation of Ketones Using New Iron(II) (P-NH-N-P') Catalysts: Changing the Steric and Electronic Properties at Phosphorus P'

Samantha A. M. Smith, Demyan, E. Prokopchuk and Robert H. Morris

Supporting Information for

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Experimental Section

All manipulations were done under inert atmosphere of either nitrogen or argon using Schlenk techniques or a glovebox, unless otherwise stated. Solvents were dried and degassed under standard procedures prior to use. NMR spectra were recorded at ambient temperature and pressure using Varian Gemini 600 MHz, 500 MHz and 400 MHz spectrometers [^1H (600 MHz, 500 MHz and 400 MHz), $^{13}\text{C}\{^1\text{H}\}$ (150 MHz, 125 MHz and 100 MHz) and $^{31}\text{P}\{^1\text{H}\}$ (242 MHz, 201 MHz and 161 MHz)]. The electrospray ionization mass spectrometry (ESI-MS) data were collected on an AB/Sciex QStar mass spectrometer with an ESI source. IR spectra were measured using a Bruker ALPHA FT-IR-base spectrometer with a DTGS detector, SiC globar source, and automated instrument tests with integrated polystyrene standard.

(S,S) -[FeBr(CO)(PPh₂CH₂CH₂NHCHPhCHPhN=CHCH₂PEt₂)] [BPh₄] ((S,S) -1). In the glovebox, sodium methoxide (64 mg, 1.18 mmol) was added to a 100 mL Schlenk flask charged with a stir bar and diethyl-phosphonium bromide (D1) (5.88×10^{-1} mmol) and 25 mL methanol was added with stirring. This solution was stirred for no more than 2 minutes. A solution of dissolved [Fe(H₂O)₆][BF₄]₂ (496 mg, 1.47 mmol) in 20 mL acetonitrile was added to the Schlenk flask, followed by a solution of 1.18 mmol of (S,S) -PPh₂CH₂CH₂NHCH(Ph)CH(Ph)NH₂ in 10 mL methanol. This resulted in a purple solution. This was left to stir at room temperature for 16 hours, after which a colour change to pink or orange was observed. The solvent was removed *in vacuo*. KBr (140 mg, 4.70 mmol) was added to the flask, the flask was sealed and removed from the glovebox. The flask was purged and placed under CO atmosphere using Schlenk techniques. 20 mL distilled acetone in a syringe was injected into the flask with stirring for 1.5 hours, after which the solvent was removed under vacuum. The residual yellow or orange solid was dissolved in 20 mL acetone while under CO atmosphere. This was stirred for 1 additional hour, after which the solvent was removed and the flask brought into the glovebox. The solid residue was dissolved in 20 mL dichloromethane and filtered through a pad of Celite, then through a 25 mm Syringe Filter PTFE membrane (pore size 0.45 μm). The clear yellow or orange solution was dried *in vacuo*, then dissolved in minimal methanol. This solution was added to a vial charged with a stir bar and NaBPh₄ (402 mg, 1.294 mmol) dissolved in minimal methanol, from which a yellow solid precipitated. This solid was filtered off and washed with diethyl ether (3x15 mL) and dried overnight. If the purity by NMR was not sufficient, the solid was dissolved in minimal dichloromethane and precipitated out by addition of diethyl ether. Yield: 42 mg (35%). FT-IR (KBr, cm^{-1}): 1956 (ν_{CO} , $w_{1/2}$ 20 cm^{-1}). HRMS (ESI-TOF, CH₂Cl₂) m/z calculated for [C₃₅H₅₄BrFeN₂OP₂]⁺: 701.1145, found: 701.1151 ^1H NMR (300 MHz; CD₂Cl₂) δ : 1.03 (bs, 6H, P(CH₂CH₃)₂), 1.58 (bs, 4H, P(CH₂CH₃)₂), 2.99 (m, 2H, CH₂CH=N), 2.87 (m, 2H, CH₂PPh₂), 4.00 (d, 2H, CH₂NH, $J_{\text{HH}} = 10.9$ Hz), 4.38 (t, 1H, NCHPh, $J_{\text{HH}} = 11.9$ Hz), 5.05 (t, 1H, NCHPh, $J_{\text{HH}} = 11.9$ Hz), 5.52 (m, 1H, NCHPh), 6.83-7.56 (m, 40H, ArH), 7.79 (m, 1H, N=CH). The air sensitivity of this compound prevented the measuring of acceptable elemental analysis. The spectroscopic evidence and reproducible catalytic activity of separate batches provide support for acceptable purity.

Figure S1 $^{31}\text{P}\{^1\text{H}\}$ NMR (242 MHz, CD_2Cl_2) spectrum of **(*S,S*)-1** $\text{PR}_2 = \text{PEt}_2$

Figure S2 ^1H NMR (300 MHz, CD_2Cl_2) spectrum of **(*S,S*)-1** $\text{PR}_2 = \text{PEt}_2$

Figure S3. $^1\text{H}/^{31}\text{P}$ gHBMBC spectrum (600 MHz, CD_2Cl_2) of **(S,S)-1** $\text{PR}_2 = \text{PEt}_2$.

Figure S4 The FT-IR spectrum (KBr pellet) of **(S,S)-1** $PR_2 = PEt_2$. The peak at 1956 cm^{-1} was assigned to the CO stretch.

(S,S)-[FeBr(CO)(PPh₂CH₂CH₂NHCHPhCHPhN=CHCH₂P(*o*-Tol)₂)] [BPh₄] (**(S,S)-2**). The procedure follows that of **(S,S)-1**. Yield: 90 mg (56%). FT-IR (KBr, cm^{-1}): 1963 (ν_{CO} , $w_{1/2}$ 20 cm^{-1}). HRMS (ESI-TOF, CH_2Cl_2) m/z calculated for $[\text{C}_{45}\text{H}_{45}\text{BrFeN}_2\text{OP}_2]^+$: 825.1454, found: 825.1459. ^1H NMR (300 MHz; CD_2Cl_2) δ : 1.27 (s, 6H, $\text{P}(\text{C}_6\text{H}_4(\text{CH}_3))_2$), 2.40 (m, 2H, PCH_2), 3.70 (m, 2H, $\text{CH}_2\text{CH}=\text{N}$), 3.89 (m, 2H, NCH_2), 5.04 (m, 1H, NCHPh ; the other CHPh must overlap with CDHCl_2), 6.5-7.60 (m, 48H, ArH), 7.6-7.8 (m, 1H, $\text{N}=\text{CH}$). $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz; CD_2Cl_2) δ : 68.82 (d, $J_{\text{PP}} = 36.7\text{ Hz}$), 63.70 (d, $J_{\text{PP}} = 38.8\text{ Hz}$), 61.58 (d, $J_{\text{PP}} = 41.4\text{ Hz}$), 55.37 (d, $J_{\text{PP}} = 41.4\text{ Hz}$), 54.13 (d, $J_{\text{PP}} = 38.8\text{ Hz}$). EA $[\text{C}_{69}\text{H}_{64}\text{BBFeN}_2\text{OP}_2]$ Expected: C 72.33%, H 5.63%, N 2.44%. Analysis: C 72.61%, H 6.24%, N 2.57%.

Figure S9 $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, CD_2Cl_2) spectrum of **(*S,S*)-2** $\text{PR}_2 = \text{PoTol}_2$

Figure S10 ^1H NMR (300 MHz, CD_2Cl_2) spectrum of **(*S,S*)-2** $\text{PR}_2 = \text{PoTol}_2$

Figure S11 H-H COSY NMR (300 MHz, CD_2Cl_2) spectrum of **(*S,S*)-2** $\text{PR}_2 = \text{PoTol}_2$

Figure S12 The FT-IR spectrum (KBr pellet) of **(*S,S*)-2** $\text{PR}_2 = \text{PoTol}_2$. The peak at 1963 cm^{-1} was assigned to the CO stretch.

Observation by NMR of the Iron amido-eneamido and hydride

Fe(H)(CO)(PPh₂CH₂CH₂NHCHPhCHPhNCH=CHPCy₂) (S,S)-3. Amido-eneamido: (S,S)-1 (20 mg, 1.96x10⁻⁵ mol) and KOtBu (8 eq., 18 mg) were stirred in THF for 5 min, then dried *in vacuo*. The residue was dissolved in C₆D₆ and filtered through a Syringe Filter PTFE membrane (pore size 0.45 μm). Two compounds were present in NMR. Compound 1: ¹H NMR (400 MHz; C₆D₆) δ: 3.32 (t, 1H, PCH, J_{HH} = 4.7 Hz), 4.58 (t, 1H, C(H)(Ph), J_{HH} = 8.7 Hz), 5.36 (d, 1H, C(H)(Ph), J_{HH} = 10.3 Hz), 7.65 (t, 1H, NCH=CH, J_{HH}=8.7 Hz). ³¹P{¹H} NMR (161 MHz; C₆D₆) δ: 86.30 (d, J_{PP} = 25.2 Hz), 82.68 (d, J_{PP} = 25.2 Hz); Compound 2: ¹H NMR (400 MHz; C₆D₆) δ: 3.44 (dd, 1H, PCH, J_{HH} = 5.0, 3.0 Hz), 4.40 (d, 1H, C(H)(Ph), J_{HH} = 3.0 Hz), 4.73 (d, 1H, C(H)(Ph), J_{HH} = 3.5 Hz), 7.62 (m, 1H, NCH=CH). ³¹P{¹H} NMR (161 MHz; C₆D₆) δ: 91.42 (d, J_{PP} = 27.5 Hz), 82.71 (d, J_{PP} = 27.5 Hz).

Hydride (S,S)-3: The solution from above was dried then dissolved in ⁱPrOH and stirred for 2 mins. This solution was dried overnight. FT-IR (KBr, cm⁻¹): 1894 (ν_{CO}). ¹H NMR (400 MHz; C₆D₆) δ: -10.27 (dd, 1H, FeH, J_{HP} = 82.2, 59.8). ³¹P{¹H} NMR (161 MHz; C₆D₆) δ: 91.19 (d, J_{PP} = 36.6 Hz), 83.02 (d, J_{PP} = 36.6 Hz).

Figure S16 ¹H NMR (400 MHz, C₆D₆) spectrum of **Amido-eneamido** PR₂ = PCy₂

Figure S17 ^1H - ^1H COSY NMR (400 MHz, C_6D_6) spectrum of **Amido-eneamido** $\text{PR}_2 = \text{PCy}_2$

Figure S18 $^{31}\text{P}\{^1\text{H}\}$ NMR (161 MHz, C_6D_6) spectrum of **Amido-eneamido** $\text{PR}_2 = \text{PCy}_2$

Figure S19 The FT-IR spectrum (KBr pellet) of **Amido-eneamido** $PR_2 = PCy_2$. The peak at 1895 cm^{-1} was assigned to the CO stretch

Figure S20 1H NMR (400 MHz, C_6D_6) spectrum of **Hydride (S,S)-3** $PR_2 = PCy_2$

Figure S21 $^{31}\text{P}\{^1\text{H}\}$ NMR (161 MHz, C_6D_6) spectrum of Hydride (*S,S*)-3 $\text{PR}_2 = \text{PCy}_2$

Figure S22 The FT-IR spectrum (KBr pellet) of Hydride (*S,S*)-3 $\text{PR}_2 = \text{PCy}_2$. The peak at 1894 cm^{-1} was assigned to the CO stretch

General procedure for ATH (C/B/S=1/2/500):

A 20 mL vial was charged with a stir bar and precatalyst (8.9×10^{-3} mmol). The substrate (4.43×10 mmol) was added and the mixture was stirred. For liquid substrates, the mixture was stirred until the catalyst was completely dissolved. 3.61 g i PrOH was added and the solution was stirred for 5 minutes, or longer for solid substrates to allow them to fully dissolve. A stock solution of K Ot Bu (20 mg, 0.18 mmol) in 0.98 g i PrOH was stirred until all the base was dissolved. 0.1 g stock solution (2 eq.) was diluted by 1.0 g i PrOH and added to the 20-mL vial to activate the precatalyst and start catalysis. 0.1 mL samples were taken *via* syringe and injected into Teflon-sealed GC vials prepared with wet, aerated i PrOH to quench catalysis.

General procedure for ATH (C/B/S=1/8/6121):

The quantity of the precatalyst was measured via a stock solution method. A concentrated stock solution was made by dissolving the precatalysts (1.97×10^{-2} mmol) in 6.08 g cold dichloromethane. After all the solid was dissolved, the solution was immediately sucked into a syringe. The solution was then divided into equal portions into several 20 mL vials such that each portion has 0.2 g of the stock solution, and then dichloromethane was removed under vacuum. These operations led to a precatalyst quantity of 6.48×10^{-4} mmol in each vial. The base was prepared by dissolving K Ot Bu (10 mg, 0.089 mmol) in i PrOH (1.02 g, 1.30 mL). i PrOH (6.63 g, 8.44 mL), substrate (3.95 mmol) and a clean stirring bar were added to the vial that contains the precatalyst and the solution was stirred for 5 minutes, or until it was dissolved. 0.015 g of the base stock solution was added into a vial that contains 0.546 g of i PrOH and the mixed solution was then added into the catalyst solution to start the catalytic reaction. 0.1 mL samples were taken *via* syringe and injected into Teflon-sealed GC vials prepared with wet, aerated i PrOH to quench catalysis.

Data for analysis of the structures of the isomers of complexes

Position of the NH relative to the chiral centre on dpen. All of the structures of metal derivatives of racemic or enantiopure dpen in the Cambridge Crystallographic Data Bank containing the structure C-NH-CHPh- have the NH and CH hydrogens positioned anti to each other with the phenyl group equatorial in the five member ring. See the structures with refcodes ABALAR, BEPGAF, BOXVOA, CAGLUT, CAGMAA, DAQDIJ, DAQDOP, DOZMAH, GASGUD, IJIHIS, KUPDIJ, KUPDOP, KUYHET, LIPDUL, LIPFAT, MIMKAW, NIDXEE, ONOXOG, ONOXUM, OPOSOC, OPOSUI, QENJEY, QOPHAG, RAZNUD, RAZPAL, RAZPEP, RILYES, SITSEU, SOJTUG, TANROQ, TEJLAX, TEJLEB, TIXNAQ, TIXNEU, TIXNIY, TUSPOO, VEDPUQ, XOSCEP, YOSXEJ, YUFJOZ, YUFJUF, ZOWNIK, TAQJIH.

Analysis of the NMR spectra of the *trans* isomers

The complexes **C1** to **C3** are thought to have the *trans*-configuration with structure E in Figure S23.

Figure S23. Structure E of **C3** (left) and proposed structure E' of **C4** in solution.

³¹P NMR

Analysis of the ¹H NMR spectra of the backbone regions of **C1, **C4-1** and (**S,S**)-**1** in CD₂Cl₂ solution.**

2D NMR spectra and spin simulation software MNova-11 were used to assign the proton spectra between 2 and 6 ppm where the signals of the backbone of the tetradentate ligand are found apart from the imine CH=N proton which is hidden under the aryl proton resonances. The results are found in Table S1 and the simulated spectra in Figures S24-S27.

Table S1. Chemical shifts and coupling constants for the ¹H NMR of backbone resonances of **C1**, **C4-1** and (**S,S**)-**1** in CD₂Cl₂ solution; refer to the structures with the spectra for the lettering of hydrogen and phosphorus atoms.

	³¹ P NMR		³¹ P NMR			¹ H NMR											
PR2	PPh2	PR2	JPP		H	A	B	C	D	E	F	G	A2	B2	C2		
	ppm	ppm	Hz			ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm
PPh2, C1	CD ₂ Cl ₂					J, Hz	J, Hz	J, Hz	J, Hz	J, Hz	J, Hz	J, Hz	J, Hz	J, Hz	J, Hz	J, Hz	J, Hz
Isomer 1	57.9	62.7	40	δ		3.00	2.84	2.99	3.42	5.59	5.08	5.32	3.98	4.00	7.84		
	H	D2			JHH	AB	12 AB	12 AC	6 AD	12 DE	12 EF	10 FG	10 A2B2	12 A2B2	12		
					JHH	AC	6 BC	2 BC	2 BD	7 EF	10 FG	10	A2C2	4 B2C2	4		
					JHH	AD	12 BD	7 CD	12 CD	12							
					JHH				DE	12							
					JHP	AH	6 BH	55	10 DH	10 EH	4 FH	4 GH	4 A2D2	10 B2D2	10		
PEt2, (S,S)- 1	PPh2	PR2	JPP		H	A	B	C	D	E	F	G	A2	B2	C2		
SS1-1	59.3	65.5	37.9	δ		2.34	3.10	2.97	2.38	4.16	4.36	4.92	2.89	3.09	7.33		
	H	D2			JHH	AB	12 AB	12 AC	7 AD	14 CE	7 EF	10 FG	10 A2B2	12.5 A2B2	12.5		
					JHH	AC	7 BC	2 BC	7 BD	7 DE	13 FG	10	A2C2	6 B2C2			
					JHH	AD	14 BD	7 CD	12 CD	12 EF	10						
					JHH			CE	7 DE	13							
					JHP	AH	6 BH	22 CH	15 DH	10 EH	6 FH	0	A2D2	5 B2D2	10		
PEt2, (S,S)- 1	PPh2	PR2	JPP		H	A	B	C	D	E	F	G	A2	B2	C2		
SS1-2	53.7	67.1	36.4	δ		2.70	2.90	3.24	2.63	3.58	4.80	4.97	2.97	3.10	7.40		
	H	D2			JHH	AB	13 AB	12 AC	7 AD	13 CE	7 EF	12 FG	10 A2B2	12.5 A2B2	12.5		
					JHH	AC	7 BC	2 BC	2 BD	7 DE	13 FG	10					
					JHH	AD	13 BD	7 CD	12 CD	12 EF	12						
					JHH			CE	7 DE	13							
					JHP	AH	6 BH	22 CH	15 DH	0 EH	12 FH	4 GH	4 A2D2	5 A2D2	10		
PCy2, C4	PPh2	PR2	JPP		H	A	B	C	D	E	F	G	A2	B2	C2		
C4-1	47.3	78.4	33	δ		3.19	2.57	2.74	3.14	4.70	4.38	4.83	3.12	3.32	7.30		
	H	D2			JHH	AB	12 AB	12 AC	7 AD	13 CE	7 EF	11.7 FG	11.7 A2B2	12.5 A2B2	12.5		
					JHH	AC	7 BC	2 BC	13 BD	7 DE	12.1 FG	11.7					
					JHH	AD	13 BD	7 CD	12 CD	12 EF	11.7						
					JHH			CE	7 DE	12.1							
					JHP	AH	6 BH	22 CH	15 DH	12 EH	12 FH	GH	4 A2D2	5 A2D2	5

Figure S24. Simulation of the ¹H NMR spectrum at 500 MHz of **C1** (PR₂ = PPh₂) in CD₂Cl₂. The parameters used are listed in Table S1. A small amount of a second isomer, **C1-2**, is present in this sample as indicated.

