DFT Insight into Metals and Ligands Substitution Effects on Reactivity of Phenoxy-Imine Catalysts for Ethylene Polymerization

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ABSTRACT

The reaction mechanism of ethylene (ET) polymerization catalyzed by the phenoxy-imine (FI) ligands using DFT calculations was studied. Among five possible isomers, isomer A which has an octahedral geometry and a (*cis*-N/*trans*-O/*cis*-Cl) arrangement is the most stable pre-reaction Ti-FI dichloride complex. The isomer A can be activated by MAO to form the active catalyst and the active form was used for the study of the mechanism for Ti-FI. The second ethylene insertion was found to be the rate-determining step of the catalyzed ethylene polymerization. To examine the effect of group IV_B transition metals (M = Ti, Zr, Hf) substitutions, calculated activation energies at the rate-determining step (E_a^{RDS}) were compared, where values of E_a^{RDS} of Zr < Hf < Ti agree with experiments. Moreover, we examined the effect of substitution on (O, X) ligands of the Ti-phenoxy-imine (Ti-1) based catalyst. The results revealed that E_a^{RDS} of (O, N) > (O, O) > (O, P) > O, S). Hence, the (O, S) ligand has the highest potential to improve the catalytic activity of the Ti-FI catalyst. We also found the activation energy to be related to the Ti-X distance. In addition, a novel Ni-based FI catalyst was investigated. The results indicated that the nickel (II) complex based on the phenoxy-imine (O, N) ligand in the square-planar geometry is more active than in the octahedral geometry. This work provides fundamental insights into the reaction mechanism of M-FI catalysts which can be used for the design and development of M-FI catalysts for ET polymerization.

KEYWORDS

FI catalyst, Ethylene polymerization, DFT calculations, Nickel, Mechanism

1. INTRODUCTION

Polyethylene (PE) is the most used plastic material and has the simplest basic structure of any polymer [1]. Around 8,300 million metric tons of plastics were produced worldwide using the catalytic olefin polymerization [2]. Most of the catalytic systems used to produce PE are the Ziegler-Natta catalysts [3]. However, the disadvantages of these catalysts are the controllability of the polymer chain growth because of multiple metal sites, the difficulty in removing the catalyst from the final product, and the encapsulation effect on the polymer chains [4]. Therefore, single-site post-metallocene catalysts have been developed for the polyolefin industry [5]. The general formula for these kinds of catalysts is L_nMR, where L_n is an organic ligand that is connected to the active metal center (M). The reactivity and selectivity of these catalysts could be tuned by modifying the ligand. For example, by adapting the coordination environment of the metal center, the single-site catalysts are possible to control the molecular weight, molecular weight distribution, comonomer incorporation, and stereochemistry of a polymer [6, 7]. Phenoxy-imine catalyst (M-FI), one type of post-metallocene catalyst, was introduced as a high-performance catalyst for olefin polymerization [8, 9]. The M-FI system is composed of group IV_B transition metal (M) complexes with two phenoxy-imine (FI) ligands. Several studies [10-12] reported that FI catalysts show high activity for ethylene (ET) polymerization when activated with methyl aluminoxane (MAO). All basic olefin monomers as well as their polymerization processes are advantageously catalyzed by FI-based complexes with high activity and selectivity [13].

Fujita et al. [14, 15] firstly introduced M-FI catalysts (M = Zr and Ti) and investigated their macroscopic properties and catalytic behaviors. They proposed five possible isomers of the Zr-FI catalysts (isomers A-E) as displayed in **Fig. 1**. Their result revealed that isomer A (having *cis*-N/*trans*-O/*cis*-Cl arrangement) has lower formation energy than isomers B, C, D, and E by 19.5,

25.3, 33.3, and 37.3 kJ mol^{-1}, respectively. Thus, the octahedral Zr-FI dichloride complex in isomer A form is the most stable. However, there is still no theoretical report on the relative stability of the Ti-FI catalysts.

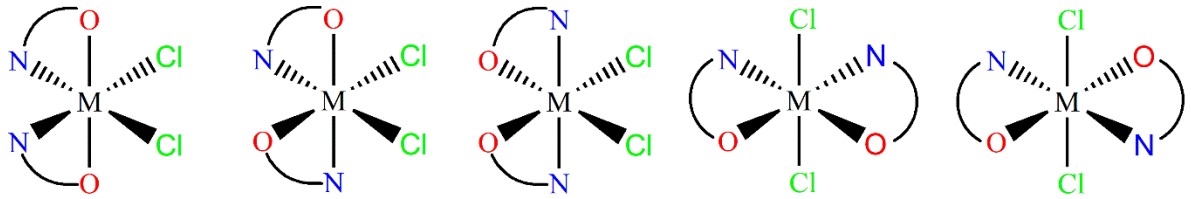
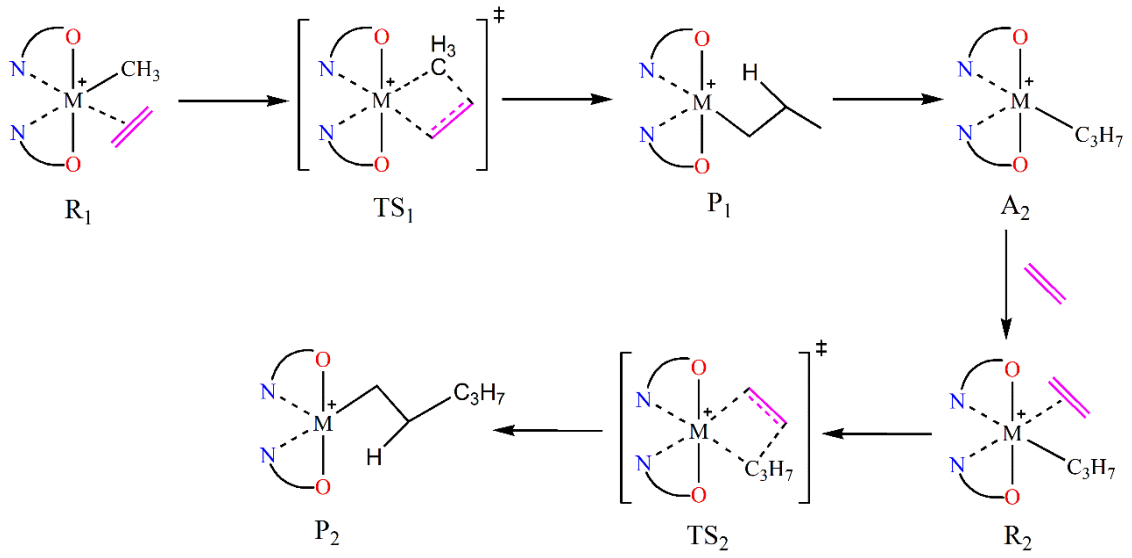


Fig. 1 Structures of the five possible isomers (A-E) of the M-FI (M = Zr and Ti) catalysts.