Figure S25. Simulation of the 600 MHz ^1H NMR spectrum of the peaks due to isomer 1, (*S,S*)-1-1 ($\text{PR}_2 = \text{PEt}_2$) in CD_2Cl_2 . The parameters used are listed in Table S2. The other peaks are from isomer (*S,S*)-1-2 as in Figure S26.

Figure S26. Simulation of the 600 MHz ^1H NMR spectrum of the peaks due to isomer 2, **(*S,S*)-1-2** ($\text{PR}_2 = \text{PEt}_2$) in CD_2Cl_2 . The parameters used are listed in Table S1. The other peaks are from isomer **(*S,S*)-1-1** as in Figure S25.

Figure S27. Simulation of the 600 MHz ^1H NMR spectrum of **C4** ($\text{PR}_2 = \text{PCy}_2$) in CD_2Cl_2 . The parameters used are listed in Table S2. This sample had 75% of a *trans* isomer **C4-1** and 25% of a second isomer, **C4-1**, possibly with a *cis*- β structure since this is the isomer that crystallized from solution. The other peaks are from the second isomer and solvent impurities. This sample was used for the catalytic runs described here and in reference 3c of the main article.

Figure S28. gHBMC ^1H - ^{31}P NMR spectrum (600 MHz, CD_2Cl_2) of a sample of **C4** mixed with some *trans*-[FeBr(CO)(PCy₂CH₂CH=NCHPhCHPhN=CHCH₂PCy₂)]BPh₄ (67, 70 ppm, see reference 6a of the main article) which formed in the synthesis due to the presence of a dpen impurity. In this case both E (47, 78 ppm) and E' (72, 52 ppm) isomers of **C4** are observed under the conditions of the synthesis.

Full table of catalytic results

Figure S29: Substrate Scope.

Table S2: Full catalytic results for the ATH of substrates in **Figure S29**.

Entry	Subst.	Catalyst	Conv. (%)	Time (min)	e.e. (%)	TON
1	A1	(<i>S,S</i>)-1	>99	1	N/A	500
2 ^[b]		C4	>99	1	N/A	500
3		(<i>S,S</i>)-2	>99	1	N/A	500
4		C1	>99	1	N/A	500
5	K1	(<i>S,S</i>)-1	78	40	48	390
6 ^[b]		C4	84	40	83	420
7		(<i>S,S</i>)-2	78	40	80	390
8 ^[a]		(<i>S,S</i>)-1	87	120	84	5325
9 ^{[a][b]}	K2	C4	71	120	98	4346
10 ^[a]		(<i>S,S</i>)-2	67	120	89	4101
11		(<i>S,S</i>)-1	79	3	86	395
12 ^[b]		C4	80	60	94	400
13	K3	(<i>S,S</i>)-2	82	30	90	410
14		C1	82	10	31	410
15		(<i>S,S</i>)-1	52	60	12	260
16 ^[b]		C4	0	60	N/A	0
17	K4	(<i>S,S</i>)-2	0	60	N/A	0
18		C1	88	40	40	440
19		(<i>S,S</i>)-1	90	10	38	450
20 ^[b]		C4	92	10	52	460
21	K5	(<i>S,S</i>)-2	92	10	58	460
22		C1	90	3	6	450
23		(<i>S,S</i>)-1	>99	1	90	500
24 ^[b]		C4	>99	10	94	500
25	K6	(<i>S,S</i>)-2	>99	20	84	500
26		C1	>99	1	94	500
27		(<i>S,S</i>)-1	63	60	86	315
28 ^[b]		C4	38	40	95	190
29		(<i>S,S</i>)-2	>99	30	93	500

30		C1	>99	1	91	500
31	K7	(S,S)-1	62	20	15	310
32 ^[b]		C4	60	20	65	300
33		(S,S)-2	60	40	63	300
34		C1	60	30	3	300
35	K8	(S,S)-1	>99	3		500
36 ^[b]		C4	>99	20		500
37		(S,S)-2	>99	30		500
38		C1	>99	2		500
39	K9	(S,S)-1	0	60	N/A	0
40 ^[b]		C4	0	60	N/A	0
41		(S,S)-2	0	60	N/A	0
42		C1	0	60	N/A	0
43	K10	(S,S)-1	63	60	27	315
44 ^[b]		C4	44	60	43	220
45		(S,S)-2	75	40	55	375
46		C1	90	20	23	450
47	K11	(S,S)-1	33	60	N/A	165
48 ^[b]		C4	0	60	N/A	0
49		(S,S)-2	>99	2	N/A	500
50		C1	>99	50	N/A	500
51	K12	(S,S)-1	81	30	23	405
52 ^[b]		C4	88	40	82	440
53		(S,S)-2	84	40	59	420
54		C1	76	20	3	380
55	K13	(S,S)-1	0	60	N/A	0
56 ^[b]		C4	11	60	53	55
57		(S,S)-2	0	60	N/A	0
58		C1	0	60	N/A	0
59	K14	(S,S)-1	90	20	N/A	450
60 ^[b]		C4	89	20	N/A	445
61		(S,S)-2	91	20	N/A	455
62		C1	89	1	N/A	445
63	K15	(S,S)-1	57	5	4	285
64 ^[b]		C4	40	20	5	200
65		(S,S)-2	22	30	46	110
66		C1	78	50	3	390

^[a] C/B/S=1/2/6121; ^[b] from reference 12

GC Traces for reduction of acetophenone K1

(S,S)-1

GC analysis conditions: Oven temperature 130 °C

Retention time: (R)-isomer = 6.693; (S)-isomer = 7.193; starting material = 4.093.

(S,S)-2

GC analysis conditions: Oven temperature 130 °C

Retention time: (*R*)-isomer = 6.693; (*S*)-isomer = 7.193; starting material = 4.093.

(S,S)-1

GC analysis conditions: Oven temperature 130 °C

Retention time: (*R*)-isomer = 6.693; (*S*)-isomer = 7.193; starting material = 4.093.

(S,S)-2

GC analysis conditions: Oven temperature 130 °C

Retention time: (*R*)-isomer = 6.693; (*S*)-isomer = 7.193; starting material = 4.093.

GC Traces for Table 3 of the Main Article.

Propiophenone K2

GC analysis conditions: Oven temperature 120 °C

Retention time: (*R*)-isomer = 10.966; (*S*)-isomer = 11.992; starting material = 5.349.

Entry 1 (*S,S*)-4

Entry 3 (*S,S*)-2

Butyrophenone K3

GC analysis conditions: Oven temperature 140 °C

Retention time: (*R*)-isomer = 47.884; (*S*)-isomer = 50.454; starting material = 11.762.

Entry 4 (*S,S*)-1

p-Chloroacetophenone K4

GC analysis conditions: Oven temperature 145 °C

Retention time: (*R*)-isomer = 4.737; (*S*)-isomer = 5.213; starting material = 2.588

Entry 7 (*S,S*)-2

o-Chloroacetophenone K5

GC analysis conditions: Oven temperature 145 °C

Retention time: (*R*)-isomer = 5.654; (*S*)-isomer = 6.924; starting material = 2.752.

Entry 8 (*S,S*)-1

3',5'-(CF₃)₂acetophenone K6

GC analysis conditions: Oven temperature 140 °C

Retention time: (*R*)-isomer = 2.735; (*S*)-isomer = 2.606; starting material = 1.399.

Entry 11 (*S,S*)-2

p-Methylacetophenone K7

GC analysis conditions: Oven temperature 130 °C

Retention time: (*R*)-isomer = 6.034; (*S*)-isomer = 6.637; starting material = 4.142.

Entry 15 (*S,S*)-2

2-Acetylpyridine K8

GC analysis conditions: Oven temperature 100 °C

Retention time: (*R*)-isomer = 13.779; (*S*)-isomer = 14.208; starting material = 5.865.

Entry 16 (*S,S*)-1

Entry 17 (*S,S*)-2

2-acetylfuran K9

GC analysis conditions: Oven temperature 90 °C

Retention time: (*R*)-isomer = 8.827; (*S*)-isomer = 9.263; starting material = 4.165.

3-Methylbutan-2-one K10

GC analysis conditions: Oven temperature 60 °C

Retention time: (*R*)-isomer = 9.41; (*S*)-isomer = 9.92; starting material = 3.74.

Entry 21 (*S,S*)-2

Cyclohexanone K11

GC analysis conditions: Oven temperature 110 °C

Retention time: alcohol product = 2.941; starting material = 2.285.

Entry 23 (S,S)-1

Entry 24 (S,S)-2

2-Acetonaphthone K12

GC analysis conditions: Oven temperature 150 °C

Retention time: (*R*)-isomer = 6.119; (*S*)-isomer = 6.378; starting material = 4.403.

Entry 26 (S,S)-1

Entry 29 (S,S)-2

Benzophenone K14

GC analysis conditions: Oven temperature 180 °C

Retention time: product = 5.013; starting material = 3.228.

Entry 31 (S,S)-1

Entry 33 (S,S)-2

Benzylidene acetone K15

GC analysis conditions: Oven temperature 125 °C

Retention time: (R)-isomer = 15.743; (S)-isomer = 16.157; RED-(R)-isomer = 10.677; RED-(S)-isomer = 11.051; REDK = 6.416; starting material = 12.175.

Entry 35 (S,S)-2

DFT Calculations.

DFT calculations were performed using Gaussian 09 (Rev. D.01)¹ at the M06L²/TZVP³/TZVPfit level of theory. Either normal (opt) or tight (opt = tight) convergence criteria were used for all optimizations, and a pruned (99,590) integration grid was used throughout (grid = ultrafine). Optimizations were performed in a 2-propanol solvent continuum using the integral equation formalism polarizable continuum model (IEF-PCM)^{4,5} with radii and non-electrostatic terms from the SMD solvation model (scrf = smd).⁶ Full vibrational and thermochemical analyses (1 atm, 298 K) were performed on optimized structures to obtain solvent-corrected free energies (G°) and enthalpies (H°). Optimized ground states were found to have zero imaginary frequencies. Calculations were performed in part by the facilities of the Shared Hierarchical Academic Research Computing Network (SHARCNET) and Compute/Calcul Canada.⁷ Complexes *trans*-(*S,S*)-**C1** and **G1-1** have been reported elsewhere using the same level of theory.⁸

Scheme S1 and Tables S3 and S4 compare the calculated and observed energies and structures of the two isomers of the starting complex **C4** that were observed in the crystalline state.⁹

Scheme S2 compares the energies of some of the possible isomers of the alkoxide complexes (the complete set of isomers is found in Scheme 4 of the main article) derived from the reaction of **C4** with KOtBu and then 2-propanol. The intermediate alkoxide complexes are found to be less stable than the corresponding hydrides produced from them.

Scheme S3 compares the energies of possible isomers of the amido and hydride complexes derived from the reaction of **C1** with KOtBu and then isopropanol in an analogous fashion to those of **C4** found in Scheme 4 of the main article. Some of these were not considered in the original DFT study of such complexes.⁸ Here too the calculations show that *cis*- β hydride isomers cannot be ruled out as intermediates or resting states in catalysis.

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Scheme S1. Ground state energies of the *cis*- β isomers of **C4** (relative to Δ -(*S,S*)-**C4**).

Table S3. Selected experimental and calculated metrical parameters for complex Δ -*cis*- β -**C4** **R_{NH}**.

Parameter	Experimental	Calculated
	Length (Å)	
Fe1B–Br1B	2.5183(8)	2.564
Fe1B–P1B	2.246(1)	2.307
Fe1B–P2B	2.260(2)	2.278
Fe1B–N1B	2.071(5)	2.075
Fe1B–N2B	1.989(4)	2.010
Fe1B–C7B	1.756(7)	1.764
N2B–C5B	1.265(7)	1.275
Parameter	Angle (°)	
P1B–Fe1B–P2B	102.70(6)	101.5
N1B–Fe1B–N2B	82.4(2)	81.7
N1B–Fe1B–P1B	80.2(1)	80.5
N1B–Fe1B–P2B	165.7(1)	165.6
N2B–Fe1B–P1B	101.3(1)	96.5
N2B–Fe1B–P2B	83.3(1)	83.9
C7B–Fe1B–Br1B	85.1(2)	86.4

Table S4. Selected experimental and calculated metrical parameters for complex Λ -*cis*- β -**C4** **S_{NH}**.

Parameter	Experimental	Calculated
	Length (Å)	
Fe1A–Br1A	2.4970(8)	2.565
Fe1A–P1A	2.240(1)	2.278

Fe1A–P2A	2.256(2)	2.277
Fe1A–N1A	2.089(5)	2.015
Fe1A–N2A	1.976(4)	2.021
Fe1A–C7A	1.758(7)	1.762
N2A–C5A	1.280(8)	1.275
Angle (°)		
P1A–Fe1A–P2A	104.36(6)	100.9
N1A–Fe1A–N2A	82.1(2)	80.8
N1A–Fe1A–P1A	82.9(1)	82.9
N1A–Fe1A–P2A	165.6(1)	164.9
N2A–Fe1A–P1A	95.7(1)	94.5
N2A–Fe1A–P2A	84.8(1)	84.3
C7A–Fe1A–Br1A	87.5(2)	85.8

Scheme S2 – Reactions of some of the possible eneamido structures **(S,S)-4** (for a more complete set see Scheme S4 of the main article) with alcohol to give alkoxide isomers **(S,S)-5** which lead to some of the possible hydride isomers **(S,S)-3**. Ground state energies in kcal/mol (relative to Δ -cis- β -(S,S)-**4A**).

Scheme S3 – Relative energies of possible amido and hydride isomers derived from **C1**.