Mitani et al. [16] reported the catalytic activities for M-FI catalysts with different transition metals. Under mild conditions, the Zr-FI exhibited the highest activity followed by Hf-FI and Ti-FI. Matsugi and Fujita [17] discovered that transition metal complexes containing FI ligands provide higher activity for ET polymerization than when containing other ligands, for instance, pyrrolide-imine (M-PI catalyst), indolide-imine (M-II catalyst), phenoxy-ether (M-FE catalyst), imine-phenoxy (M-IF catalyst), phenoxy-pyridine (M-FP catalyst). The (O,N)-phenoxy-imine is one of these catalysts that has been essential to several important developments. The catalytic activities of the metal catalysts as well as the structural and electrical properties of the resulting high molecular weight polymers have a crucial role in controlling the appearance of these N-containing ligands [18]. Terao et al. [19] studied the significance of substituent effects on the activity of M-FI catalysts. They summarized that the increase in the steric bulkiness of the substituent can enhance the catalytic activity. Damavandi et al. [20] introduced the Ni complexes with naphtholato imine group ligands and moderate ET polymerization activities were observed. Nikitin et al. [21] investigated the reaction mechanism of Ti-FI catalyzed ET polymerization. Their

results suggested that HOMO-LUMO gaps of the active cations can affect the catalytic activities. Theoretical and experimental data on Ti-FI catalysts with different substitutions as well as activity values have been vastly reported. The M-3 model (see **Fig. 2**) displayed the highest activity among Ti-FI series. Chasing et al. [22] performed the quantitative structure-activity relationship (QSAR) for a series of Ti-FI catalysts. From the QSAR study, a new M-FI catalyst with a Ni metal center was proposed as a candidate for ET polymerization.

The most commonly accepted mechanism for the olefin polymerization was proposed by Cossée-Arlman mechanism [23] and Brookhart and Green [24]. The mechanism of ET polymerization by M-FI catalyst was proposed by Nikitin et al. [21]. The proposed mechanism is depicted in **Scheme 1**.



Scheme 1 Proposed reaction mechanism of ethylene polymerization on phenoxy-imine (FI) catalysts.

In this mechanism, ethylene is first inserted into the transition metal (M) and the reactant π-complex (R_1) is formed. Then, a four-membered ring transition state (TS_1) is generated which results in the β-agostic product (P_1) with an exothermic process [25, 26]. After that, the structure

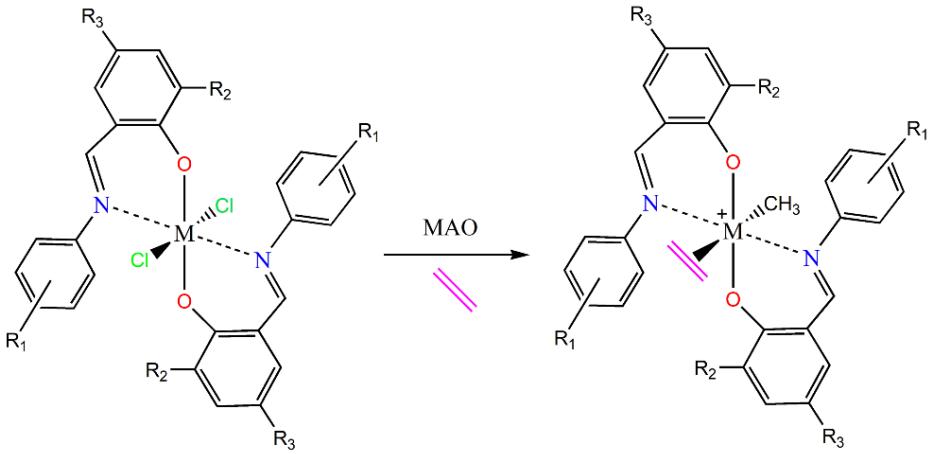
is rearranged to the active complex (A_2) which is ready for the second ethylene insertion. The reaction is continued with a new ethylene monomer being inserted to transition metal like the first insertion. The reaction proceeds along with reactant π-complex (R_2), then four-membered ring transition state (TS_2), and the β-agostic product (P_2).

Here, density functional theory (DFT) calculations were performed to elucidate the reaction mechanism of ET polymerization by phenoxy-imine (M-FI) catalysts. The relative stability of five possible isomers of pre-reaction Ti-FI dichloride complexes was firstly determined to select the most stable isomer as the starting structure. Then, the potential energy profiles of the ET polymerization catalyzed by M-FI catalysts with different group IV_B transition metals (M = Ti, Zr, Hf) were calculated to gain insight into the reaction mechanism. Both activation energies and structural properties were mainly compared to catalytic activities. The effect of ligand substitutions was as well investigated by replacing the parent nitrogen (O, N) of FI ligands with oxygen (O, O), phosphorus (O, P), and sulfur (O, S). Finally, using the information obtained in this work we investigated the possibility of using other transition metals such as Ni as a new candidate for M-FI catalysts for catalyzed ET polymerization.

2. COMPUTATIONAL DETAILS

2.1 M-FI models

Since methyl aluminoxane (MAO) is the most widely used activator for olefin polymerization [27-29], we employed MAO to generate the vacant site before the ethylene insertion on M-FI catalysts. The structure of M-FI catalysts is based on the X-ray structure of the dichloride complex (**Fig. 2**, left) [14]. Thus, the reactant π-complex (**Fig. 2**, right) was constructed as a starting structure.



M-1: R_1 = H, R_2 = *t*-Bu, R_3 = H
M-3: R_1 = *p*-OAll, R_2 = *t*-Bu, R_3 = H

Fig. 2 Structures of FI catalyst for pre-reaction complex (left) and reactant π-complex (right). Where M is group IV_B transition metals (Ti, Zr, Hf).

Selected from experimental activities, [16] two models of M-FI catalysts, M-1 and M-3, were used in this study. The M-1 model is referred to as the parent M-FI catalyst containing two phenoxy-imine (O, N) ligands with substituents R_1 = H, R_2 = *t*-Bu, and R_3 = H. The M-3 is referred to as the M-FI catalyst containing two phenoxy-imine (O, N) ligands with substituents R_1 = *para*-allyloxy (*p*-OAll), R_2 = *t*-Bu, and R_3 = H. The M-3 model gives the highest activity among the Ti-FI series of Nikitin et al. [21]. Here, the M-1 was utilized for the investigation of the reaction mechanism for the ET polymerization with different group IV_B transition metals (M = Ti, Zr, Hf). For the effect of ligand substitution, we used the Ti-1 model and modified the parent phenoxy-imine (O, N) ligand to (O, P), (O, O), and (O, S). In addition, the Ti-3 model was also employed to assess the effect of substituents on the parent phenoxy-imine ligand. Finally, the M-3 model was applied to the nickel (II) complexes based on the (O, N) ligand system.

Based on the proposed reaction mechanism as shown in **Scheme 1**. The activation energy and reaction energy were represented as E_{ax} and ΔE_{rx} which were determined according to Eq. (1) and (2).

$$E_{ax} = E_{TSx} - E_{Rx} \quad (1)$$

$$\Delta E_{rx} = E_{Px} - E_{Rx} \quad (2)$$

Where E_{Rx}, E_{TSx}, and E_{Px} are the energy of the reactant π-complex (R), transition-state (TS), and the β-agostic product (P) for the ethylene insertion. The subscript x=1 and 2 are referred to as the first and second ethylene insertion, respectively.

2.2 DFT calculations

Several methods of quantum chemical calculations have been used for the study of the ethylene polymerization reaction [19, 21, 30-32]. According to, the M06-2X functional showed a great performance for molecular ethylene polymerization catalysts and is well suited for a broad range of applications on transition-metal chemistry, and molecular structure prediction. Hence, we employed the M06-2X [33, 34] with the correlation consistent cc-pVDZ basis set of Dunning [35] was used for non-metal atoms and the LANL2DZ basis set with effective core potential (ECP) [36] was used for transition metal atoms in all calculations. All the calculations were carried out using the Gaussian 09 program [37]. The comparison of bond lengths and bond angles obtained from different theoretical methods were given in **Table S1** of the supplementary material.

The optimized stationary and transition state structures were confirmed by their vibrational frequency calculations with zero and one imaginary frequency, respectively. Moreover, the transition state structures were verified by intrinsic reaction coordinate (IRC) calculations. Our calculations were performed in gas phase conditions. We assessed the solvent effect with the

implicit SMD solvation model [38] using toluene as a solvent (Eps = 2.3741). The Gibbs free energy profiles at 298.15 K and 1 atm were reported in both gas phase and toluene solvent as given in **Fig. S1** of supplementary material. In the calculation, the standard self-consistent energy convergence is $1.0x10^{-6}$ Hartree. The standard maximum displacement and maximum force convergence in the calculation are $1.8x10^{-3}$ Å and $4.5x10^{-4}$ Hartree/Bohr, respectively. The spin-multiplicity were set to the singlet-state for all geometries. The potential energy reported in **Figs. 3 and 4** are in the gas phase without zero-point correction.

3. RESULTS AND DISCUSSION

3.1 Stability of pre-reaction Ti-FI complex

Group IV_B transition metal complexes have octahedral geometry. For their complexes with phenoxy-imine (FI) ligands, the metal (M) center is attached to two imine nitrogen, two phenolic oxygens, and two chloro ligands. Thus, there are five possible isomeric structures for the complex between the group IV_B metal and phenoxy-imine ligand as suggested by Fujita et al. [13, 14]. As displayed in **Fig. 3**, five isomers of the Ti-FI dichloro complex are *cis*-N/*trans*-O/*cis*-Cl (isomer A), *cis*-N/*cis*-O/*cis*-Cl (isomer B), *trans*-N/*cis*-O/*cis*-Cl (isomer C), *cis*-N/*cis*-O/*trans*-Cl (isomer D), and *trans*-N/*trans*-O/*trans*-Cl (isomer E). Moreover, relative potential energies (RE) to isomer A of the five possible isomers were given in **Fig. 3**. Our calculations revealed that for Ti-FI catalyst isomer A is the most stable form, which is followed by isomer B (RE = 2.0 kcal mol^{-1}), D (RE = 6.6 kcal mol^{-1}), C (RE = 7.9 kcal mol^{-1}), and E (RE = 11.2 kcal mol^{-1}). The coordination energy (E_{co}) in each isomer were calculated by equation: $E_{co} = E_{cpx+ET} - (E_{cpx} + E_{ET})$. We found that E_{co} were -20.46, -18.85, -17.98, -9.85, and -10.97 kcal mol^{-1} for isomer A, B, C, D, and E, respectively. The relative stabilities and coordination energy of the FI complexes show a similar result in which

isomer A is the most preferred complex [15]. Our results showed that the complex and ethylene monomer interactions were strongest in the most stable form. Moreover, isomer A corresponds to the X-ray structure reported by Makio et al. [14]. From our observation, the octahedral geometry of isomer A allows polymer chain and ethylene monomer to be inserted into the *cis*-position easier than other isomers. Thus, the structures of isomer A complexes were used to investigate the reaction mechanism in the next part.