Free Energies (G° , Hartree), Enthalpies (H° , Hartree) and Cartesian Coordinates (Å) of Optimized Structures

acetone

$H^\circ = -193.115521$

$G^\circ = -193.149197$

C	0.00000	0.17857	0.00000
C	-1.27170	-0.60888	-0.00329
H	-2.13449	0.03240	-0.16508
H	-1.24103	-1.39249	-0.76166
H	-1.38181	-1.11751	0.95723
C	1.27170	-0.60888	0.00329
H	1.24103	-1.39249	0.76166
H	1.38181	-1.11751	-0.95723
H	2.13449	0.03240	0.16508
O	-0.00000	1.39880	0.00000

isopropanol

$H^\circ = -194.291128$

$G^\circ = -194.324792$

C	0.00260	0.03438	0.36276
H	-0.01064	0.08668	1.46070
C	1.33435	-0.51028	-0.08819
H	2.15412	0.12418	0.24946
H	1.49682	-1.51151	0.30996
H	1.37657	-0.56879	-1.17775
C	-1.16167	-0.81100	-0.10246
H	-1.10031	-1.82070	0.30624
H	-2.11275	-0.38249	0.21842
H	-1.17376	-0.88550	-1.19179
O	-0.09186	1.36929	-0.16410
H	-0.94685	1.72521	0.10490

Δ -cis- β -C4-R_{NH}

$H^\circ = -6374.602957$

$G^\circ = -6374.730671$

Fe	0.14177	-0.62700	-0.79009
Br	-0.13214	-3.15504	-1.12166
P	-0.04073	1.66986	-0.89850
P	1.84774	-0.87800	0.69860
O	1.87526	-0.76502	-3.13417
N	-1.70522	-0.47377	-1.72232
H	-1.87224	-1.39923	-2.11941
N	-1.02181	-0.87169	0.83042
C	-2.75770	-0.19725	-0.70046

H	-2.63352	0.84690	-0.39929
C	-2.45920	-1.05698	0.52656
H	-2.55127	-2.11034	0.23670
C	-1.70104	0.52298	-2.81470
H	-2.68651	0.58405	-3.28595
H	-0.99886	0.16537	-3.56713
C	-1.28495	1.87543	-2.27333
H	-2.14536	2.42118	-1.88970
H	-0.85146	2.49113	-3.05878
C	-0.57158	-1.06747	2.00755
H	-1.25231	-1.28218	2.83306
C	0.87802	-1.06050	2.28381
H	1.14230	-2.00678	2.76681
H	1.11754	-0.29482	3.02598
C	1.18663	-0.66554	-2.21097
C	-4.16170	-0.36694	-1.21828
C	-4.61645	-1.60057	-1.68227
H	-3.95222	-2.46009	-1.68615
C	-5.91821	-1.74242	-2.13718
H	-6.26131	-2.70579	-2.49409
C	-6.78179	-0.65457	-2.13054
H	-7.79939	-0.76762	-2.48381
C	-6.33764	0.57671	-1.67075
H	-7.00688	1.42832	-1.66400
C	-5.03323	0.71859	-1.21873
H	-4.68298	1.67963	-0.85485
C	-3.40188	-0.76965	1.66300
C	-4.23978	-1.76585	2.15294
H	-4.19114	-2.76080	1.72377
C	-5.13562	-1.49036	3.17780
H	-5.78521	-2.27327	3.54979
C	-5.19715	-0.21697	3.72453
H	-5.89483	-0.00252	4.52488
C	-4.36080	0.78296	3.24293
H	-4.40381	1.78062	3.66386
C	-3.47119	0.50818	2.21722
H	-2.82202	1.29139	1.83977
C	2.81720	-2.46966	0.68405
H	2.01450	-3.19801	0.86149
C	-0.16875	2.26779	1.81156
H	0.65312	1.56742	1.88795
C	-0.63358	2.89285	2.95784
H	-0.17846	2.66600	3.91459
C	-1.68155	3.79911	2.87401
H	-2.05606	4.28283	3.76769
C	-2.24478	4.08673	1.63880
H	-3.05502	4.80155	1.56417
C	-1.77283	3.46759	0.48891
H	-2.21974	3.72652	-0.46246
C	-0.73430	2.53935	0.56510
C	1.32862	2.77922	-1.42772
C	1.89720	2.58776	-2.68872
H	1.54513	1.79059	-3.33299

C	2.89637	3.43391	-3.14291
H	3.32500	3.27694	-4.12507
C	3.33616	4.48465	-2.34839
H	4.11257	5.14874	-2.70755
C	2.77520	4.68199	-1.09562
H	3.11134	5.50011	-0.47016
C	1.78065	3.83178	-0.63210
H	1.35142	4.00050	0.34816
C	3.83470	-2.60263	1.81767
H	3.38422	-2.35285	2.78195
H	4.65163	-1.89053	1.66211
C	4.40727	-4.01441	1.85359
H	5.14633	-4.09285	2.65445
H	3.60604	-4.71998	2.10112
C	5.02236	-4.39764	0.51665
H	5.88996	-3.75601	0.32257
H	5.40005	-5.42218	0.55159
C	4.01948	-4.23810	-0.61536
H	3.19829	-4.95159	-0.47809
H	4.48125	-4.48198	-1.57496
C	3.44574	-2.82761	-0.66216
H	2.69856	-2.75699	-1.45322
H	4.24441	-2.12276	-0.90784
C	3.02186	0.55664	0.91814
H	2.41269	1.42317	0.63472
C	3.53919	0.83211	2.32942
H	2.70926	0.92771	3.03382
H	4.15381	-0.00103	2.68031
C	4.36193	2.11511	2.34057
H	3.70651	2.95949	2.09087
H	4.73724	2.30435	3.34879
C	5.50779	2.05603	1.34256
H	6.20959	1.27060	1.64642
H	6.07062	2.99218	1.35426
C	4.99793	1.76214	-0.05922
H	5.82825	1.68153	-0.76478
H	4.37992	2.59796	-0.40268
C	4.16909	0.48649	-0.09255
H	3.78019	0.31067	-1.10037
H	4.81376	-0.36447	0.14749

Λ -cis- β -C4-S_{NH}

$H^\circ = -6374.599956$

$G^\circ = -6374.727772$

Fe	0.14177	-0.62700	-0.79009
Br	-0.13214	-3.15504	-1.12166
P	-0.04073	1.66986	-0.89850
P	1.84774	-0.87800	0.69860
O	1.87526	-0.76502	-3.13417
N	-1.70522	-0.47377	-1.72232
H	-1.87224	-1.39923	-2.11941
N	-1.02181	-0.87169	0.83042
C	-2.75770	-0.19725	-0.70046
H	-2.63352	0.84690	-0.39929
C	-2.45920	-1.05698	0.52656
H	-2.55127	-2.11034	0.23670
C	-1.70104	0.52298	-2.81470
H	-2.68651	0.58405	-3.28595
H	-0.99886	0.16537	-3.56713
C	-1.28495	1.87543	-2.27333
H	-2.14536	2.42118	-1.88970
H	-0.85146	2.49113	-3.05878
C	-0.57158	-1.06747	2.00755
H	-1.25231	-1.28218	2.83306
C	0.87802	-1.06050	2.28381
H	1.14230	-2.00678	2.76681
H	1.11754	-0.29482	3.02598
C	1.18663	-0.66554	-2.21097
C	-4.16170	-0.36694	-1.21828
C	-4.61645	-1.60057	-1.68227
H	-3.95222	-2.46009	-1.68615
C	-5.91821	-1.74242	-2.13718
H	-6.26131	-2.70579	-2.49409
C	-6.78179	-0.65457	-2.13054
H	-7.79939	-0.76762	-2.48381
C	-6.33764	0.57671	-1.67075
H	-7.00688	1.42832	-1.66400
C	-5.03323	0.71859	-1.21873
H	-4.68298	1.67963	-0.85485
C	-3.40188	-0.76965	1.66300
C	-4.23978	-1.76585	2.15294
H	-4.19114	-2.76080	1.72377
C	-5.13562	-1.49036	3.17780
H	-5.78521	-2.27327	3.54979
C	-5.19715	-0.21697	3.72453
H	-5.89483	-0.00252	4.52488
C	-4.36080	0.78296	3.24293
H	-4.40381	1.78062	3.66386
C	-3.47119	0.50818	2.21722
H	-2.82202	1.29139	1.83977
C	2.81720	-2.46966	0.68405
H	2.01450	-3.19801	0.86149
C	-0.16875	2.26779	1.81156
H	0.65312	1.56742	1.88795
C	-0.63358	2.89285	2.95784
H	-0.17846	2.66600	3.91459
C	-1.68155	3.79911	2.87401
H	-2.05606	4.28283	3.76769
C	-2.24478	4.08673	1.63880
H	-3.05502	4.80155	1.56417
C	-1.77283	3.46759	0.48891
H	-2.21974	3.72652	-0.46246

Δ -(S,S)-4A S36

C	1.86841	2.71989	-2.48256
H	1.44333	2.07959	-3.24704
C	2.91990	3.56110	-2.81172
H	3.30883	3.56119	-3.82273
C	3.46489	4.40641	-1.85394
H	4.28368	5.06612	-2.11388
C	2.95458	4.40231	-0.56432
H	3.37263	5.05884	0.18946
C	1.90662	3.55582	-0.22909
H	1.51900	3.56825	0.78264
C	3.63730	-3.26575	1.21957
H	3.24641	-3.14739	2.23366
H	4.49613	-2.59151	1.13467
C	4.11500	-4.69503	0.99833
H	4.88597	-4.94764	1.73070
H	3.28257	-5.38599	1.17508
C	4.63566	-4.88535	-0.41738
H	5.52399	-4.25870	-0.56159
H	4.96018	-5.91731	-0.57131
C	3.57840	-4.50261	-1.44079
H	2.73048	-5.19197	-1.35416
H	3.96521	-4.61874	-2.45623
C	3.08041	-3.07669	-1.23659
H	2.27789	-2.86069	-1.94432
H	3.89010	-2.37504	-1.46063
C	3.09375	0.06211	0.88962
H	2.53819	1.00400	0.78127
C	3.66735	0.05299	2.30515
H	2.85645	0.07333	3.03837
H	4.22445	-0.87154	2.48356
C	4.59357	1.24612	2.50653
H	4.00677	2.17083	2.42989
H	5.01161	1.23058	3.51601
C	5.70402	1.26841	1.46676
H	6.34184	0.38713	1.60433
H	6.34818	2.13858	1.61443
C	5.13691	1.26298	0.05539
H	5.94165	1.24414	-0.68394
H	4.58371	2.19307	-0.11485
C	4.19816	0.08471	-0.16560
H	3.76382	0.13049	-1.16920
H	4.77222	-0.84666	-0.11627

Δ -(S,S)-4B

$H^\circ = -3799.366002$

$G^\circ = -3799.492309$

Fe	-0.08897	0.87641	-0.91530
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P	0.02067	-1.55080	-0.95916
P	-1.87502	1.13737	0.51403
O	0.07132	3.75176	-1.28050
N	1.67698	0.63918	-1.85436
N	1.01172	0.97549	0.67415
C	2.70126	0.36452	-0.86157
H	2.64110	-0.66867	-0.46098
C	2.40607	1.25441	0.35980
H	2.52337	2.30510	0.04030
C	1.59786	-0.39643	-2.86321
H	2.52633	-0.45909	-3.45302
H	0.81499	-0.11566	-3.57625
C	1.28057	-1.79167	-2.30133
H	2.17524	-2.25068	-1.87957
H	0.89810	-2.47249	-3.06203
C	0.44765	1.35419	1.82613
H	1.11225	1.57872	2.66398
C	-0.91150	1.41857	1.99550
H	-1.33976	1.66745	2.95860
C	-0.02480	2.60315	-1.13244
C	4.11071	0.54142	-1.37597
C	4.48842	1.71108	-2.03434
H	3.74079	2.47695	-2.21333
C	5.79588	1.89533	-2.45885
H	6.07588	2.81247	-2.96434
C	6.74854	0.90735	-2.23719
H	7.76950	1.05042	-2.57067
C	6.38267	-0.26577	-1.59200
H	7.11772	-1.04386	-1.42176
C	5.07257	-0.44376	-1.16547
H	4.78580	-1.35898	-0.65389
C	3.37195	0.98797	1.48533
C	4.34807	1.92081	1.82397
H	4.37079	2.87463	1.30672
C	5.29167	1.63845	2.80391
H	6.04704	2.37444	3.05299
C	5.26625	0.41803	3.46372
H	5.99994	0.19726	4.22975
C	4.29108	-0.51800	3.13917
H	4.26354	-1.47280	3.65200
C	3.35436	-0.23492	2.15734
H	2.59430	-0.96591	1.90142
C	-2.88975	2.69394	0.29746
H	-2.11001	3.45886	0.42001
C	0.10401	-2.05339	1.77024
H	-0.62310	-1.25117	1.83058
C	0.51833	-2.68803	2.93174
H	0.09453	-2.39217	3.88442
C	1.48525	-3.68258	2.87344
H	1.81684	-4.17361	3.78034
C	2.03014	-4.04282	1.64831
H	2.78371	-4.81943	1.59597
C	1.60699	-3.41784	0.48306
H	2.03065	-3.72505	-0.46579
C	0.63998	-2.41370	0.53285
C	-1.39073	-2.59429	-1.51104
C	-2.14622	-2.13995	-2.59510
H	-1.90672	-1.18628	-3.05705

C	-3.19643	-2.89774	-3.08966
H	-3.77135	-2.53436	-3.93299
C	-3.51285	-4.11615	-2.50191
H	-4.33437	-4.70765	-2.88708
C	-2.77820	-4.56761	-1.41485
H	-3.02433	-5.51375	-0.94790
C	-1.72499	-3.81108	-0.91753
H	-1.15809	-4.17778	-0.06946
C	-3.94589	2.96104	1.36655
H	-3.51517	2.85214	2.36555
H	-4.74663	2.21756	1.28897
C	-4.54094	4.35434	1.19735
H	-5.31533	4.52585	1.94937
H	-3.75969	5.10026	1.38377
C	-5.10335	4.55492	-0.20212
H	-5.95519	3.87969	-0.34717
H	-5.49483	5.56901	-0.31347
C	-4.05568	4.26876	-1.26847
H	-3.24702	5.00576	-1.19259
H	-4.48491	4.38433	-2.26691
C	-3.47106	2.87225	-1.10504
H	-2.69990	2.68723	-1.85961
H	-4.25781	2.13278	-1.28124
C	-3.04960	-0.28604	0.83513
H	-2.41792	-1.15901	0.62087
C	-3.52890	-0.44238	2.27584
H	-2.67641	-0.41238	2.96017
H	-4.17794	0.39565	2.55030
C	-4.28815	-1.75322	2.43805
H	-3.59390	-2.58590	2.26431
H	-4.64401	-1.85908	3.46592
C	-5.44735	-1.85454	1.45718
H	-6.18909	-1.08333	1.69670
H	-5.95766	-2.81460	1.56747
C	-4.97389	-1.66643	0.02358
H	-5.81667	-1.70998	-0.67128
H	-4.30702	-2.49282	-0.24812
C	-4.21895	-0.35481	-0.14391
H	-3.86489	-0.24784	-1.17405
H	-4.90189	0.48158	0.03824

Λ -(S,S)-4A

$H^\circ = -3799.380057$

$G^\circ = -3799.504910$

Fe	0.00746	0.28250	-0.88823
P	0.29909	-1.84864	-0.52106
P	1.62723	1.31130	0.35616

O	1.50690	0.13864	-3.37977
N	-1.73639	-0.31783	-1.67353
N	-1.12868	0.88106	0.57354
C	-2.81075	0.43822	-1.00748
H	-2.70389	1.48165	-1.33587
C	-2.53532	0.47428	0.50355
H	-2.63774	-0.54380	0.91644
C	-2.03420	-1.74113	-1.78798
H	-2.66117	-1.95899	-2.66712
H	-2.60772	-2.11855	-0.92553
C	-0.75021	-2.53588	-1.86650
H	-0.21704	-2.34265	-2.80043
H	-0.90198	-3.61411	-1.79026
C	-0.62513	1.40826	1.71016
H	-1.31681	1.62844	2.52602
C	0.70372	1.67817	1.84649
H	1.10154	2.17552	2.72132
C	0.93680	0.17643	-2.36144
C	-4.19805	0.00417	-1.41465
C	-4.72618	0.48762	-2.61231
H	-4.14081	1.18866	-3.19867
C	-5.97516	0.08574	-3.06122
H	-6.36472	0.47550	-3.99446
C	-6.72719	-0.81102	-2.31354
H	-7.70506	-1.12491	-2.65865
C	-6.21789	-1.29877	-1.11831
H	-6.79787	-1.99742	-0.52660
C	-4.96491	-0.89665	-0.67508
H	-4.58049	-1.29502	0.25754
C	-3.48155	1.37825	1.24483
C	-3.56140	2.73903	0.93814
H	-2.90525	3.15481	0.18061
C	-4.45690	3.56410	1.59999
H	-4.50619	4.61699	1.34777
C	-5.28761	3.04696	2.58746
H	-5.98613	3.69302	3.10548
C	-5.20982	1.69976	2.91006
H	-5.84715	1.28885	3.68431
C	-4.31171	0.87549	2.24466
H	-4.24868	-0.17778	2.50133
C	-0.45076	-2.42959	1.04513
C	-0.08075	-1.78601	2.22664
H	0.65927	-0.99252	2.19647
C	-0.66874	-2.13350	3.43233
H	-0.37471	-1.62254	4.34157
C	-1.63866	-3.12768	3.47031
H	-2.10827	-3.39268	4.40987
C	-2.00271	-3.78301	2.30274
H	-2.75266	-4.56445	2.32905
C	-1.40861	-3.44227	1.09428
H	-1.69798	-3.96968	0.19379
C	1.87422	-2.78979	-0.64485
C	2.56078	-2.80271	-1.86167
H	2.18894	-2.23168	-2.70420
C	3.71245	-3.56018	-2.01074
H	4.22938	-3.56678	-2.96267
C	4.19820	-4.31059	-0.94786
H	5.09629	-4.90413	-1.06736

C	3.53138	-4.29195	0.26849
H	3.90634	-4.87030	1.10431
C	2.37822	-3.53451	0.42228
H	1.86371	-3.53579	1.37599
C	2.18882	2.99856	-0.24670
H	1.25261	3.56785	-0.15542
C	3.22771	3.67413	0.64637
H	2.90225	3.65895	1.68987
H	4.16545	3.10979	0.60227
C	3.49708	5.10361	0.19472
H	2.58495	5.69890	0.31802
H	4.25347	5.56140	0.83716
C	3.93230	5.14451	-1.26138
H	4.89111	4.62265	-1.36516
H	4.10780	6.17463	-1.58079
C	2.89806	4.47966	-2.15565
H	1.96952	5.06152	-2.12277
H	3.22746	4.48729	-3.19762
C	2.60173	3.05044	-1.71742
H	3.48719	2.42843	-1.88378
H	1.80877	2.63097	-2.33894
C	3.11198	0.28997	0.83416
H	2.67204	-0.71256	0.93163
C	3.75290	0.61124	2.18363
H	2.99122	0.61718	2.96727
H	4.19323	1.61207	2.16828
C	4.83661	-0.40984	2.50894
H	5.30156	-0.16922	3.46806
H	4.37259	-1.39695	2.63017
C	5.88406	-0.48177	1.40795
H	6.41161	0.47774	1.34834
H	6.64071	-1.23222	1.64957
C	5.24365	-0.78941	0.06297
H	4.79887	-1.78992	0.09736
H	5.99685	-0.81322	-0.72882
C	4.15531	0.21821	-0.27853
H	3.68015	-0.04116	-1.23055
H	4.60806	1.20621	-0.41662

Λ -(*S,S*)-4B

$H^\circ = -3799.360481$

$G^\circ = -3799.485408$

Fe	-0.01861	0.50472	-0.96916
P	0.36199	-1.82825	-0.71126
P	1.73043	1.27281	0.33016
O	-0.54313	3.30499	-1.59929
N	-1.73045	-0.16673	-1.78127
N	-1.08945	0.71680	0.63427
C	-2.79310	0.50094	-1.01206