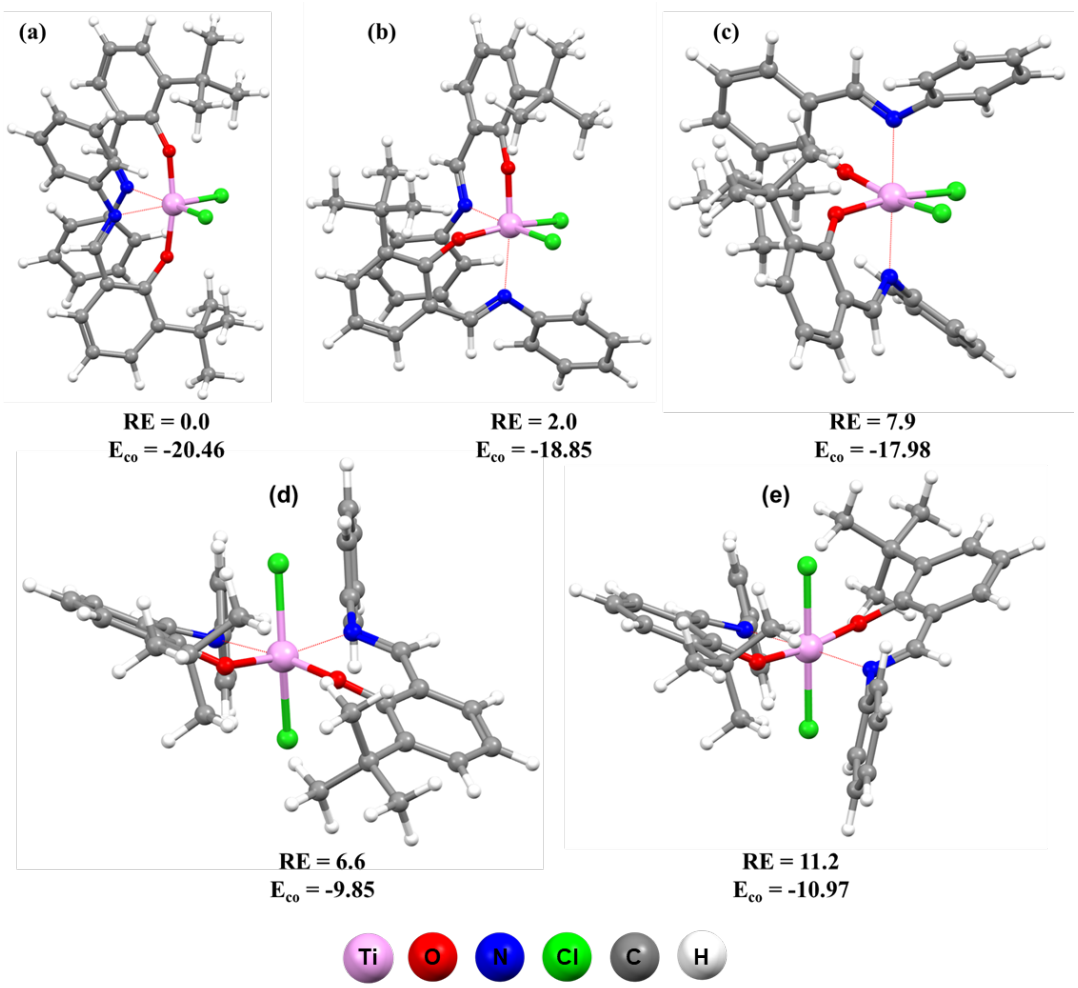


Fig. 3 Structures of the five possible isomers (A-E) at the pre-reaction Ti-FI states and their relative potential energies (RE) and coordination energy (E_{co}) in kcal mol^{-1}. Isomer A is the most stable and the reference.

3.2 Effect of metal substitutions

To generate the reactant π-complex (R_1) in **Scheme 1**, firstly the most stable octahedral dichloride complex (isomer A) is activated by MAO. After the activation, the cationic FI catalyst with one vacant site is created representing the activated catalyst. Finally, ethylene is inserted into the vacant site of the activated catalyst to form R_1. Methyl and propyl groups were used to represent the growing chain for the first and the second ethylene insertions, respectively.

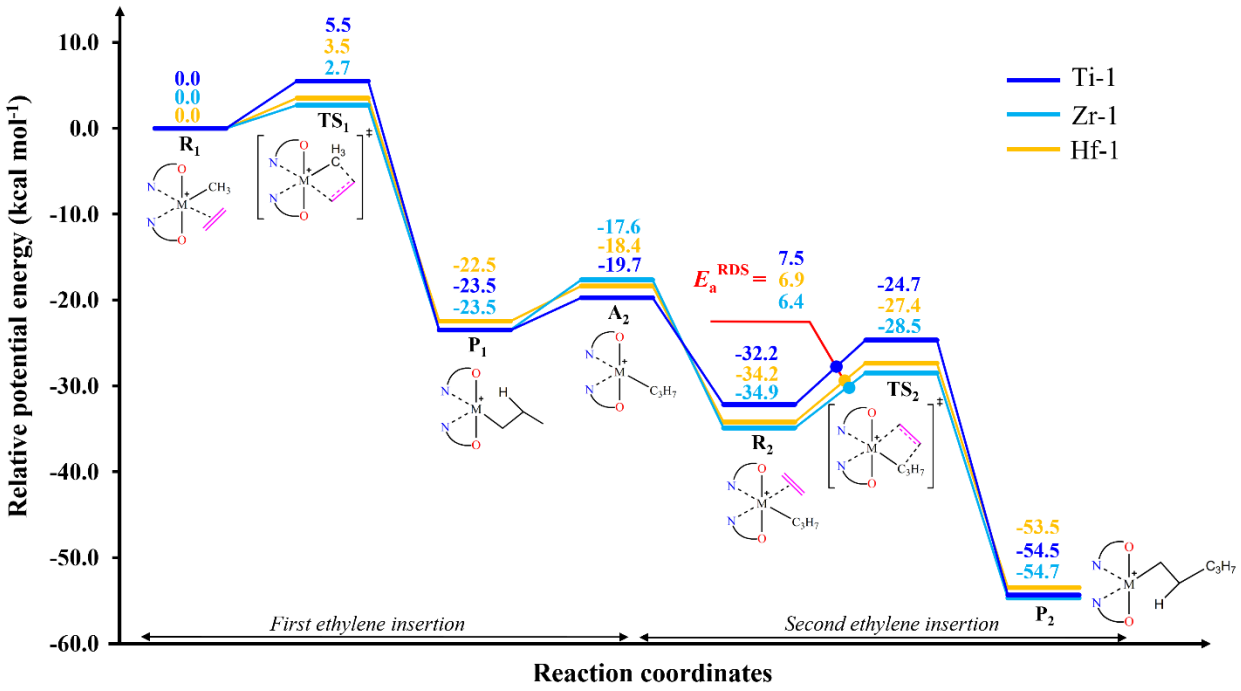
Activities for ethylene polymerization of general M-FI catalysts (M-1) with different metal substitutions were reported by Mitani et al. [16]. The highest activity was obtained when using Zr as the metal center followed by Hf and Ti, respectively. In this part, we investigated the reaction mechanism and examined the effect of group IV_B transition metal (M = Ti, Zr, Hf) substitutions on ET polymerization by phenoxy-imine (M-FI) catalysts using DFT calculations. The study is based on the proposed mechanism in **Scheme 1**.

All the optimized structures of intermediates and transition states for ET polymerization catalyzed by Ti-1-FI, Zr-1-FI, and Hf-1-FI were given in **Figs. S2, S3, and S4** of the supplementary material, respectively. The relative potential energy profiles of ET polymerization by the M-FI catalysts were shown in **Fig. 4**. From R_1 to P_1, the activation energies (E_{a1}) are 5.5, 2.7, and 3.5 kcal mol^{-1} and the reaction energies (ΔE_{r1}) are -23.5, -23.5, and -22.5 kcal mol^{-1} for Ti-1-FI, Zr-1-FI, and Hf-1-FI, respectively. For the second ethylene insertion, the activation energies (E_{a2}) are 7.5, 6.4, and 6.9 kcal mol^{-1}, and the reaction energies (ΔE_{r2}) are -22.2, -19.8, and -19.3 kcal mol^{-1}

for Ti-1-FI, Zr-1-FI, and Hf-1-FI, respectively. The experimental activities and our DFT results were listed in **Table S2** of the supplementary material. It was found that the trend of E_{a1} as well as E_{a2}, which is Zr-1-FI < Hf-1-FI < Ti-1-FI, agrees with experimental activities. However, the second ethylene insertion shows higher activation energy than the first ethylene insertion. Thus, the second insertion is the rate-determining (RD) step of this reaction which corresponds to Nikitin's work [21]. Therefore, the structures related to the second ethylene insertion were further analyzed to investigate the key factors of ET polymerization by the M-FI catalyst. In addition, the exothermic reaction energy was exhibited for both the first and second insertions. However, the trend of ΔE_{r1} and ΔE_{r2} is not related to experimental activities.

From the structures (see **Figs. S2-S4** of the supplementary material), we found the distance between the transition metal center (M) and nitrogen (at the nearest ethylene insertion site), M-N distance, to be related to the catalytic activities. The M-N distance of TS_1 (Zr-N (2.33 Å) > Hf-N (2.30 Å) > Ti-N (2.21 Å)) and TS_2 (Zr-N (2.34 Å) > Hf-N (2.30 Å) > Ti-N (2.23 Å)) show the similar trend to experimental activity. Furthermore, we employed the molecular electrostatic potential (MEP) maps and NBO charges of Ti-1-FI, Zr-1-FI, and Hf-1-FI of the TS_1 and TS_2 structures. Their results were given in **Fig. 5a-c**. The NBO charges of the transition metals are in the following order: Hf (+1.86) > Zr (+1.68) > Ti (+0.81) for TS_1 and Hf (+1.81) > Zr (+1.63) > Ti (+0.79) for TS_2. It can be seen that the electrostatic and electronic effects rather correspond to the size of metal cations but unrelated to the experiment trend.

Therefore, the M-N distance should be focused on as a key factor for ET polymerization. The elongation of the M-N distance would provide a larger space for the ethylene monomer to easily be inserted into the metal center. According to the RD step, the $R_2/TS_2/P_2$ structures were mainly focused on determining the factors related to the experimental activities in the next part.



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240 **Fig. 4** Relative potential energy profiles of ethylene polymerization by M-FI catalysts using
241 different group IV_B (Ti, Zr, Hf) transition metals were compared. The potential energies relative
242 to R_1 are given in kcal mol^{-1}.

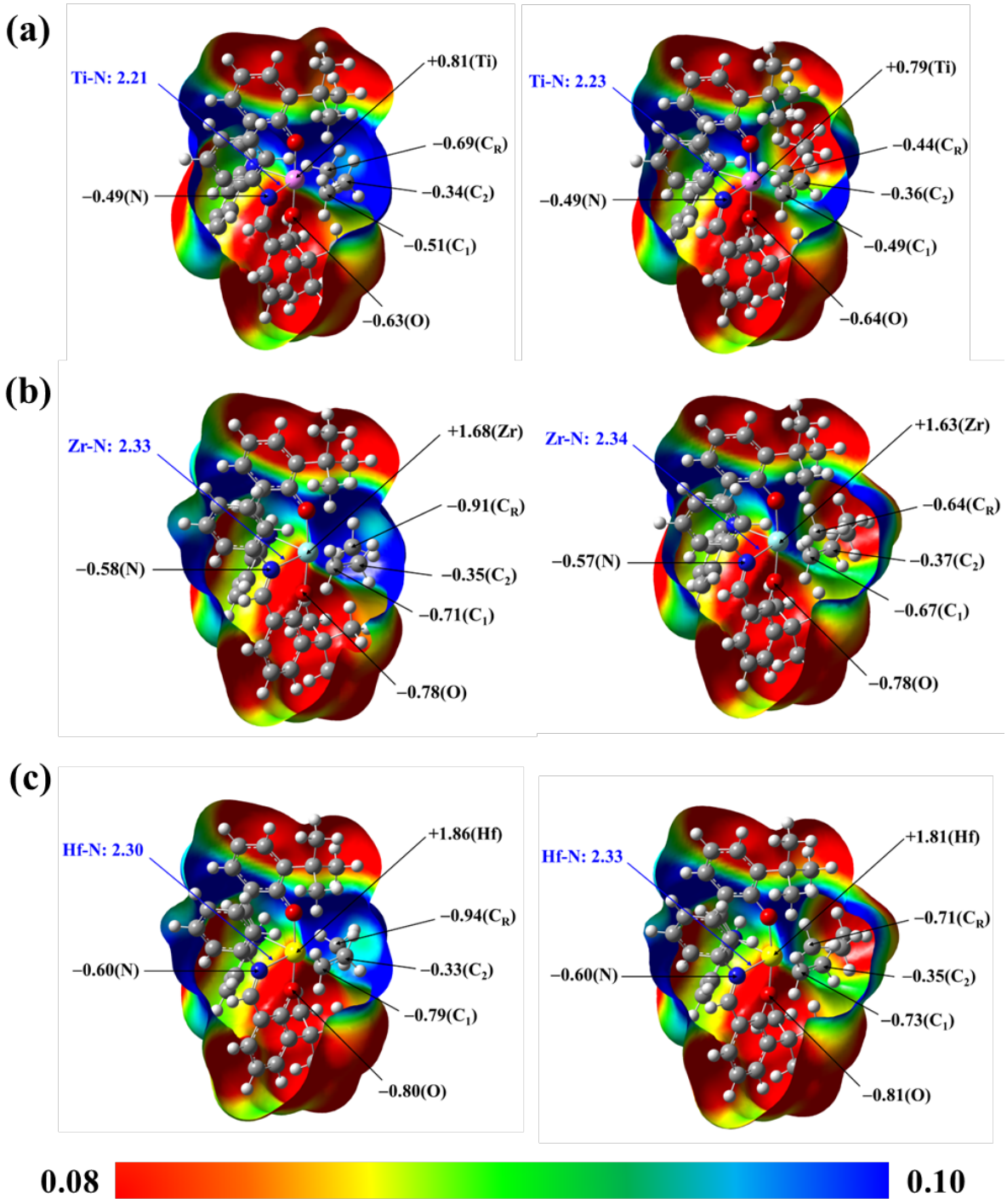

Fig 5. The molecular electrostatic potential (MEP) maps and NBO charges of (a) Ti-1-FI, (b) Zr-1-FI, and (c) Hf-1-FI of the TS_1 (left) and TS_2 (right) structures. The isosurface value is 0.002 with a range for the MEPs map of 0.08 to 0.10 a.u. for all structures. Distances (Å) are given in blue and NBO charges are shown in black.

3.3 Effect of ligand substitutions

In the previous section, among group IV_B transition metals the parent (Ti-1)-FI catalyst which contains (O, N) ligands possess the highest activation energy at the RD step. Thus, there has been an interest to study the catalytic activity of (Ti-1)-FI catalyst with other (O, X) ligands such as (O, O) [39], (O, P) [40, 41], or (O, S) [42, 43].

Table 1 displayed calculated activation energies (E_a^{RDS}) and reaction energies (ΔE_r^{RDS}) at the RD step for Ti-1 catalysts with different ligand substitutions. We observed E_a^{RDS} of 7.5, 4.7, 5.0, and 2.3 kcal mol^{-1} and ΔE_r^{RDS} of -28.1, -24.3, -22.1, and -21.7 kcal mol^{-1} when using (O, N), (O, P), (O, O), and (O, S) ligands, respectively. Thus, by substituting heteroatom in the ligand with P, O, and S, E_a^{RDS} of Ti-1-FI is decreased and the reaction becomes less exothermic. The catalyst with (O, S) ligand showed the lowest activation energy and is, therefore, the most active Ti-1-FI catalyst. For the Ti-3 catalyst, E_a^{RDS} are 4.2 and 2.4 kcal mol^{-1} and ΔE_r^{RDS} are -23.6 and -19.3 kcal mol^{-1} for (O, N) and (O, S) ligands, respectively. E_a^{RDS} of Ti-3 with (O, N) ligands is lower than that of Ti-1 in agreement with experimental activities reported by Nikitin et al. [21]. Interestingly, the Ti-1 with (O, S) ligand provides a lower E_a^{RDS} than Ti-1 with (O, N) ligands and has similar activity to Ti-3 with (O, S) ligands.