H	-2.69750	1.57496	-1.21785
C	-2.49516	0.33923	0.49788
H	-2.59628	-0.73088	0.74849
C	-2.00161	-1.59576	-1.92804
H	-2.66208	-1.78305	-2.78917
H	-2.53516	-2.02135	-1.06216
C	-0.71582	-2.36693	-2.09824
H	-0.19773	-2.07823	-3.01681
H	-0.86224	-3.44793	-2.12907
C	-0.56027	1.27622	1.71340
H	-1.21425	1.44886	2.57118
C	0.77106	1.62664	1.78933
H	1.16985	2.09184	2.68191
C	-0.34798	2.18511	-1.36080
C	-4.18984	0.10416	-1.43177
C	-4.74234	0.70777	-2.56242
H	-4.16932	1.46859	-3.08319
C	-5.99941	0.35139	-3.02684
H	-6.40782	0.83599	-3.90611
C	-6.73602	-0.62091	-2.36259
H	-7.71997	-0.90035	-2.71982
C	-6.20226	-1.22961	-1.23555
H	-6.76904	-1.98944	-0.71009
C	-4.94164	-0.87130	-0.77657
H	-4.53973	-1.36522	0.10141
C	-3.43198	1.11411	1.38345
C	-3.56382	2.49802	1.24541
H	-2.95745	3.02166	0.51285
C	-4.44787	3.20809	2.04209
H	-4.54097	4.28089	1.91998
C	-5.21178	2.54897	2.99880
H	-5.90109	3.10530	3.62254
C	-5.07970	1.17685	3.15528
H	-5.66402	0.65691	3.90537
C	-4.19449	0.46793	2.35343
H	-4.08730	-0.60554	2.47832
C	-0.39407	-2.52620	0.80013
C	-0.07552	-1.93526	2.02330
H	0.62438	-1.10581	2.05409
C	-0.66579	-2.38302	3.19551
H	-0.41390	-1.91207	4.13842
C	-1.58576	-3.42254	3.15679
H	-2.05671	-3.76532	4.07024
C	-1.89989	-4.02407	1.94557
H	-2.61097	-4.84077	1.91232
C	-1.30430	-3.58279	0.77177
H	-1.55632	-4.06480	-0.16533
C	1.88993	-2.81735	-0.96444
C	2.63657	-2.61132	-2.12728
H	2.33797	-1.84429	-2.83464
C	3.75465	-3.38742	-2.39098
H	4.32065	-3.22150	-3.29977
C	4.14789	-4.37297	-1.49423
H	5.02057	-4.97981	-1.70253
C	3.42273	-4.57137	-0.32824
H	3.72702	-5.33373	0.37884
C	2.30157	-3.79709	-0.06123
H	1.73936	-3.96794	0.84959

trans-(*S,S*)-4

$$G^{\circ} = -3799.520870$$

H	-0.20966	2.66898	-2.30855
Fe	-0.32317	0.06468	0.13194
P	1.01508	1.82723	-0.39814
P	1.03727	-1.81767	0.30113
C	-0.37086	0.33483	1.81378
O	-0.59508	0.50945	2.94767
C	-0.22047	-2.97862	0.82094
H	-0.02776	-4.00131	1.11581
C	-1.58065	2.56530	-0.66571
H	-2.36980	3.01040	-1.28521
H	-1.69845	3.01279	0.33766
C	2.33672	1.61330	-1.65715
C	3.68971	1.75244	-1.34762
C	1.97771	1.18388	-2.93759
C	4.66041	1.48497	-2.30350
H	3.99129	2.06986	-0.35556
C	2.94864	0.93027	-3.89371
H	0.93205	1.03673	-3.18779
C	4.29315	1.07865	-3.57854
H	5.70750	1.59826	-2.04932
H	2.65443	0.60593	-4.88468
H	5.05194	0.87337	-4.32383
C	1.79819	2.97051	0.81819
C	2.29294	4.19806	0.36665
C	1.91717	2.65871	2.16945
C	2.89027	5.08555	1.24624
H	2.21965	4.45859	-0.68367
C	2.51765	3.54839	3.05161
H	1.54741	1.71518	2.54611
C	3.00434	4.76199	2.59268
H	3.26934	6.03184	0.87965
H	2.60179	3.28701	4.09964
H	3.47186	5.45618	3.28030
C	-4.19120	1.26049	-0.96452
C	-5.29702	1.81296	-0.32516
C	-4.19535	1.18243	-2.35731
C	-6.38666	2.27137	-1.05460
H	-5.30295	1.87670	0.75865
C	-5.27838	1.64399	-3.08958
H	-3.33449	0.76045	-2.86599
C	-6.38047	2.18723	-2.43946
H	-7.24097	2.69537	-0.54006
H	-5.26574	1.57935	-4.17142
H	-7.22803	2.54560	-3.01135
C	-4.21013	-1.37508	0.63080
C	-5.36797	-1.83770	0.01196
C	-4.15887	-1.35451	2.02484
C	-6.45478	-2.26508	0.76400
H	-5.41616	-1.85577	-1.07250
C	-5.24029	-1.78403	2.77848
H	-3.25771	-1.00295	2.51728
C	-6.39365	-2.23889	2.14981
H	-7.34913	-2.62098	0.26622
H	-5.18551	-1.76414	3.86070
H	-7.23829	-2.57489	2.73928
C	1.73521	-2.56209	-1.29152
C	3.10422	-2.01399	-1.68640
C	1.78043	-4.08951	-1.25400

H	1.00931	-2.25917	-2.05927
C	3.55919	-2.57587	-3.02732
H	3.83727	-2.29935	-0.92259
H	3.09442	-0.92367	-1.71673
C	2.26146	-4.66839	-2.57875
H	2.45312	-4.40813	-0.44724
H	0.79559	-4.49057	-1.01114
C	3.60506	-4.09485	-2.99853
H	4.53755	-2.16463	-3.29002
H	2.86577	-2.24541	-3.80995
H	2.31181	-5.75820	-2.51050
H	1.51790	-4.44445	-3.35260
H	3.90275	-4.49022	-3.97284
H	4.37508	-4.41671	-2.28752
C	2.46959	-1.91519	1.49751
C	3.32367	-0.65059	1.40324
C	1.99153	-2.13124	2.93212
H	3.07629	-2.78105	1.19846
C	4.47149	-0.64188	2.40122
H	2.67371	0.20810	1.60015
H	3.70220	-0.51035	0.38958
C	3.15000	-2.12904	3.92012
H	1.28899	-1.33363	3.20108
H	1.43079	-3.06499	3.00623
C	3.96861	-0.85132	3.82022
H	5.01990	0.30150	2.32106
H	5.18422	-1.43490	2.14574
H	2.77022	-2.26447	4.93585
H	3.79839	-2.98958	3.71735
H	4.80231	-0.87245	4.52622
H	3.34187	0.00213	4.10831

Δ -(*S,S*)-3A

$H^\circ = -3800.586861$

$G^\circ = -3800.712638$

Fe	0.17636	-0.74125	-0.94857
H	0.08269	-2.26980	-1.22015
P	-0.03531	1.55343	-0.75344
P	1.80523	-1.25222	0.50950
O	1.88811	-0.64576	-3.29297
N	-1.67287	-0.50309	-1.89067
H	-1.83676	-1.34960	-2.43010
N	-1.03398	-1.10547	0.62066
C	-2.74438	-0.39515	-0.86110
H	-2.65243	0.60327	-0.42177
C	-2.41138	-1.38235	0.26464
H	-2.50899	-2.40096	-0.15283

C	-1.66890	0.64396	-2.82496
H	-2.64704	0.75788	-3.30550
H	-0.94681	0.40936	-3.60704
C	-1.28754	1.92123	-2.09808
H	-2.16592	2.38380	-1.64878
H	-0.87751	2.64878	-2.79684
C	-0.51437	-1.54618	1.76619
H	-1.19846	-1.85213	2.56324
C	0.84168	-1.59212	1.97581
H	1.26005	-1.86561	2.93648
C	1.20411	-0.64350	-2.34276
C	-4.13292	-0.54230	-1.41776
C	-4.51672	-1.69586	-2.10094
H	-3.79804	-2.49380	-2.26035
C	-5.81348	-1.83629	-2.57252
H	-6.10005	-2.73818	-3.10004
C	-6.74451	-0.82633	-2.36588
H	-7.75755	-0.93792	-2.73294
C	-6.37150	0.32683	-1.68956
H	-7.09232	1.11918	-1.52753
C	-5.07266	0.46654	-1.22076
H	-4.77853	1.36504	-0.68605
C	-3.41182	-1.24391	1.38813
C	-4.30476	-2.27046	1.67678
H	-4.24849	-3.19530	1.11174
C	-5.26310	-2.11957	2.67148
H	-5.95143	-2.92885	2.88475
C	-5.33715	-0.93605	3.39133
H	-6.08349	-0.81655	4.16747
C	-4.44590	0.09447	3.11431
H	-4.49794	1.02187	3.67336
C	-3.49190	-0.05901	2.12044
H	-2.79503	0.74556	1.90537
C	2.74973	-2.84512	0.20067
H	1.93924	-3.57796	0.31929
C	-0.27268	1.79530	1.99688
H	0.46909	1.00302	2.00318
C	-0.75185	2.29792	3.19750
H	-0.36879	1.90872	4.13379
C	-1.73167	3.28161	3.19683
H	-2.11578	3.66874	4.13294
C	-2.21872	3.76700	1.99083
H	-2.97850	4.53952	1.98307
C	-1.72910	3.27374	0.78834
H	-2.10848	3.68416	-0.13981
C	-0.75482	2.27577	0.77895
C	1.31841	2.74560	-1.13796
C	1.92162	2.69441	-2.39733
H	1.58135	1.97438	-3.13328
C	2.94505	3.57004	-2.72628
H	3.39820	3.51951	-3.70909
C	3.38271	4.51168	-1.80357
H	4.17999	5.19758	-2.06269
C	2.79410	4.56700	-0.54889
H	3.13042	5.29622	0.17864
C	1.77292	3.68710	-0.21447
H	1.32516	3.74420	0.77083
C	3.80932	-3.16201	1.25456

H	3.38957	-3.06221	2.25942
H	4.62513	-2.43454	1.18367
C	4.38368	-4.55900	1.05678
H	5.15183	-4.75795	1.80865
H	3.59278	-5.30039	1.21958
C	4.94929	-4.72540	-0.34484
H	5.80094	-4.04617	-0.47198
H	5.34072	-5.73636	-0.48307
C	3.89680	-4.41335	-1.39711
H	3.09235	-5.15543	-1.33024
H	4.31751	-4.50835	-2.40146
C	3.30280	-3.02189	-1.21146
H	2.50694	-2.86119	-1.94092
H	4.07137	-2.26968	-1.41646
C	3.04113	0.09698	0.90513
H	2.41931	0.99720	0.79488
C	3.58651	0.12652	2.33136
H	2.76295	0.07039	3.04855
H	4.21968	-0.74637	2.51598
C	4.39921	1.39489	2.55898
H	3.73369	2.26378	2.47262
H	4.79549	1.41198	3.57739
C	5.52602	1.52319	1.54425
H	6.24071	0.70542	1.69648
H	6.08271	2.44963	1.70682
C	4.99460	1.46819	0.11966
H	5.81569	1.52134	-0.60008
H	4.36663	2.34667	-0.06460
C	4.16503	0.21430	-0.12241
H	3.75347	0.22395	-1.13689
H	4.81407	-0.66581	-0.05900

Δ -(*S,S*)-**3B**

$H^\circ = -3800.580262$

$G^\circ = -3800.705384$

Fe	0.13029	-0.83274	-0.95532
H	0.95179	-0.49322	-2.24483
P	0.03266	1.48090	-0.94512
P	1.82687	-1.13395	0.51684
O	0.34552	-3.58432	-1.84970
N	-1.73477	-0.57205	-1.87388
H	-1.95980	-1.43634	-2.36060
N	-1.04415	-1.07786	0.65796
C	-2.76664	-0.36864	-0.81589
H	-2.62032	0.64626	-0.43352
C	-2.44011	-1.31384	0.35136
H	-2.59291	-2.34675	-0.01293
C	-1.71757	0.51200	-2.88069
H	-2.70460	0.62928	-3.34225

H	-1.02224	0.20097	-3.65921
C	-1.27250	1.81399	-2.24743
H	-2.11299	2.32018	-1.77286
H	-0.88119	2.49391	-3.00271
C	-0.49476	-1.48146	1.80045
H	-1.15417	-1.76561	2.62645
C	0.86944	-1.51561	1.98052
H	1.29934	-1.75116	2.94648
C	0.25282	-2.49047	-1.44880
C	-4.17795	-0.49097	-1.32045
C	-4.62403	-1.65929	-1.93817
H	-3.93937	-2.48885	-2.08674
C	-5.94005	-1.77441	-2.36077
H	-6.27457	-2.68758	-2.83828
C	-6.82930	-0.72486	-2.16816
H	-7.85747	-0.81663	-2.49655
C	-6.39527	0.44204	-1.55491
H	-7.08361	1.26467	-1.40305
C	-5.07697	0.55676	-1.13642
H	-4.73541	1.46659	-0.65159
C	-3.39643	-1.07504	1.49611
C	-4.31328	-2.04588	1.88494
H	-4.32007	-3.00333	1.37409
C	-5.21539	-1.79799	2.91291
H	-5.92323	-2.56461	3.20524
C	-5.20787	-0.57400	3.56586
H	-5.90887	-0.38089	4.36902
C	-4.29323	0.40225	3.18640
H	-4.27870	1.36158	3.69134
C	-3.39777	0.15225	2.15924
H	-2.68359	0.91349	1.86264
C	2.88962	-2.65203	0.23550
H	2.11583	-3.43289	0.25228
C	-0.18976	1.92620	1.79152
H	0.42350	1.03451	1.86816
C	-0.60385	2.57418	2.94695
H	-0.29090	2.19784	3.91429
C	-1.43213	3.68449	2.86183
H	-1.76536	4.18644	3.76223
C	-1.83403	4.15031	1.61655
H	-2.47514	5.02060	1.54304
C	-1.40715	3.51192	0.46018
H	-1.70953	3.90773	-0.50266
C	-0.58322	2.38755	0.53548
C	1.43475	2.54426	-1.50229
C	2.11356	2.19940	-2.67273
H	1.83180	1.29930	-3.20894
C	3.14504	2.99263	-3.15078
H	3.66046	2.71038	-4.06102
C	3.51579	4.14382	-2.46765
H	4.32142	4.76359	-2.84214
C	2.85210	4.49167	-1.30076
H	3.13850	5.38367	-0.75646
C	1.82103	3.69631	-0.81693
H	1.31767	3.98169	0.09913
C	3.87433	-2.98596	1.35356
H	3.38157	-2.93249	2.32812
H	4.68039	-2.24392	1.36897

C	4.47335	-4.37222	1.14322
H	5.19795	-4.59303	1.93130
H	3.67753	-5.12000	1.23868
C	5.12134	-4.50177	-0.22748
H	5.99061	-3.83526	-0.27806
H	5.50483	-5.51487	-0.37246
C	4.15024	-4.13367	-1.34045
H	3.32886	-4.85987	-1.36390
H	4.64429	-4.19571	-2.31349
C	3.57544	-2.73926	-1.12808
H	2.87685	-2.48130	-1.92800
H	4.38837	-2.01100	-1.18603
C	2.98039	0.29234	0.92402
H	2.35235	1.17133	0.72448
C	3.40402	0.39042	2.38782
H	2.52453	0.34392	3.03581
H	4.03297	-0.46497	2.65675
C	4.16931	1.68416	2.63461
H	3.49256	2.53199	2.46530
H	4.48140	1.74401	3.68042
C	5.37003	1.81036	1.70841
H	6.08971	1.01691	1.94318
H	5.88964	2.75599	1.88242
C	4.95147	1.69386	0.25067
H	5.82232	1.75271	-0.40758
H	4.31069	2.54319	-0.00929
C	4.18663	0.40237	-0.00530
H	3.86856	0.34558	-1.05116
H	4.85716	-0.44618	0.16460

Λ -(*S,S*)-**3A**

$H^\circ = -3800.582115$

$G^\circ = -3800.707382$

Fe	0.07894	0.45362	-0.96232
P	0.28750	-1.79875	-0.54803
P	1.64679	1.34857	0.38057
O	1.68326	0.35873	-3.37921
N	-1.78103	-0.14171	-1.79546
H	-1.78109	0.23448	-2.73871
N	-1.13130	0.77264	0.61711
C	-2.83759	0.59854	-1.02918
H	-2.65198	1.64871	-1.26671
C	-2.53124	0.41666	0.46201
H	-2.66840	-0.65038	0.71337
C	-2.05552	-1.60384	-1.89619
H	-2.68480	-1.81137	-2.76476