The bond distances are significantly affected the catalytic activities. Cohen et al. [44] found that the long Ti-S distance makes ligand more recessed. In Lapenta study [45], the Ti-S distance of was 2.60 Å which is longer than Ti-N bond distance (2.20 Å) [46]. Therefore, the formation of olefin into the complex of (O, S) is easier than (O, N). Herein, the Ti-S distance of the active cation form was 2.62 Å which is longer than Ti-N distance (2.17 Å) and the range of angle of S-Ti-S (105.2˚) is wider than N-Ti-N (83.6˚). We expected that a longer distance and a wide range of angle can produce more vacant site which assists the coordination-insertion polymerization.

Based on Nikitin's work [21], the high activities of FI catalysts were attributed to smaller HOMO-LUMO gaps in the active cations. Therefore, we calculated the HOMO and LUMO of active cation species as shown in **Fig. S5** of the supplementary material. We found that Ti-1(O, S) have smaller energy gaps (E_g = 5.32 eV) than Ti-1(O, N) complex (E_g = 5.66 eV). Our results indicated that the Ti with (O, S) complexes are good candidate for high active catalysts.

Table 1 The calculated activation energy (E_a^{RDS}) and reaction energy (ΔE_r^{RDS}) of different ligands substitutions of Ti-1(O, X) and Ti-3(O, X) systems at the RD site.

Energy	**Ti-1(O, X) system**				**Ti-3(O, X) system**	
(kcal mol^{-1})	**(O, N)**	**(O, P)**	**(O, O)**	**(O, S)**	**(O, N)**	**(O, S)**
E_a^{RDS}	7.5	4.7	5.0	2.3	4.2	2.4
ΔE_r^{RDS}	-28.1	-24.3	-22.1	-21.7	-23.6	-19.3

From the previous section, we suggested that the M-N distance plays a key role in controlling the catalytic activity of the M-FI catalyst. Hence, the distance between titanium and heteroatom (Ti-X) is of interest. Geometry optimized parameters of reactant π-complex (R_2), transition state (TS_2), β-agostic product (P_2) for the ethylene polymerization catalyzed by Ti-1 with (O, P), (O, O), and (O, S) ligands and Ti-3 with (O, N) and (O, S) ligands were given in **Figs. S6-S10** of the supplementary material, respectively. **Fig. 6a-d** displayed the optimized TS structures of Ti-1 with (O, N), (O, P), (O, O), and (O, S) ligands. We found the trend of Ti-X distance to be related to the activation energy, Ti-S (2.70 Å) > Ti-P (2.55Å) > Ti-O (2.25 Å) > Ti-N (2.23 Å). The longer Ti-S distance indicates the weaker interaction between the metal center and heteroatom. Thus, it allows ethylene to easily be inserted into the metal center and is resulted in a lower E_a^{RDS}. Moreover, Ti-X distances for the optimized TS structures of Ti-3 with (O, N) and (O, S) ligands as shown in **Fig. 6e and 6f** are 2.20 and 2.70 Å, respectively. Our results showed that the Ti (O,S)

292 is the best candidate for high activity catalysts similar to Lapenta et al. [45]. We compared the
293 E_a^{RDS} of Ti-3(O, N) complex with the different basis set and the M06-2X plus D3 correction was
294 elucidated as shown in **Table S3** of the supplementary material. While using M06-2X, the results
295 exhibit that using cc-pVDZ basis set is similar result to cc-pVTZ and cc-pVQZ. The additional of
296 dispersion interaction (D3) was not affected in M06-2X method.
297 Therefore, we summarized that the M-X distance is an important parameter for designing
298 Ti-FI based catalysts. In addition, our calculations revealed that all product structures still provided
299 a strong β-agostic interaction which is supported by the elongated C_R-H_β bond distance (1.13-1.15
300 Å) as compared to the normal C-H bond distance of 1.10 Å [47, 48].
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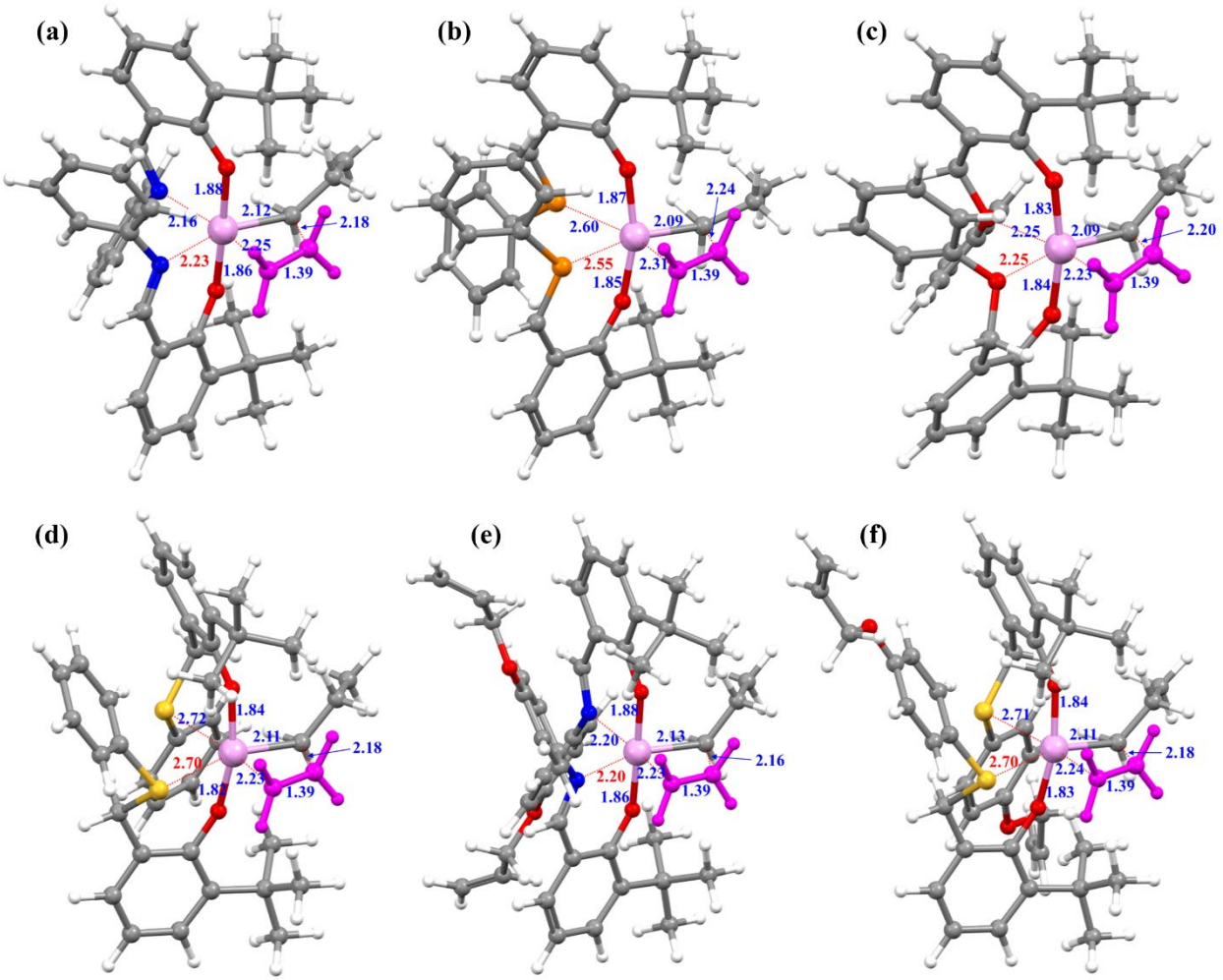

Fig. 6 Optimized TS structures of Ti-1 with (a) (O, N) (b) (O, P) (c) (O, O) (d) (O, S) ligands and Ti-3 with (e) (O, N) (f) (O, S) ligands. The carbon, hydrogen, oxygen, nitrogen, phosphorus, sulfur, and titanium atoms are shown in grey, white, red, blue, orange, yellow, and light pink colors, respectively. The ethylene (ET) molecule is shown in magenta color. Distance (Å) is given in blue and red colors.

3.4 Novel Ni-based FI catalyst with (O, N) ligand

Chasing et al. [22] performed a QSAR study on varieties of M-FI catalysts and proposed nickel (II) complex with phenoxy-imine (O,N) ligand as a candidate catalyst for ethylene polymerization. To verify their suggestion, we calculated the activation energy at the RD step for

313 the Ni-phenoxy-imine (Ni-FI) catalyst using Ti-3 as the template catalyst. The Ti-3-FI catalyst was
314 chosen because this structure provides a lower activation at the RD step for Ti-FI. This is supported
315 by our calculations and Nikitin et al. [21]. It turned out that the calculated E_a^{RDS} of the Ni-3-FI
316 catalyst is very high (29.6 kcal mol^{-1}) and has ΔE_r^{RDS} of -22.4 kcal mol^{-1}. From our observation,
317 the high E_a^{RDS} value probably comes from the C_2 symmetric octahedral geometry of the Ni-FI
318 catalyst. From **Figure 7a** and according to Makio et al. [9] , it could be viewed that this octahedral
319 structure of Ni-3-FI yields high steric interaction for the ethylene insertion. Therefore, the Ni-FI
320 catalyst that used Ti-3 as the template structure is inactive for the ethylene polymerization [49, 50].
321 The metal center in the Ni-FI catalyst is hexacoordinate and the catalyst contains two phenoxy-
322 imine (O, N) ligands. Since Ni can also form a stable four coordination complex, we generated an
323 active form of the Ni-FI catalyst with four coordination on nickel by removing one phenoxy-imine
324 (O, N) ligand and performed geometry optimization. The optimized tetracoordinate nickel
325 complex has a square-planar geometry [51-53]. We determined E_a^{RDS} and ΔE_r^{RDS} for the reaction
326 from the active catalyst structure (see **Figure 7b.** Values of 12.3 and the -20.8 kcal mol^{-1} for E_a^{RDS}
327 and ΔE_r^{RDS} were obtained, respectively. However, this nickel (II) complex with one phenoxy-
328 imine (O, N) ligand still has higher activation energy at the RD step than Ti-FI catalysts.
329 To understand why Ni-FI prefers square-planar geometry, we compared the coordination
330 energy of ET to Ni-FI for the octahedral and square-planar complexes. The coordination energy
331 for the octahedral complex is -7.7 kcal mol^{-1}, whereas that for the square-planar complex is -29.1
332 kcal mol^{-1} (see **Table S4** of the supplementary material). One reason which might explain the
333 preference for a four-coordinate nickel is the neutrality of the tetracoordinate nickel complex,
334 while the hexacoordinate one adopts a negative charge. Thus, Ni-FI in a square-planar geometry
335 provides a stronger interaction between ET and Ni metal center. Due to the higher stability of the

nickel complex and being less steric for ethylene coordination, the nickel (II) complex with one phenoxy-imine (O, N) ligand in square-planar geometry is more reactive than the C_2 symmetric octahedral geometry.