H	-2.62751	-1.90146	-1.01566
C	-0.77058	-2.39408	-1.94374
H	-0.21644	-2.18923	-2.86301
H	-0.96179	-3.46802	-1.91271
C	-0.64532	1.31320	1.72661
H	-1.32453	1.49474	2.56372
C	0.68582	1.64440	1.85190
H	1.06580	2.12095	2.74688
C	1.05760	0.36742	-2.38972
C	-4.23781	0.25458	-1.47317
C	-4.76497	0.90867	-2.58686
H	-4.16881	1.66771	-3.08350
C	-6.03292	0.60652	-3.05980
H	-6.42486	1.12787	-3.92496
C	-6.80078	-0.35687	-2.41975
H	-7.79380	-0.59252	-2.78293
C	-6.29085	-1.01310	-1.30824
H	-6.88505	-1.76439	-0.80189
C	-5.01961	-0.71168	-0.83990
H	-4.63516	-1.23592	0.02824
C	-3.48178	1.20345	1.33139
C	-3.64426	2.57798	1.15527
H	-3.08060	3.08960	0.38185
C	-4.50784	3.29700	1.96672
H	-4.62690	4.36336	1.81539
C	-5.21787	2.65462	2.97447
H	-5.89146	3.21783	3.60910
C	-5.05449	1.29072	3.16678
H	-5.59821	0.78369	3.95509
C	-4.19021	0.57302	2.34975
H	-4.05861	-0.49428	2.50055
C	-0.50683	-2.47910	0.95929
C	-0.17616	-1.88818	2.17973
H	0.54730	-1.07775	2.20269
C	-0.77676	-2.31252	3.35541
H	-0.51123	-1.84305	4.29537
C	-1.72404	-3.32759	3.32434
H	-2.20220	-3.65333	4.24028
C	-2.05854	-3.92325	2.11581
H	-2.79376	-4.71866	2.08721
C	-1.45136	-3.50529	0.93903
H	-1.72215	-3.98572	0.00617
C	1.80183	-2.82938	-0.74159
C	2.51202	-2.76637	-1.94345
H	2.18045	-2.10835	-2.73826
C	3.63748	-3.55233	-2.13948
H	4.17152	-3.49697	-3.08055
C	4.07812	-4.40569	-1.13620
H	4.95661	-5.02003	-1.29135
C	3.38984	-4.46234	0.06707
H	3.72904	-5.12073	0.85794
C	2.26064	-3.67881	0.26577
H	1.73073	-3.73927	1.20938
C	2.33535	3.02183	-0.11615
H	1.43065	3.64129	-0.03839
C	3.36968	3.59545	0.85046
H	3.00326	3.54270	1.87947
H	4.28041	2.98815	0.81199

C	3.72778	5.03069	0.48689
H	2.84139	5.66471	0.60520
H	4.47794	5.41752	1.18148
C	4.22571	5.12344	-0.94681
H	5.16341	4.56204	-1.03825
H	4.46211	6.15872	-1.20485
C	3.20215	4.55348	-1.91627
H	2.30136	5.17794	-1.89372
H	3.57810	4.59593	-2.94173
C	2.81908	3.12166	-1.56144
H	3.68232	2.46632	-1.71698
H	2.03680	2.77137	-2.23715
C	3.07957	0.23710	0.84676
H	2.58067	-0.74211	0.88378
C	3.69232	0.45201	2.22958
H	2.90387	0.49385	2.98553
H	4.21562	1.41152	2.27075
C	4.67497	-0.66763	2.55070
H	5.11890	-0.50931	3.53685
H	4.12716	-1.61729	2.60833
C	5.75825	-0.77707	1.48775
H	6.36528	0.13610	1.49851
H	6.43924	-1.60004	1.71932
C	5.15341	-0.96357	0.10437
H	4.63005	-1.92553	0.06931
H	5.93638	-1.01101	-0.65726
C	4.16042	0.14265	-0.22660
H	3.70917	-0.03384	-1.20870
H	4.69273	1.09807	-0.29701
H	-0.26371	1.90918	-1.39031

Λ -(*S,S*)-**3B**

$$H^\circ = -3800.576161$$

$$G^\circ = -3800.701765$$

Fe	0.05919	0.49904	-1.00587
P	0.34413	-1.77073	-0.71664
P	1.71008	1.24874	0.35635
O	-0.20583	3.12540	-2.21375
N	-1.81017	-0.14211	-1.81107
H	-1.84726	0.25709	-2.74444
N	-1.11042	0.76234	0.60887
C	-2.85992	0.55616	-0.99242
H	-2.71836	1.61626	-1.21955
C	-2.49926	0.36098	0.48698
H	-2.58949	-0.71572	0.71938
C	-2.05741	-1.60459	-1.94727
H	-2.72477	-1.79883	-2.79010
H	-2.57653	-1.94508	-1.04956

C	-0.75568	-2.35115	-2.08352
H	-0.24633	-2.09849	-3.01543
H	-0.90946	-3.43114	-2.07710
C	-0.59630	1.29242	1.70925
H	-1.25372	1.47384	2.56434
C	0.74149	1.61655	1.80851
H	1.13819	2.07063	2.70819
C	-0.10590	2.08324	-1.69515
C	-4.26541	0.17767	-1.38844
C	-4.86328	0.84224	-2.45896
H	-4.31674	1.63545	-2.95930
C	-6.13980	0.50728	-2.88501
H	-6.58762	1.03771	-3.71687
C	-6.84456	-0.50047	-2.24079
H	-7.84368	-0.76181	-2.56791
C	-6.26363	-1.16782	-1.17159
H	-6.80820	-1.95366	-0.66188
C	-4.98476	-0.83302	-0.74993
H	-4.54506	-1.36697	0.08546
C	-3.44895	1.09452	1.40206
C	-3.67353	2.46375	1.25567
H	-3.16349	3.00993	0.46837
C	-4.53078	3.13460	2.11382
H	-4.69925	4.19728	1.98537
C	-5.17156	2.44881	3.13923
H	-5.84041	2.97444	3.81006
C	-4.94563	1.08997	3.30217
H	-5.43537	0.54947	4.10353
C	-4.08816	0.42059	2.43842
H	-3.90717	-0.64257	2.56565
C	-0.36542	-2.54281	0.79208
C	-0.05858	-1.95189	2.01900
H	0.59992	-1.08896	2.04816
C	-0.60772	-2.43881	3.19571
H	-0.36113	-1.96700	4.13977
C	-1.48196	-3.51700	3.16029
H	-1.92110	-3.89177	4.07702
C	-1.79401	-4.11262	1.94567
H	-2.47245	-4.95681	1.91275
C	-1.23646	-3.63245	0.76833
H	-1.48642	-4.11648	-0.16844
C	1.87534	-2.73938	-1.03445
C	2.62388	-2.46222	-2.17992
H	2.32725	-1.64587	-2.83023
C	3.74044	-3.22336	-2.49115
H	4.30945	-2.99967	-3.38569
C	4.12940	-4.26612	-1.66001
H	5.00193	-4.85977	-1.90433
C	3.39920	-4.53943	-0.51257
H	3.69885	-5.34736	0.14417
C	2.27935	-3.78077	-0.19879
H	1.71513	-4.00906	0.69790
C	2.51653	2.86578	-0.13439
H	1.63470	3.52198	-0.16602
C	3.47566	3.46073	0.89398
H	3.02782	3.44711	1.89137
H	4.38138	2.84641	0.94893
C	3.86252	4.88389	0.50855

H	2.97072	5.51953	0.55468
H	4.56854	5.29243	1.23621
C	4.44999	4.94240	-0.89382
H	5.40257	4.39918	-0.90594
H	4.68338	5.97475	-1.16609
C	3.51159	4.31874	-1.91728
H	2.59649	4.91927	-1.98716
H	3.96625	4.33461	-2.91108
C	3.14365	2.89268	-1.52854
H	4.04826	2.27850	-1.54306
H	2.46551	2.45311	-2.26404
C	3.07791	0.06890	0.86989
H	2.56749	-0.90351	0.83341
C	3.58677	0.22944	2.30107
H	2.74486	0.26569	2.99689
H	4.12043	1.17950	2.40754
C	4.51888	-0.92032	2.66243
H	4.89176	-0.79813	3.68267
H	3.94491	-1.85643	2.65460
C	5.67617	-1.03455	1.68072
H	6.30830	-0.14256	1.76536
H	6.31199	-1.88577	1.93721
C	5.17362	-1.15796	0.25005
H	4.62742	-2.10139	0.13959
H	6.01100	-1.20366	-0.45148
C	4.24354	-0.00800	-0.11172
H	3.87622	-0.11784	-1.13681
H	4.80706	0.93089	-0.08109
H	0.92115	0.13196	-2.26175

trans-(*S,S*)-3'

$H^\circ = -3800.577825$

$G^\circ = -3800.705558$

H	2.98942	-0.74939	0.79090
C	3.04293	-0.57849	-0.28918
H	3.18970	1.07729	-1.62303
C	3.01779	0.94552	-0.53895
H	2.26740	3.36432	0.23953
N	1.78511	-1.10802	-0.85771
N	1.69591	1.40713	-0.17920
C	1.43609	2.65659	0.18118
H	-0.01818	-3.94540	-1.18125
C	0.22216	-2.88773	-1.28628
H	0.20535	-2.64806	-2.35206
Fe	0.21474	0.04127	-0.12693
P	-1.02733	-1.81038	-0.41776
P	-1.11318	1.86671	0.18990

C	0.57219	-0.14193	1.59248
O	0.87368	-0.18699	2.71859
H	-0.14022	0.29621	-1.66189
C	0.16165	3.07960	0.48725
H	-0.03120	4.11118	0.75242
C	1.58119	-2.55822	-0.71233
H	2.37103	-3.12299	-1.21837
H	1.63458	-2.79557	0.35480
H	1.78076	-0.89574	-1.85436
C	-2.48732	-1.83251	-1.53625
C	-3.78104	-1.96568	-1.03041
C	-2.32172	-1.57025	-2.89734
C	-4.88195	-1.84417	-1.86707
H	-3.93398	-2.15992	0.02543
C	-3.42215	-1.46226	-3.73392
H	-1.32744	-1.43311	-3.30763
C	-4.70568	-1.59452	-3.22060
H	-5.87987	-1.94573	-1.45761
H	-3.27618	-1.26320	-4.78888
H	-5.56487	-1.49942	-3.87338
C	-1.57537	-2.96978	0.91955
C	-2.09158	-4.22053	0.56474
C	-1.46314	-2.65781	2.27067
C	-2.48898	-5.12540	1.53485
H	-2.19004	-4.48735	-0.48222
C	-1.86336	-3.56402	3.24578
H	-1.06396	-1.70124	2.57711
C	-2.37818	-4.79743	2.88080
H	-2.88764	-6.08870	1.24008
H	-1.77045	-3.29915	4.29229
H	-2.69185	-5.50369	3.63994
C	4.29256	-1.22298	-0.82697
C	5.26964	-1.68963	0.04807
C	4.52279	-1.31067	-2.19975
C	6.45536	-2.22646	-0.43380
H	5.09746	-1.62260	1.11735
C	5.70463	-1.85171	-2.68372
H	3.77373	-0.95073	-2.89836
C	6.67587	-2.30772	-1.80159
H	7.20724	-2.58280	0.26008
H	5.87071	-1.91393	-3.75257
H	7.60001	-2.72715	-2.18034
C	4.16763	1.59843	0.19134
C	5.29211	2.03551	-0.50160
C	4.15317	1.70217	1.58226
C	6.38527	2.55906	0.17721
H	5.31083	1.95673	-1.58389
C	5.24135	2.22627	2.26209
H	3.27678	1.37051	2.13034
C	6.36301	2.65406	1.56096
H	7.25449	2.89362	-0.37666
H	5.21724	2.30043	3.34292
H	7.21337	3.06374	2.09268
C	-2.09547	2.53032	-1.26992
C	-3.37697	1.75758	-1.56456
C	-2.39133	4.02520	-1.16833
H	-1.40520	2.37798	-2.11006
C	-4.04828	2.26301	-2.83534

H	-4.07529	1.87990	-0.72725
H	-3.16699	0.68902	-1.64327
C	-3.07633	4.53929	-2.42916
H	-3.03836	4.21406	-0.30251
H	-1.46827	4.58176	-0.99323
C	-4.33833	3.75340	-2.74861
H	-4.96860	1.70312	-3.02224
H	-3.39018	2.06813	-3.69084
H	-3.30301	5.60355	-2.32438
H	-2.37768	4.45635	-3.26982
H	-4.78768	4.11281	-3.67773
H	-5.08097	3.92790	-1.96106
C	-2.37947	1.92987	1.57211
C	-3.08733	0.58000	1.68059
C	-1.77731	2.32717	2.91653
H	-3.11906	2.69037	1.28716
C	-4.12368	0.55034	2.79293
H	-2.32766	-0.18167	1.88009
H	-3.53927	0.30318	0.72486
C	-2.81915	2.29785	4.02784
H	-0.96303	1.63734	3.16594
H	-1.32262	3.31785	2.84860
C	-3.50305	0.94254	4.12481
H	-4.57298	-0.44545	2.85512
H	-4.94017	1.24186	2.55296
H	-2.35433	2.56178	4.98117
H	-3.57498	3.06773	3.83281
H	-4.25805	0.95012	4.91486
H	-2.76324	0.18467	4.41296

trans-(*S,S*)-3

$H^\circ = -3800.581199$

$G^\circ = -3800.708676$

H	-2.870744	0.622606	0.758750
C	-3.011212	0.525155	-0.321986
H	-3.183626	-1.053441	-1.750198
C	-2.985439	-0.978294	-0.664181
H	-2.200568	-3.425443	-0.029352
N	-1.805150	1.122984	-0.939626
N	-1.655036	-1.442770	-0.350389
C	-1.377555	-2.706475	-0.062957
H	-0.016468	4.004453	-0.872701
C	-0.237096	2.962167	-1.105501
H	-0.183428	2.839009	-2.190016
Fe	-0.169652	-0.101475	-0.480903
P	0.983218	1.801377	-0.314933
P	1.135093	-1.834085	0.184349
C	0.276025	-0.397483	-2.166356

O	0.598296	-0.583346	-3.273219
H	-0.478686	0.167024	1.040295
C	-0.094893	-3.127266	0.206982
H	0.110450	-4.145111	0.517047
C	-1.604027	2.548099	-0.610248
H	-2.392049	3.167216	-1.050189
H	-1.674632	2.645832	0.477302
H	-1.914523	1.059754	-1.951015
C	2.552004	2.068090	-1.232121
C	3.776958	2.002685	-0.565339
C	2.549881	2.171969	-2.623922
C	4.969103	2.046857	-1.272285
H	3.800279	1.912574	0.515371
C	3.743918	2.220371	-3.329117
H	1.613600	2.208609	-3.168329
C	4.956272	2.154900	-2.656269
H	5.910945	1.994220	-0.739181
H	3.725077	2.307074	-4.408906
H	5.887443	2.187367	-3.208735
C	1.303354	2.708179	1.265970
C	1.927376	3.958602	1.217566
C	0.871444	2.224456	2.496654
C	2.122623	4.696354	2.373661
H	2.265397	4.358923	0.267850
C	1.064417	2.965781	3.656318
H	0.376735	1.260960	2.542667
C	1.691687	4.200265	3.598046
H	2.609794	5.662485	2.318534
H	0.720845	2.573968	4.606303
H	1.843984	4.777377	4.502147
C	-4.302823	1.188395	-0.719369
C	-5.191723	1.627569	0.258174
C	-4.659452	1.326155	-2.060829
C	-6.413384	2.185327	-0.092122
H	-4.921631	1.521859	1.303830
C	-5.877532	1.888046	-2.413704
H	-3.981777	0.986859	-2.838459
C	-6.759613	2.315906	-1.429798
H	-7.095111	2.519611	0.680783
H	-6.141604	1.988401	-3.459732
H	-7.712150	2.751677	-1.705945
C	-4.108908	-1.681412	0.061009
C	-5.239756	-2.112234	-0.625010
C	-4.060956	-1.843701	1.446015
C	-6.306981	-2.686350	0.054373
H	-5.283357	-1.989352	-1.702426
C	-5.123057	-2.418154	2.126267
H	-3.178419	-1.517552	1.988385
C	-6.251809	-2.838790	1.431990
H	-7.181397	-3.015851	-0.494341
H	-5.073145	-2.537964	3.202147
H	-7.081710	-3.287935	1.964203
C	2.441639	-2.456511	-1.011976
C	3.447246	-1.426028	-1.518771
C	3.168062	-3.716864	-0.548862
H	1.811526	-2.738912	-1.867308
C	4.276872	-2.002514	-2.658731
H	4.119547	-1.129991	-0.706651

H	2.937919	-0.515906	-1.841001
C	4.005203	-4.303508	-1.679365
H	3.827452	-3.468108	0.291266
H	2.456494	-4.460215	-0.178407
C	4.985543	-3.281153	-2.235589
H	5.000698	-1.262121	-3.009887
H	3.615893	-2.214705	-3.508157
H	4.537153	-5.193162	-1.332225
H	3.336104	-4.637503	-2.480760
H	5.544105	-3.705587	-3.073592
H	5.726448	-3.039259	-1.464226
C	1.971100	-1.887528	1.859505
C	3.020529	-0.791548	2.020545
C	0.951551	-1.834758	2.993783
H	2.469427	-2.864994	1.905618
C	3.679059	-0.821211	3.393779
H	2.533856	0.180710	1.872305
H	3.782910	-0.872393	1.242870
C	1.627391	-1.891066	4.356411
H	0.373462	-0.906142	2.914214
H	0.231031	-2.649437	2.885649
C	2.649489	-0.776338	4.511707
H	4.383202	0.010534	3.485841
H	4.273214	-1.738185	3.486985
H	0.876470	-1.836382	5.148880
H	2.127589	-2.859879	4.473145
H	3.140289	-0.836014	5.486367
H	2.131732	0.189810	4.485002

Δ -cis- β -(S,S)-5A

$H^\circ = -3993.712445$

$G^\circ = -3993.849797$

Fe	-0.08136	0.63881	-0.77735
P	-0.02176	-1.65890	-0.99062
P	-1.79372	0.88320	0.74649
O	-1.71491	1.13454	-3.13851
N	1.75907	0.42190	-1.68257
H	1.85800	1.38725	-2.00275
N	1.07323	0.61996	0.86726
C	2.81421	0.12719	-0.67898
H	2.72848	-0.93731	-0.43606
C	2.47309	0.89814	0.60318
H	2.61373	1.96907	0.38703
C	1.74803	-0.51977	-2.81240
H	2.73955	-0.60110	-3.27175
H	1.07166	-0.10974	-3.56289

C	1.27047	-1.87651	-2.33241
H	2.09941	-2.45352	-1.92322
H	0.85789	-2.46056	-3.15338
C	0.53380	0.91909	2.04828
H	1.20608	1.07743	2.89728
C	-0.82293	0.99703	2.24138
H	-1.24489	1.12342	3.23058
C	-1.07942	0.86871	-2.19998
C	4.20524	0.39927	-1.18330
C	4.55846	1.66717	-1.64529
H	3.81325	2.45728	-1.67453
C	5.85520	1.92884	-2.06081
H	6.11848	2.91858	-2.41432
C	6.81707	0.92720	-2.01890
H	7.83045	1.13377	-2.34120
C	6.47438	-0.33842	-1.56435
H	7.21954	-1.12429	-1.53206
C	5.17514	-0.59903	-1.15020
H	4.90548	-1.58714	-0.78935
C	3.42352	0.51294	1.71223
C	4.34716	1.42742	2.20811
H	4.35432	2.43861	1.81377
C	5.25461	1.05696	3.19325
H	5.96788	1.78090	3.56935
C	5.24521	-0.23574	3.69686
H	5.95047	-0.52589	4.46639
C	4.32312	-1.15622	3.21148
H	4.30830	-2.16818	3.60028
C	3.42174	-0.78364	2.22680
H	2.70064	-1.50120	1.84835
C	-2.85091	2.43121	0.76675
H	-2.07422	3.19577	0.88458
C	0.12830	-2.37871	1.69254
H	-0.51212	-1.51729	1.84223
C	0.50878	-3.14614	2.78347
H	0.14588	-2.88868	3.77203
C	1.36347	-4.22591	2.60864
H	1.66863	-4.82307	3.45947
C	1.82570	-4.53897	1.33741
H	2.48683	-5.38486	1.19249
C	1.43457	-3.77915	0.24308
H	1.78530	-4.06025	-0.74280
C	0.58651	-2.68402	0.41169
C	-1.40772	-2.69337	-1.63794
C	-1.99432	-2.34866	-2.85796
H	-1.64050	-1.48340	-3.40698
C	-3.01615	-3.11860	-3.39221
H	-3.45716	-2.83829	-4.34113
C	-3.46442	-4.24855	-2.72025
H	-4.25896	-4.85220	-3.14144
C	-2.88845	-4.59904	-1.50861
H	-3.23214	-5.47772	-0.97600
C	-1.87184	-3.82421	-0.96584
H	-1.43684	-4.11256	-0.01645
C	-3.77052	2.56631	1.98070
H	-3.23980	2.31153	2.90141
H	-4.60551	1.86205	1.89248
C	-4.31640	3.98737	2.06714

H	-4.98402	4.08319	2.92722
H	-3.48099	4.67497	2.24688
C	-5.03392	4.39201	0.78799
H	-5.93614	3.77926	0.67382
H	-5.37525	5.42801	0.85420
C	-4.14751	4.19961	-0.43404
H	-3.29893	4.89413	-0.38452
H	-4.69618	4.44865	-1.34604
C	-3.61804	2.77286	-0.51143
H	-2.98619	2.64872	-1.39277
H	-4.46223	2.09199	-0.64103
C	-2.96594	-0.57700	0.90395
H	-2.35417	-1.41900	0.55559
C	-3.39202	-0.92081	2.32989
H	-2.51309	-0.99827	2.97605
H	-4.01053	-0.11797	2.74386
C	-4.17628	-2.22719	2.34596
H	-3.51354	-3.04184	2.02553
H	-4.48697	-2.46754	3.36590
C	-5.38160	-2.16617	1.41926
H	-6.08680	-1.41628	1.79734
H	-5.91672	-3.11901	1.42517
C	-4.96886	-1.79866	0.00213
H	-5.84596	-1.71442	-0.64482
H	-4.35351	-2.60203	-0.41529
C	-4.17429	-0.50026	-0.02517
H	-3.85905	-0.26607	-1.04781
H	-4.82644	0.31736	0.29704
O	0.57024	2.56288	-1.03157
C	-0.12756	3.76253	-0.93066
H	-1.21435	3.59388	-0.98391
H	-0.01967	3.78224	1.23361
C	0.17664	4.45467	0.39434
H	-0.41558	5.36317	0.54107
H	1.23377	4.73410	0.43983
H	-0.28244	5.62780	-2.05657
H	1.30830	4.85816	-2.11877
C	0.23159	4.66403	-2.10434
H	-0.03368	4.18777	-3.05085

Λ -cis- β -(S,S)-5A

$H^\circ = -3993.713887$

$G^\circ = -3993.849890$

Fe	0.08232	0.39232	-0.75102
P	0.39349	-1.87311	-0.77222
P	1.70690	1.04071	0.71189
O	1.70782	0.70112	-3.14941

N	-1.78587	-0.14312	-1.62851
H	-1.83413	0.42779	-2.46843
N	-1.06479	0.28325	0.89617
C	-2.83972	0.37050	-0.69561
H	-2.69931	1.45238	-0.73060
C	-2.46463	-0.07516	0.72189
H	-2.56775	-1.17319	0.78677
C	-1.99124	-1.56316	-2.02172
H	-2.62115	-1.62400	-2.91200
H	-2.53697	-2.06006	-1.21782
C	-0.67012	-2.26211	-2.23201
H	-0.14781	-1.86617	-3.10637
H	-0.80167	-3.33323	-2.39252
C	-0.56882	0.68862	2.05576
H	-1.22765	0.70903	2.92811
C	0.74540	1.06969	2.20884
H	1.12712	1.38380	3.17151
C	1.06312	0.56868	-2.18554
C	-4.23657	0.04336	-1.15881
C	-4.82740	0.86291	-2.12139
H	-4.28069	1.72864	-2.48257
C	-6.09335	0.58921	-2.61584
H	-6.53459	1.24057	-3.36083
C	-6.79678	-0.51358	-2.14981
H	-7.78823	-0.72865	-2.52958
C	-6.22389	-1.33607	-1.18999
H	-6.76718	-2.19706	-0.81917
C	-4.95405	-1.06176	-0.70048
H	-4.51966	-1.71715	0.04674
C	-3.40159	0.52473	1.74266
C	-3.59110	1.90592	1.81123
H	-3.04895	2.55374	1.12874
C	-4.44723	2.45539	2.75228
H	-4.58690	3.52928	2.79142
C	-5.12343	1.63345	3.64672
H	-5.79180	2.06408	4.38266
C	-4.93334	0.26057	3.59541
H	-5.45099	-0.38641	4.29376
C	-4.07617	-0.28726	2.64911
H	-3.92472	-1.36169	2.60937
C	-0.33773	-2.82584	0.61434
C	0.03001	-2.47556	1.91401
H	0.73697	-1.66678	2.07258
C	-0.51717	-3.13522	3.00350
H	-0.22513	-2.84947	4.00718
C	-1.44416	-4.15099	2.80780
H	-1.88033	-4.66029	3.65871
C	-1.81119	-4.51128	1.51911
H	-2.52891	-5.30712	1.36026
C	-1.25818	-3.85625	0.42630
H	-1.55236	-4.15751	-0.57184
C	1.93135	-2.81143	-1.16181
C	2.62813	-2.51416	-2.33557
H	2.28674	-1.71853	-2.98658
C	3.75354	-3.24212	-2.69070
H	4.27897	-3.00190	-3.60717
C	4.20202	-4.27633	-1.87999
H	5.07903	-4.84678	-2.16034

C	3.52283	-4.57247	-0.70732
H	3.86724	-5.37503	-0.06616
C	2.39719	-3.84393	-0.34655
H	1.87619	-4.09135	0.57066
C	2.35308	2.77796	0.47520
H	1.39440	3.30419	0.36507
C	3.07572	3.36761	1.68471
H	2.52338	3.16532	2.60573
H	4.05616	2.88856	1.79209
C	3.26815	4.86970	1.50745
H	2.28361	5.35223	1.49233
H	3.80064	5.28585	2.36669
C	4.00699	5.19386	0.21710
H	5.03507	4.81926	0.28866
H	4.08499	6.27581	0.08444
C	3.33178	4.55535	-0.98811
H	2.34537	5.01024	-1.14032
H	3.90630	4.75432	-1.89659
C	3.16448	3.05369	-0.79056
H	4.15685	2.60354	-0.70484
H	2.69598	2.60280	-1.66669
C	3.13948	-0.12872	0.99418
H	2.64762	-1.10649	0.88753
C	3.74630	-0.10333	2.39581
H	2.95819	-0.16293	3.15050
H	4.26653	0.84626	2.56066
C	4.72823	-1.25623	2.56721
H	5.16975	-1.22976	3.56665
H	4.17706	-2.20332	2.49868
C	5.81474	-1.23130	1.50198
H	6.43209	-0.33577	1.63978
H	6.48524	-2.08611	1.62033
C	5.21482	-1.21629	0.10390
H	4.68415	-2.15804	-0.07092
H	6.00108	-1.16016	-0.65395
C	4.23685	-0.06193	-0.06378
H	3.80676	-0.06231	-1.07090
H	4.78278	0.88049	0.04369
O	-0.59946	2.28355	-0.76540
C	-0.34265	3.19966	-1.78255
H	0.73709	3.23999	-2.03005
C	-1.08345	2.87009	-3.07544
H	-0.90760	3.61631	-3.85494
H	-0.76946	1.90518	-3.48047
H	-2.16193	2.82754	-2.89174
C	-0.74225	4.58238	-1.28533
H	-0.21230	4.82813	-0.36226
H	-0.52745	5.36413	-2.01821
H	-1.81417	4.61002	-1.06689

trans-(*S,S*)-5

$H^\circ = -3993.715729$

$G^\circ = -3993.853788$

Fe	-0.21949	-0.03893	-0.07657
P	1.01753	1.91626	-0.33589
P	1.16380	-1.81303	0.44575
H	-3.00281	0.80279	0.89385
C	-3.05007	0.56703	-0.17447
H	-3.31456	-1.17547	-1.37950
C	-3.02501	-0.97273	-0.33558
H	-2.19558	-3.37221	0.37473
N	-1.80093	1.08246	-0.76971
N	-1.66212	-1.41705	-0.10065
C	-1.37655	-2.65131	0.30740
H	-0.05070	3.92803	-1.30074
C	-0.25515	2.85742	-1.31134
H	-0.21609	2.51182	-2.34621
C	-0.58904	0.17764	1.60601
O	-0.93021	0.26144	2.71853
C	-0.10493	-3.05224	0.64486
H	0.08710	-4.07553	0.94087
C	-1.61413	2.54014	-0.72148
H	-2.40732	3.05933	-1.26921
H	-1.68043	2.85309	0.32565
H	-1.71979	0.78072	-1.74457
C	2.55683	1.96212	-1.33050
C	3.79197	2.05315	-0.68150
C	2.53740	1.76135	-2.71146
C	4.97530	1.94014	-1.39423
H	3.83027	2.21112	0.39081
C	3.72468	1.64783	-3.42195
H	1.59355	1.67173	-3.23188
C	4.94501	1.73228	-2.76718
H	5.92332	2.01287	-0.87467
H	3.69198	1.48754	-4.49343
H	5.86974	1.63775	-3.32365
C	1.39844	3.15978	0.97959
C	1.94958	4.38772	0.59674
C	1.12369	2.94787	2.32739
C	2.22931	5.36444	1.53737
H	2.16798	4.57840	-0.44859
C	1.40488	3.92791	3.27246
H	0.68722	2.01682	2.65787
C	1.96069	5.13497	2.88141

H	2.65862	6.30738	1.22080
H	1.18627	3.74021	4.31689
H	2.18238	5.89748	3.61814
C	-4.30987	1.16527	-0.74349
C	-5.31653	1.61689	0.10503
C	-4.51596	1.22065	-2.12156
C	-6.50812	2.10956	-0.40914
H	-5.16354	1.57290	1.17852
C	-5.70323	1.71772	-2.63771
H	-3.73958	0.87172	-2.79633
C	-6.70402	2.16060	-1.78199
H	-7.28383	2.45492	0.26376
H	-5.85013	1.75689	-3.71043
H	-7.63244	2.54635	-2.18529
C	-4.08813	-1.59099	0.54324
C	-5.28344	-2.03891	-0.01109
C	-3.92218	-1.66145	1.92640
C	-6.29718	-2.54026	0.79531
H	-5.41999	-1.98658	-1.08674
C	-4.93107	-2.16365	2.73347
H	-2.99101	-1.32322	2.36865
C	-6.12377	-2.60249	2.17018
H	-7.22215	-2.88441	0.34796
H	-4.78799	-2.21278	3.80649
H	-6.91122	-2.99578	2.80180
C	2.36783	-2.51372	-0.80608
C	3.58436	-1.62013	-1.03051
C	2.78382	-3.94884	-0.48346
H	1.79044	-2.54339	-1.73416
C	4.52319	-2.19407	-2.08479
H	4.13927	-1.51019	-0.09044
H	3.25600	-0.61773	-1.31974
C	3.71198	-4.50491	-1.55649
H	3.29799	-3.98249	0.48451
H	1.89979	-4.58317	-0.38818
C	4.93260	-3.61973	-1.75138
H	5.40361	-1.55404	-2.18637
H	4.02167	-2.18204	-3.05973
H	4.01153	-5.52404	-1.29875
H	3.16230	-4.57552	-2.50299
H	5.57940	-4.02517	-2.53337
H	5.52746	-3.61898	-0.83020
C	2.23971	-1.72616	1.98329
C	2.76633	-0.30430	2.16857
C	1.54160	-2.22447	3.24497
H	3.09890	-2.38163	1.79272
C	3.65427	-0.16935	3.39483
H	1.91221	0.36864	2.27656
H	3.29106	0.02706	1.26802
C	2.43120	-2.07165	4.47273
H	0.61260	-1.66518	3.39748
H	1.24608	-3.26878	3.12022
C	2.92335	-0.64199	4.64180
H	3.97718	0.87007	3.50572
H	4.56576	-0.76338	3.25798
H	1.89268	-2.40073	5.36503
H	3.29680	-2.73747	4.37417
H	3.56664	-0.56048	5.52127

H	2.06535	0.01786	4.82488
H	-2.26528	-0.97290	-2.96368
C	-1.42639	-1.01720	-3.65818
H	-1.40480	-0.07648	-4.21801
H	-1.63160	-1.82329	-4.36793
H	-0.17310	-2.17157	-2.37175
C	-0.10329	-1.21359	-2.92445
C	1.01768	-1.33863	-3.95265
H	0.90474	-2.22929	-4.57658
H	1.02300	-0.46803	-4.61545
O	0.16904	-0.15522	-2.05915
H	1.99461	-1.38367	-3.46859

Δ -(S,S)-6A (from *trans*-(S,S)-C1)

$H^\circ = -3792.279027$

$G^\circ = -3792.399730$

Fe	0.21202	-0.77386	-0.77230
P	0.24284	1.40358	-0.96447
P	1.82448	-1.27493	0.74476
O	2.07268	-1.21597	-2.97224
N	-1.46416	-0.63716	-1.73333
N	-0.96776	-1.07432	0.74381
C	-2.56340	-0.30459	-0.82530
H	-2.49215	0.74160	-0.46893
C	-2.38723	-1.18127	0.41945
H	-2.61580	-2.21732	0.12064
C	-1.39249	0.30573	-2.84765
H	-2.36034	0.39696	-3.35886
H	-0.68711	-0.08984	-3.58265
C	-0.93115	1.68800	-2.38543
H	-1.77057	2.28551	-2.02835
H	-0.44751	2.26646	-3.17352
C	-0.49673	-1.40602	1.95652
H	-1.21848	-1.63227	2.74425
C	0.84605	-1.45424	2.22451
H	1.23655	-1.75405	3.18812
C	1.31648	-0.97438	-2.11874
C	-3.93332	-0.46092	-1.43908
C	-4.29451	-1.63605	-2.09699
H	-3.56104	-2.42800	-2.20384
C	-5.57125	-1.79260	-2.61535
H	-5.83855	-2.71207	-3.12314
C	-6.50837	-0.77445	-2.48520
H	-7.50557	-0.89713	-2.89066
C	-6.15804	0.40215	-1.83789
H	-6.88157	1.20257	-1.73668

C	-4.87812	0.55524	-1.32078
H	-4.60239	1.47438	-0.81066
C	-3.34857	-0.79143	1.51358
C	-4.42951	-1.60977	1.82916
H	-4.54242	-2.55967	1.31644
C	-5.36195	-1.22041	2.78256
H	-6.19865	-1.86869	3.01493
C	-5.22162	-0.00516	3.43716
H	-5.94628	0.29928	4.18280
C	-4.14336	0.81804	3.13359
H	-4.02480	1.76885	3.64092
C	-3.21745	0.42769	2.17848
H	-2.37738	1.07118	1.93995
C	0.11639	2.01034	1.73377
H	0.84489	1.21284	1.81910
C	-0.30691	2.67818	2.87202
H	0.10598	2.40839	3.83716
C	-1.26940	3.67415	2.77215
H	-1.61214	4.19161	3.65998
C	-1.79504	4.00202	1.52990
H	-2.54707	4.77726	1.44602
C	-1.36004	3.34373	0.38686
H	-1.77543	3.62644	-0.57256
C	-0.39970	2.33733	0.47988
C	1.78606	2.29393	-1.40324
C	2.32788	2.10634	-2.67738
H	1.81662	1.48073	-3.40049
C	3.51541	2.72518	-3.03414
H	3.92087	2.57502	-4.02735
C	4.17853	3.53867	-2.12441
H	5.10624	4.02270	-2.40427
C	3.64704	3.73011	-0.85767
H	4.15849	4.36334	-0.14260
C	2.45961	3.10998	-0.49489
H	2.05832	3.27039	0.49877
C	3.25110	-0.16805	1.05712
C	3.39519	0.53311	2.25200
H	2.65859	0.41014	3.03933
C	4.47929	1.38151	2.44154
H	4.58328	1.92013	3.37595
C	5.43043	1.52986	1.44307
H	6.27658	2.18976	1.59225
C	5.29503	0.83162	0.24839
H	6.03346	0.94786	-0.53608
C	4.21037	-0.00753	0.05324
H	4.10880	-0.54827	-0.88266
C	2.65474	-2.90441	0.48590
C	3.82404	-3.26292	1.15688
H	4.31419	-2.55052	1.81196
C	4.36690	-4.52898	0.99226
H	5.27672	-4.79590	1.51684
C	3.74833	-5.45158	0.15875
H	4.17641	-6.43820	0.02890
C	2.58201	-5.10499	-0.50972
H	2.09730	-5.81947	-1.16431
C	2.04057	-3.83804	-0.34957
H	1.13193	-3.56414	-0.87866

Δ -(*S,S*)-**6B** (from *trans*-(*S,S*)-**C1**)

$H^\circ = -3792.250009$

$G^\circ = -3792.372174$

Fe	-0.24488	0.87738	-0.93605
P	-0.28214	-1.55341	-0.88268
P	-1.97819	1.32295	0.51997
O	0.22440	3.69240	-1.48932
N	1.48152	0.49638	-1.89423
N	0.88475	0.96015	0.63103
C	2.50558	0.18811	-0.90967
H	2.39112	-0.82696	-0.47779
C	2.29079	1.13081	0.28967
H	2.46926	2.16081	-0.06409
C	1.31258	-0.56410	-2.86562
H	2.22358	-0.70451	-3.46849
H	0.53523	-0.25455	-3.57237
C	0.91790	-1.91479	-2.24933
H	1.79172	-2.42137	-1.83950
H	0.46850	-2.59175	-2.97586
C	0.36499	1.36311	1.78877
H	1.05320	1.54744	2.61671
C	-0.98792	1.51486	1.98247
H	-1.38555	1.83553	2.93700
C	-0.00988	2.58270	-1.25049
C	3.91147	0.26684	-1.45538
C	4.34084	1.39121	-2.15914
H	3.63323	2.19123	-2.35193
C	5.64880	1.48735	-2.61056
H	5.97028	2.36989	-3.15169
C	6.54873	0.45533	-2.36987
H	7.56989	0.52947	-2.72444
C	6.13022	-0.67326	-1.67891
H	6.82417	-1.48479	-1.49338
C	4.82023	-0.76330	-1.22561
H	4.49173	-1.64334	-0.67852
C	3.25785	0.83352	1.40570
C	4.33000	1.68227	1.66592
H	4.42838	2.60218	1.09864
C	5.27364	1.35761	2.63261
H	6.10458	2.02728	2.82083
C	5.15297	0.17962	3.35647
H	5.88738	-0.07311	4.11184
C	4.08246	-0.67173	3.10925
H	3.97812	-1.59363	3.67019
C	3.14592	-0.34688	2.14044

H	2.31181	-1.01138	1.94372
C	-0.22197	-1.97958	1.85145
H	-0.97313	-1.19771	1.86892
C	0.19295	-2.56177	3.03958
H	-0.24540	-2.23944	3.97688
C	1.17754	-3.54070	3.02583
H	1.51182	-3.98992	3.95321
C	1.73435	-3.94125	1.81868
H	2.49997	-4.70764	1.80111
C	1.31179	-3.36734	0.62713
H	1.75147	-3.70269	-0.30440
C	0.33242	-2.37475	0.63348
C	-1.76646	-2.53548	-1.33793
C	-2.36513	-2.27757	-2.57459
H	-1.94158	-1.52729	-3.23537
C	-3.49653	-2.97322	-2.96811
H	-3.94640	-2.76676	-3.93184
C	-4.05289	-3.93096	-2.12857
H	-4.93876	-4.47376	-2.43488
C	-3.47234	-4.18352	-0.89476
H	-3.90372	-4.92472	-0.23238
C	-2.33628	-3.49006	-0.49798
H	-1.89342	-3.70154	0.46827
C	-3.32613	0.11060	0.83615
C	-3.56097	-0.40548	2.10905
H	-2.93893	-0.08833	2.93943
C	-4.57876	-1.32659	2.31868
H	-4.74755	-1.72337	3.31283
C	-5.38075	-1.73313	1.26150
H	-6.17669	-2.44936	1.42673
C	-5.15412	-1.22603	-0.01163
H	-5.77057	-1.54646	-0.84305
C	-4.12465	-0.32207	-0.22528
H	-3.93904	0.05153	-1.22726
C	-2.92075	2.91083	0.34378
C	-4.23107	2.99003	-0.12663
H	-4.78129	2.08952	-0.36978
C	-4.85686	4.22095	-0.27266
H	-5.87835	4.26121	-0.63227
C	-4.18455	5.39196	0.04491
H	-4.67619	6.35078	-0.06678
C	-2.87901	5.32505	0.51315
H	-2.34532	6.23252	0.76995
C	-2.25414	4.09654	0.66081
H	-1.23783	4.05058	1.03821

Λ -(*S,S*)-**6A** (from *trans*-(*S,S*)-**C1**)

$H^\circ = -3792.267780$

$G^\circ = -3792.389181$

Fe	0.14900	0.43384	-0.88363
P	0.57433	-1.68379	-0.61936
P	1.69146	1.46117	0.41541
O	1.81400	0.58344	-3.26520
N	-1.53477	-0.23064	-1.70513
N	-1.03622	0.89798	0.59896
C	-2.67351	0.39980	-1.00776
H	-2.65216	1.46350	-1.28205
C	-2.40136	0.37389	0.50258
H	-2.40453	-0.67374	0.84783
C	-1.72602	-1.65901	-1.93658
H	-2.31584	-1.85010	-2.84641
H	-2.29068	-2.13802	-1.12045
C	-0.38589	-2.35476	-2.03631
H	0.14718	-2.05952	-2.94240
H	-0.46104	-3.44346	-2.03713
C	-0.57634	1.45843	1.72941
H	-1.28264	1.64199	2.54167
C	0.73831	1.81054	1.87729
H	1.10597	2.35847	2.73494
C	1.15543	0.47573	-2.30908
C	-4.02023	-0.12487	-1.44214
C	-4.58799	0.37788	-2.61321
H	-4.06126	1.15238	-3.16150
C	-5.80412	-0.09508	-3.08262
H	-6.22640	0.31174	-3.99405
C	-6.48228	-1.08404	-2.38226
H	-7.43495	-1.45317	-2.74279
C	-5.93248	-1.59274	-1.21403
H	-6.45465	-2.36376	-0.65954
C	-4.71239	-1.11920	-0.75001
H	-4.29508	-1.53499	0.16089
C	-3.42032	1.13238	1.30676
C	-3.69034	2.47764	1.04539
H	-3.13818	2.99268	0.26640
C	-4.64689	3.16343	1.77751
H	-4.84679	4.20592	1.55890
C	-5.34750	2.51993	2.79112
H	-6.09415	3.05736	3.36327
C	-5.07931	1.18751	3.06926
H	-5.61442	0.67952	3.86299
C	-4.12150	0.50261	2.33301

H	-3.91002	-0.53953	2.55307
C	-0.17464	-2.40503	0.88675
C	0.06539	-1.77232	2.10711
H	0.71782	-0.90571	2.14183
C	-0.53967	-2.22736	3.26747
H	-0.34612	-1.72518	4.20803
C	-1.40067	-3.31682	3.21936
H	-1.88494	-3.66668	4.12303
C	-1.63785	-3.95800	2.01200
H	-2.30405	-4.81130	1.97137
C	-1.02446	-3.51028	0.84897
H	-1.21545	-4.02604	-0.08406
C	2.24086	-2.43912	-0.73378
C	2.91454	-2.42778	-1.95820
H	2.45873	-1.97841	-2.83209
C	4.17012	-3.00339	-2.07280
H	4.67723	-2.99501	-3.03001
C	4.77357	-3.59019	-0.96852
H	5.75496	-4.03955	-1.06012
C	4.11635	-3.59493	0.25303
H	4.58338	-4.04441	1.12120
C	2.85855	-3.02161	0.37295
H	2.35419	-3.03889	1.33200
C	2.34212	3.07950	-0.18763
C	3.40850	3.72157	0.44345
H	3.91757	3.23949	1.27161
C	3.82312	4.97465	0.01853
H	4.65369	5.46351	0.51388
C	3.17774	5.60168	-1.03994
H	3.50582	6.57890	-1.37316
C	2.11387	4.97255	-1.67069
H	1.60893	5.45635	-2.49828
C	1.69965	3.71706	-1.24834
H	0.86977	3.22378	-1.74559
C	3.23293	0.59762	0.90244
C	3.43902	0.14633	2.20356
H	2.67689	0.31702	2.95645
C	4.61842	-0.50708	2.54080
H	4.77153	-0.84862	3.55768
C	5.59901	-0.71286	1.58228
H	6.51872	-1.22143	1.84559
C	5.39661	-0.27251	0.27894
H	6.15733	-0.43774	-0.47480
C	4.21981	0.37409	-0.06107
H	4.06893	0.71799	-1.07989

$H^\circ = -3792.246943$

$G^\circ = -3792.368937$

Fe	0.09338	0.60210	-0.95237
P	0.58718	-1.68265	-0.73512
P	1.78111	1.38141	0.39665
O	-0.52602	3.41579	-1.47369
N	-1.56748	-0.11288	-1.81170
N	-1.00519	0.74484	0.63805
C	-2.67283	0.47562	-1.03586
H	-2.63053	1.55888	-1.20827
C	-2.38203	0.28033	0.47169
H	-2.40878	-0.80283	0.67978
C	-1.75154	-1.55324	-1.99226
H	-2.39418	-1.75703	-2.86226
H	-2.26213	-2.03330	-1.14048
C	-0.41620	-2.23439	-2.17199
H	0.09326	-1.87087	-3.06807
H	-0.49120	-3.31985	-2.25232
C	-0.51735	1.30027	1.73367
H	-1.18644	1.42844	2.58686
C	0.80103	1.70607	1.83490
H	1.17936	2.15449	2.74420
C	-0.29557	2.29397	-1.29706
C	-4.04256	0.01956	-1.48218
C	-4.62127	0.63568	-2.59252
H	-4.08629	1.44340	-3.08210
C	-5.85817	0.23449	-3.07446
H	-6.28855	0.73068	-3.93657
C	-6.54681	-0.79680	-2.44906
H	-7.51542	-1.11050	-2.81952
C	-5.98573	-1.41960	-1.34324
H	-6.51535	-2.22496	-0.84774
C	-4.74570	-1.01609	-0.86623
H	-4.32284	-1.52096	-0.00457
C	-3.36954	0.95425	1.38307
C	-3.60364	2.32815	1.29171
H	-3.04663	2.91828	0.57047
C	-4.52607	2.94471	2.12204
H	-4.69913	4.01117	2.03789
C	-5.22608	2.20031	3.06494
H	-5.94517	2.68399	3.71506
C	-4.99310	0.83696	3.17363
H	-5.52768	0.25133	3.91227
C	-4.06964	0.22168	2.33853
H	-3.88183	-0.84451	2.42522
C	-0.12036	-2.54196	0.71197
C	0.05331	-1.96619	1.97022
H	0.62555	-1.05014	2.06413
C	-0.51616	-2.54729	3.09339
H	-0.37721	-2.08898	4.06547
C	-1.27178	-3.70527	2.96779
H	-1.72690	-4.15433	3.84232
C	-1.44385	-4.28843	1.71936
H	-2.02737	-5.19553	1.61869
C	-0.86878	-3.71332	0.59510
H	-1.01058	-4.17946	-0.37261
C	2.23583	-2.42631	-1.01611

Λ -(*S,S*)-**6B** (from *trans*-(*S,S*)-**C1**)

C	2.90986	-2.09906	-2.19584
H	2.46166	-1.40763	-2.90282
C	4.15060	-2.65065	-2.47044
H	4.66018	-2.39614	-3.39200
C	4.74102	-3.52321	-1.56448
H	5.71211	-3.95266	-1.77855
C	4.08798	-3.83374	-0.38083
H	4.54889	-4.50394	0.33494
C	2.84105	-3.28822	-0.10437
H	2.33563	-3.54206	0.82069
C	2.67528	2.92338	-0.08878
C	3.21693	3.77165	0.87740
H	3.10661	3.53351	1.93005
C	3.89691	4.92009	0.50191
H	4.31037	5.57395	1.26070
C	4.05057	5.23180	-0.84360
H	4.58207	6.12967	-1.13500
C	3.52057	4.39156	-1.81182
H	3.63709	4.63023	-2.86230
C	2.83557	3.24386	-1.43488
H	2.41665	2.59059	-2.19460
C	3.23537	0.36132	0.91156
C	3.29384	-0.22650	2.17242
H	2.48119	-0.06671	2.87283
C	4.38887	-0.99825	2.54226
H	4.42268	-1.44451	3.52928
C	5.43722	-1.19027	1.65522
H	6.29059	-1.79326	1.94172
C	5.38847	-0.60644	0.39434
H	6.20290	-0.75548	-0.30493
C	4.29639	0.16206	0.02504
H	4.27047	0.61601	-0.96080

Δ -(S,S)-**G1A** (from **G1-1**)

$H^\circ = -3793.475113$

$G^\circ = -3793.597024$

Fe	0.26502	-0.86344	-0.85086
H	0.06219	-2.38585	-1.03122
P	0.22221	1.43441	-0.81288
P	1.82836	-1.36618	0.64486
O	2.08464	-1.12712	-3.09790
N	-1.53348	-0.57540	-1.84746
H	-1.73388	-1.43982	-2.34398
N	-0.98170	-1.08039	0.70978
C	-2.61978	-0.35060	-0.85130
H	-2.48449	0.66781	-0.47365
C	-2.37129	-1.28363	0.34083

H	-2.52721	-2.31801	-0.01175
C	-1.44094	0.51517	-2.84584
H	-2.40079	0.65635	-3.35469
H	-0.71657	0.19236	-3.59399
C	-0.99733	1.80655	-2.18329
H	-1.85086	2.33060	-1.75300
H	-0.55297	2.48012	-2.91469
C	-0.50455	-1.51458	1.87194
H	-1.21297	-1.76628	2.66607
C	0.84920	-1.62789	2.10332
H	1.24997	-1.92624	3.06391
C	1.34413	-0.96412	-2.20862
C	-4.00058	-0.46776	-1.43513
C	-4.42305	-1.64908	-2.04465
H	-3.74139	-2.49048	-2.12372
C	-5.71131	-1.76095	-2.54560
H	-6.02840	-2.68419	-3.01548
C	-6.59556	-0.69474	-2.44113
H	-7.60237	-0.78403	-2.83068
C	-6.18426	0.48519	-1.83734
H	-6.86899	1.32056	-1.75458
C	-4.89335	0.59659	-1.33958
H	-4.56938	1.51700	-0.86307
C	-3.37200	-1.00516	1.43730
C	-4.32963	-1.94927	1.79250
H	-4.33394	-2.91339	1.29454
C	-5.27530	-1.66565	2.77065
H	-6.01508	-2.41113	3.03725
C	-5.27061	-0.43290	3.40695
H	-6.00595	-0.21200	4.17127
C	-4.31530	0.51631	3.06112
H	-4.30305	1.48195	3.55377
C	-3.37642	0.23117	2.08296
H	-2.63014	0.97090	1.81284
C	-0.11099	1.87132	1.90662
H	0.46846	0.95924	1.99849
C	-0.54807	2.53378	3.04508
H	-0.29529	2.14405	4.02443
C	-1.32182	3.67983	2.92610
H	-1.67388	4.19355	3.81259
C	-1.64244	4.16941	1.66618
H	-2.23786	5.06924	1.56850
C	-1.19234	3.51632	0.52709
H	-1.43142	3.92676	-0.44739
C	-0.42856	2.35394	0.63829
C	1.70587	2.41835	-1.26817
C	2.24458	2.27528	-2.54914
H	1.75822	1.63087	-3.27379
C	3.39559	2.95873	-2.90904
H	3.79816	2.84285	-3.90820
C	4.02731	3.79189	-1.99419
H	4.92653	4.32615	-2.27583
C	3.50154	3.93542	-0.71882
H	3.99023	4.58045	0.00187
C	2.34908	3.25215	-0.35436
H	1.95229	3.37260	0.64729
C	3.16963	-0.15263	1.00293
C	3.23781	0.55353	2.20058

H	2.48945	0.37978	2.96743
C	4.26475	1.46393	2.42465
H	4.31083	2.00149	3.36462
C	5.23227	1.67624	1.45382
H	6.03254	2.38531	1.62907
C	5.16966	0.97898	0.25215
H	5.91921	1.14586	-0.51256
C	4.14510	0.07421	0.02758
H	4.10647	-0.47097	-0.91087
C	2.87635	-2.87694	0.40355
C	3.87559	-3.18066	1.33241
H	4.05861	-2.51099	2.16697
C	4.63842	-4.33041	1.19968
H	5.40619	-4.55450	1.93092
C	4.42323	-5.19001	0.12911
H	5.02291	-6.08592	0.02209
C	3.43841	-4.89435	-0.80131
H	3.26755	-5.55767	-1.64111
C	2.66777	-3.74692	-0.66300
H	1.89243	-3.52743	-1.38721

Δ -(*S,S*)-**G1B** (from **G1-1**)

$H^\circ = -3793.467426$

$G^\circ = -3793.591170$

Fe	-0.27242	0.91534	-0.88200
H	-1.15863	0.62337	-2.13686
P	-0.27766	-1.38865	-0.94136
P	-1.88285	1.24492	0.64832
O	-0.42712	3.69104	-1.72387
N	1.53877	0.61079	-1.87081
H	1.78944	1.48118	-2.33373
N	0.95874	1.10220	0.69168
C	2.58844	0.32223	-0.85092
H	2.38969	-0.68859	-0.48135
C	2.35650	1.26595	0.34102
H	2.54518	2.29446	-0.01578
C	1.43613	-0.43360	-2.91478
H	2.40281	-0.58187	-3.40866
H	0.73664	-0.05764	-3.66011
C	0.94217	-1.73514	-2.31679
H	1.77152	-2.30632	-1.89950
H	0.48222	-2.35962	-3.08117
C	0.46498	1.47253	1.86464
H	1.15807	1.70231	2.67908
C	-0.89652	1.54239	2.09430
H	-1.29283	1.75284	3.07947
C	-0.35571	2.58992	-1.34764

C	3.98917	0.36515	-1.39572
C	4.48600	1.50816	-2.02152
H	3.84735	2.37666	-2.15141
C	5.79562	1.54895	-2.47654
H	6.17023	2.44342	-2.95960
C	6.62747	0.44939	-2.30884
H	7.65091	0.48370	-2.66193
C	6.14195	-0.69357	-1.68911
H	6.78487	-1.55548	-1.55720
C	4.83004	-0.73406	-1.23812
H	4.44868	-1.62602	-0.74968
C	3.33804	0.96578	1.44813
C	4.29984	1.89596	1.82747
H	4.32389	2.86369	1.33712
C	5.22541	1.59361	2.81930
H	5.96905	2.32826	3.10455
C	5.19583	0.35599	3.44541
H	5.91518	0.12070	4.22060
C	4.23643	-0.57974	3.07503
H	4.20458	-1.54954	3.55865
C	3.31818	-0.27601	2.08311
H	2.57111	-1.00722	1.79272
C	0.08602	-1.93687	1.75530
H	-0.44441	-1.00119	1.88980
C	0.50730	-2.65865	2.86365
H	0.28759	-2.29110	3.85961
C	1.22488	-3.83383	2.69321
H	1.56495	-4.39458	3.55558
C	1.50564	-4.29158	1.41160
H	2.05883	-5.21284	1.27331
C	1.06834	-3.57990	0.30341
H	1.27321	-3.96776	-0.68795
C	0.35854	-2.38895	0.46602
C	-1.78452	-2.32164	-1.43269
C	-2.40292	-2.01605	-2.64703
H	-1.98386	-1.24547	-3.28552
C	-3.54893	-2.68750	-3.04215
H	-4.01445	-2.44297	-3.98941
C	-4.09874	-3.66939	-2.22713
H	-4.99641	-4.19176	-2.53495
C	-3.49551	-3.97328	-1.01627
H	-3.92280	-4.73095	-0.37006
C	-2.34513	-3.30450	-0.61873
H	-1.89037	-3.55074	0.33353
C	-3.16443	-0.02934	1.04606
C	-3.15543	-0.71628	2.25756
H	-2.38779	-0.49577	2.99198
C	-4.12498	-1.67255	2.53491
H	-4.10608	-2.19687	3.48327
C	-5.11706	-1.94932	1.60595
H	-5.87368	-2.69403	1.82241
C	-5.13583	-1.26773	0.39445
H	-5.90420	-1.48368	-0.33868
C	-4.16462	-0.31997	0.11420
H	-4.18278	0.19825	-0.83926
C	-3.00978	2.69241	0.39951
C	-3.36049	3.51520	1.46826
H	-2.95811	3.31607	2.45546

C	-4.21215	4.59432	1.27717
H	-4.47365	5.22854	2.11616
C	-4.72609	4.86229	0.01556
H	-5.38767	5.70712	-0.13370
C	-4.38265	4.04829	-1.05536
H	-4.77415	4.25667	-2.04411
C	-3.52846	2.97140	-0.86446
H	-3.24685	2.34981	-1.70882

Λ -(S,S)-**G1A** (from **G1-1**)

$H^\circ = -3793.470143$

$G^\circ = -3793.591878$

Fe	0.18449	0.58341	-0.94376
P	0.55072	-1.64802	-0.61125
P	1.68345	1.50308	0.41959
O	1.86628	0.79794	-3.29917
N	-1.62116	-0.10328	-1.80783
H	-1.63912	0.30071	-2.73941
N	-1.04827	0.81201	0.62917
C	-2.73286	0.53996	-1.03028
H	-2.62905	1.60533	-1.24855
C	-2.41703	0.35398	0.45919
H	-2.46294	-0.72556	0.68661
C	-1.79065	-1.57788	-1.95579
H	-2.40920	-1.80006	-2.82821
H	-2.33487	-1.94457	-1.08346
C	-0.45178	-2.27152	-2.03415
H	0.08166	-1.99248	-2.94547
H	-0.56534	-3.35641	-2.04270
C	-0.61160	1.40418	1.72828
H	-1.30762	1.56623	2.55458
C	0.70106	1.81654	1.85909
H	1.05445	2.34456	2.73564
C	1.19620	0.65933	-2.35185
C	-4.10291	0.09611	-1.48009
C	-4.68765	0.73138	-2.57552
H	-4.15829	1.54748	-3.05695
C	-5.93018	0.33864	-3.04994
H	-6.36797	0.84683	-3.90081
C	-6.61410	-0.69829	-2.43005
H	-7.58696	-1.00465	-2.79507
C	-6.04648	-1.33659	-1.33634
H	-6.57514	-2.14467	-0.84503
C	-4.80119	-0.94421	-0.86642
H	-4.37253	-1.45697	-0.01232
C	-3.42849	1.04284	1.34160

C	-3.69667	2.40447	1.19633
H	-3.17061	2.97710	0.43926
C	-4.61719	3.03410	2.01929
H	-4.81813	4.09135	1.89300
C	-5.27970	2.31423	3.00670
H	-5.99843	2.80769	3.64978
C	-5.01227	0.96274	3.16736
H	-5.51947	0.39579	3.93897
C	-4.09061	0.33448	2.33970
H	-3.87902	-0.72317	2.46457
C	-0.19859	-2.44160	0.86267
C	-0.00159	-1.81882	2.09574
H	0.60182	-0.91795	2.14618
C	-0.58025	-2.33255	3.24660
H	-0.41906	-1.83782	4.19730
C	-1.37504	-3.46893	3.17565
H	-1.83796	-3.86559	4.07124
C	-1.57645	-4.09627	1.95348
H	-2.19092	-4.98665	1.89454
C	-0.98843	-3.58961	0.80250
H	-1.15105	-4.09731	-0.14094
C	2.16256	-2.50501	-0.80705
C	2.83684	-2.42643	-2.02889
H	2.40633	-1.87486	-2.85674
C	4.05949	-3.05719	-2.19851
H	4.56648	-2.99399	-3.15393
C	4.63259	-3.76554	-1.15021
H	5.58848	-4.25735	-1.28400
C	3.97698	-3.83540	0.07003
H	4.42108	-4.37782	0.89634
C	2.75040	-3.20890	0.24310
H	2.24734	-3.27681	1.20085
H	-0.26041	2.01503	-1.33137
C	2.53263	3.08025	-0.05022
C	3.51678	3.61436	0.78587
H	3.80875	3.08130	1.68521
C	4.12599	4.82106	0.47910
H	4.88365	5.22536	1.14007
C	3.77018	5.50748	-0.67547
H	4.25101	6.44732	-0.91883
C	2.79872	4.98292	-1.51503
H	2.51947	5.51116	-2.41913
C	2.18159	3.77835	-1.20261
H	1.41596	3.37713	-1.85649
C	3.16408	0.51208	0.90411
C	3.30577	-0.01620	2.18412
H	2.53655	0.17419	2.92580
C	4.42678	-0.76725	2.51854
H	4.52804	-1.16581	3.52136
C	5.41603	-0.99911	1.57462
H	6.28956	-1.58560	1.83356
C	5.27991	-0.48233	0.29068
H	6.04721	-0.66597	-0.45245
C	4.16176	0.26513	-0.04256
H	4.06474	0.66837	-1.04647

Λ -(S,S)-**G1B** (from **G1-1**)

$H^\circ = -3793.463193$

$G^\circ = -3793.585392$

Fe	0.17827	0.60461	-0.95495
P	0.60577	-1.63327	-0.72947
P	1.73796	1.38999	0.45534
O	-0.17978	3.23313	-2.14274
N	-1.62360	-0.11445	-1.81833
H	-1.66618	0.30327	-2.74346
N	-1.03525	0.78636	0.63420
C	-2.73383	0.49854	-1.00969
H	-2.65616	1.56998	-1.21443
C	-2.39324	0.29757	0.47340
H	-2.40952	-0.78702	0.68164
C	-1.76906	-1.58672	-1.99666
H	-2.41629	-1.80077	-2.85015
H	-2.26888	-1.98853	-1.11315
C	-0.41595	-2.23610	-2.14494
H	0.08230	-1.90783	-3.05853
H	-0.49450	-3.32323	-2.18338
C	-0.57357	1.31307	1.75463
H	-1.25447	1.44224	2.60014
C	0.74973	1.69795	1.89212
H	1.11468	2.14075	2.80973
C	-0.04581	2.19431	-1.63108
C	-4.10226	0.03685	-1.44473
C	-4.71763	0.68110	-2.51767
H	-4.21328	1.51752	-2.99114
C	-5.95928	0.27152	-2.97999
H	-6.42160	0.78707	-3.81324
C	-6.61076	-0.79203	-2.37047
H	-7.58274	-1.11186	-2.72616
C	-6.01207	-1.43971	-1.29903
H	-6.51542	-2.26864	-0.81593
C	-4.76788	-1.03030	-0.84097
H	-4.31417	-1.55070	-0.00464
C	-3.40544	0.94582	1.38461
C	-3.70954	2.30267	1.26957
H	-3.21605	2.90066	0.50986
C	-4.62413	2.89589	2.12586
H	-4.85371	3.94984	2.02277
C	-5.24318	2.14373	3.11736
H	-5.95662	2.60880	3.78693
C	-4.93876	0.79684	3.24852
H	-5.41180	0.20553	4.02352
C	-4.02403	0.20494	2.38709
H	-3.78181	-0.84870	2.48917
C	-0.08075	-2.53297	0.71704
C	0.06707	-1.94083	1.97137

H	0.60134	-1.00068	2.05506
C	-0.47797	-2.53188	3.10162
H	-0.35570	-2.05832	4.06891
C	-1.19083	-3.71785	2.98858
H	-1.62863	-4.17553	3.86754
C	-1.34294	-4.31640	1.74477
H	-1.89411	-5.24462	1.65253
C	-0.78773	-3.73162	0.61504
H	-0.91284	-4.21630	-0.34604
C	2.24289	-2.40639	-1.01868
C	2.90846	-2.14187	-2.21755
H	2.46070	-1.47519	-2.94690
C	4.14061	-2.71948	-2.47865
H	4.64357	-2.51143	-3.41547
C	4.73078	-3.55852	-1.54166
H	5.69599	-4.00656	-1.74455
C	4.08261	-3.81387	-0.34254
H	4.54117	-4.45884	0.39762
C	2.84392	-3.24312	-0.08025
H	2.34600	-3.45324	0.85941
H	1.09068	0.31123	-2.19035
C	2.63526	2.94099	-0.00353
C	2.97313	3.88076	0.96944
H	2.69144	3.71255	2.00336
C	3.66366	5.03395	0.62567
H	3.91758	5.75783	1.39109
C	4.02900	5.26048	-0.69494
H	4.56600	6.16238	-0.96310
C	3.69978	4.32964	-1.67029
H	3.97835	4.50287	-2.70312
C	3.00716	3.17678	-1.32623
H	2.73981	2.45683	-2.09343
C	3.20262	0.37239	0.95303
C	3.28452	-0.20649	2.21680
H	2.48197	-0.04607	2.92900
C	4.38858	-0.97164	2.57396
H	4.44084	-1.41030	3.56369
C	5.42281	-1.16634	1.67088
H	6.28349	-1.76337	1.94803
C	5.34915	-0.59481	0.40551
H	6.15094	-0.74858	-0.30731
C	4.24784	0.16676	0.04904
H	4.19942	0.60629	-0.94230

G1-1

G1-1 from **C1** (see complex **5** in W. Zuo, D. E.

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$G^\circ = -3793.467893$

$H^\circ = -3793.59166$

C	2.97864	0.62549	-0.82895
C	2.97692	-0.66916	0.01503

H	2.20712	3.12685	-1.27713	H	-1.61588	4.09715	3.82950
N	1.65896	1.20425	-0.70005	H	-5.13471	2.08967	2.43880
C	1.38634	2.46580	-0.98648	H	-3.97324	3.42200	4.17257
N	1.71711	-1.38328	-0.29796	H	3.16587	0.31621	-1.87269
H	0.13619	-3.51617	-0.89350	H	2.90765	-0.38290	1.06930
C	0.11277	-3.14948	0.13473	C	4.11754	1.51763	-0.39365
Fe	0.17528	-0.01769	-0.15259	C	5.27710	1.61827	-1.15575
H	-0.16226	-3.99042	0.77058	C	4.04887	2.20141	0.82040
P	-1.13823	1.76224	-0.50773	C	6.35173	2.37973	-0.71399
P	-1.13561	-1.76880	0.22296	H	5.33729	1.08857	-2.10116
C	0.44591	0.37003	1.55529	C	5.11907	2.96267	1.26292
O	0.64624	0.65779	2.66567	H	3.14407	2.13482	1.41689
C	1.46887	-2.59189	0.51046	C	6.27574	3.05213	0.49719
H	1.49829	-2.29279	1.56207	H	7.24867	2.44876	-1.31805
H	2.25405	-3.33903	0.35536	H	5.05283	3.48840	2.20815
C	0.10093	2.96718	-0.91939	H	7.11172	3.64847	0.84233
H	-0.12285	4.00202	-1.14757	C	4.22378	-1.48785	-0.18934
C	-2.44886	-2.25399	-0.96998	C	5.20405	-1.52645	0.79867
C	-3.79414	-2.04267	-0.66821	C	4.44623	-2.17130	-1.38386
C	-2.10948	-2.71660	-2.24244	C	6.38608	-2.22520	0.59693
C	-4.77800	-2.30091	-1.61279	H	5.03855	-0.99435	1.72986
H	-4.07950	-1.67288	0.31057	C	5.62369	-2.87605	-1.58522
C	-3.09441	-2.98498	-3.18060	H	3.69322	-2.15264	-2.16560
H	-1.06854	-2.85496	-2.51317	C	6.59868	-2.90138	-0.59626
C	-4.43174	-2.77704	-2.86881	H	7.14148	-2.24244	1.37341
H	-5.81826	-2.12980	-1.36311	H	5.78280	-3.40426	-2.51773
H	-2.81485	-3.35000	-4.16167	H	7.51964	-3.44913	-0.75523
H	-5.19986	-2.98035	-3.60503	H	-0.10476	-0.31624	-1.68288
C	-1.98608	-2.03223	1.83556	H	1.74496	-1.66110	-1.2780
C	-2.39716	-3.30611	2.23451				
C	-2.28360	-0.94327	2.65069				
C	-3.07369	-3.48366	3.43078				
H	-2.19934	-4.16582	1.60344				
C	-2.96882	-1.11990	3.84586				
H	-1.98950	0.05360	2.34477				
C	-3.35983	-2.39044	4.23968				
H	-3.38353	-4.47747	3.73100				
H	-3.19599	-0.26031	4.46525				
H	-3.89076	-2.53144	5.17341				
C	-2.42453	1.84934	-1.83441				
C	-3.20320	3.00404	-1.95960				
C	-2.59514	0.82490	-2.76051				
C	-4.12807	3.12547	-2.98425				
H	-3.08532	3.81531	-1.24865				
C	-3.52705	0.94333	-3.78438				
H	-1.98849	-0.06954	-2.68008				
C	-4.29559	2.09216	-3.89856				
H	-4.72104	4.02850	-3.06993				
H	-3.64908	0.13462	-4.49571				
H	-5.02165	2.18524	-4.69731				
C	-2.10485	2.39391	0.93239				
C	-1.46128	3.14347	1.91545				
C	-3.43448	2.01874	1.13630				
C	-2.12895	3.51224	3.07510				
H	-0.42645	3.43677	1.76462				
C	-4.10306	2.38863	2.29389				
H	-3.94954	1.42493	0.38777				
C	-3.45111	3.13424	3.26797				