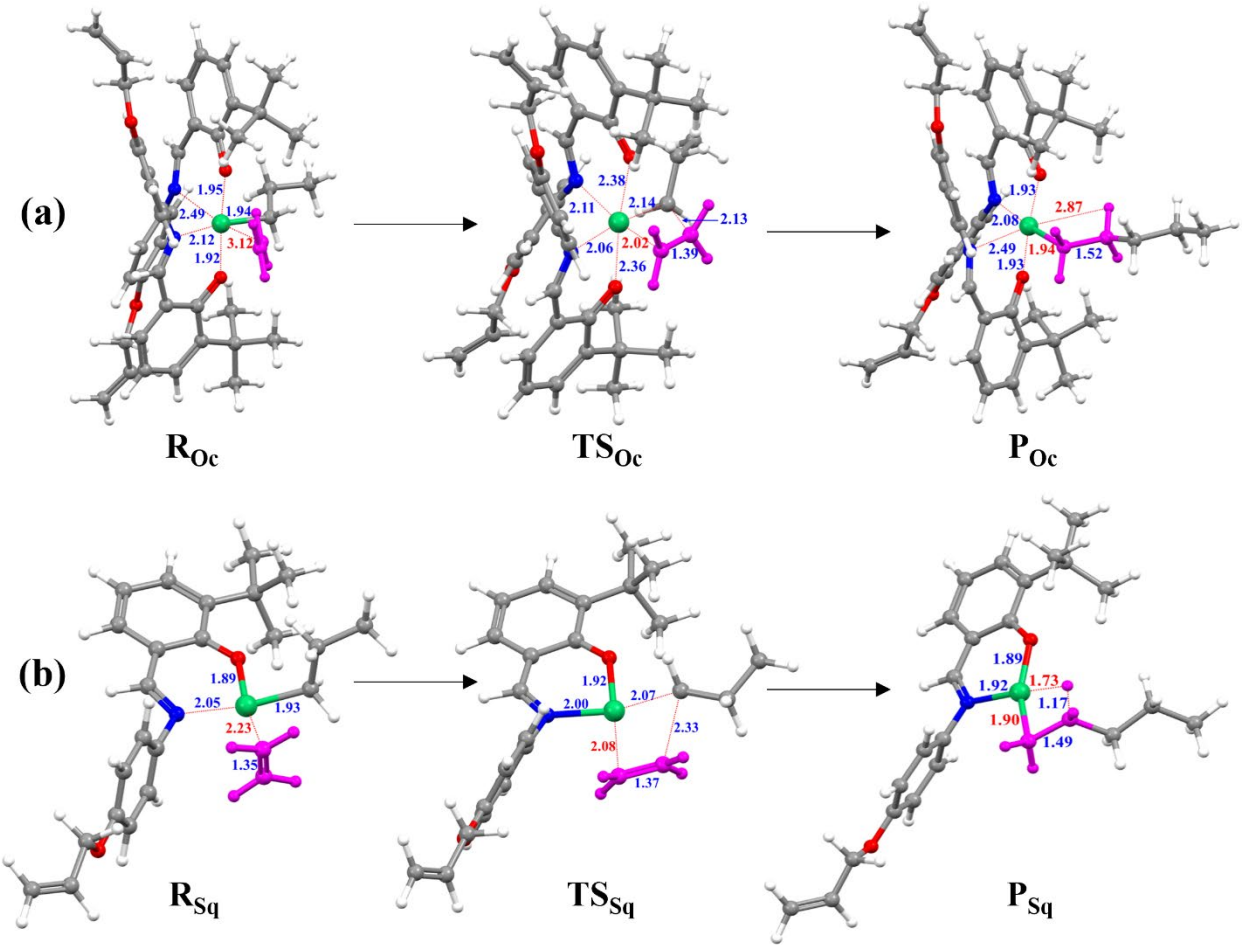

Fig. 7 Optimized structures of reactant π-complex (R), transition state (TS), β-agostic product (P) for the ethylene polymerization catalyzed by (a) octahedral Ni-FI (b) square-planar of Ni-FI. Bond distances (Å) are displayed in blue and red colors.

4. CONCLUSIONS

The reaction mechanism of phenoxy-imine (FI) catalysts for ethylene polymerization were investigated using the DFT calculations. The relative potential energy (RE) of pre-reaction Ti-FI complexes revealed that the rearrangement in *cis*-N/*trans*-O/*cis*-Cl (isomer A) is the most stable form and corresponded to the X-ray structure. The reaction mechanism for ethylene polymerization catalyzed using M-FI catalyst was elucidated based on Ti-1-FI and isomer A structure. The obtained results indicated that the second ethylene insertion is the rate-determining (RD) step for this reaction. Then, the potential energy profiles of the different group IV_B transition metals were employed for comparison. Among three group IV_B transition metals, the activation energy at the RD step (E_a^{RDS}) is as the following: Zr < Hf < Ti, which agrees with the experimental results. Furthermore, we found that the distance between the transition metal center (M) and nitrogen is related to the catalytic activities. For the effect of ligand substitutions, the Ti-1 model with (O, N) ligands was used as the parent system to compare the E_a^{RDS} with other (O, X (=P, O, and S)) ligand substitutions. We observed that using X=P, O, and S instead of N can provide a more potent catalyst and that the (O, S) ligands give the lowest E_a^{RDS} and the longest Ti-X distance. Concerning the R substitution on the ligand, the Ti-3 model exhibited a lower E_a^{RDS} than the Ti-1 model for all kinds of the (O, X) substitutions. Finally, we investigated the Ni-phenoxy-imine (Ni-FI)-based catalyst. The results revealed that the nickel (II) complexes based on the one phenoxy-imine (O, N) ligand in the square-planar geometry is more active than that of the octahedral geometry, but their activation energies are higher than that of Ti-FI. This work provides information on the reaction mechanism of the M-FI catalysts with different metal and ligand substitutions, which will be useful for the design of M-FI catalysts for ethylene polymerization.

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Supplementary material

DFT Insights into Metals and Ligands Substitutions Effects on Reactivity of Phenoxy-Imine Catalysts for Ethylene Polymerization

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Table S1 Comparison of bond distances (Å) and bond angles (˚) of the pre-reaction complex (Ti-1) between the structure reported by Makio et al. [14] and seven theoretical methods with the cc-pVDZ basis set.

Bond distances (Å)	Ref. [14]	HF	B3LYP	B3LYP-D3	M06	M06-2X	M06L	MP2
Ti-O	1.85	1.84	1.87	1.86	1.86	1.85	1.87	1.85
Ti-N	2.23	2.23	2.28	2.27	2.26	2.25	2.28	2.27
Ti-Cl	2.30	2.29	2.27	2.27	2.26	2.26	2.27	2.27
Bond angles (˚)	Ref. [14]	HF	B3LYP	B3LYP-D3	M06	M06-2X	M06L	MP2
O-Ti-O	171.6	168.6	169.6	167.6	168.2	168.5	168.5	166.1
N-Ti-N	76.4	85.4	77.7	74.7	75.9	74.1	73.9	71.3
Cl-Ti-Cl	103.1	99.6	103.5	104.7	104.5	104.8	104.8	106.3

Table S2 Experimental activities and our DFT calculation results. The energies are given in kcal mol^{-1}.

Metal	Experimental results* [16]		DFT calculation results				
	Activity (kg $mmol^{-1}$ h^{-1})	log activity	E_{a1}	E_{a2}	$E_{(A2-P1)}$	ΔE_{r1}	ΔE_{r2}
Ti	3.3	0.52	5.5	7.5	3.8	-23.5	-22.2
Zr	519.0	2.72	2.7	6.4	5.9	-23.5	-19.8
Hf	6.5	0.81	3.5	6.9	4.1	-22.5	-19.3

*Conditions: co-cat. MAO, 25˚C, $p(C_2H_4)$ 0.1 MPa. E_{a2} is the RDS.

Table S3 Comparison of the activation energy at the rate-determining step (E_a^{RDS}) of the Ti-3(O, N) complex with the different basis set and the M06-2X plus D3 correction. The E_a^{RDS} are given in kcal mol^{-1}.

Complex	E_a^{RDS}			
	M06-2X cc-pVDZ	M06-2X cc-pVTZ	M06-2X cc-pVQZ	M06-2X-D3 cc-pVDZ
Ti-3(O, N)	4.2	4.2	4.0	4.1

Table S4 The coordination energy of ethylene (ET) determined by the reactant π-complex (R_2) using equation: $\Delta E_{co} = E_{R_2} - (E_{R_2\text{-without ET}} + E_{ET})$.

Ni-FI geometry	$\Delta E_{coordination}$ (kcal mol^{-1})
Octahedral	-7.7
Square planar	-29.1

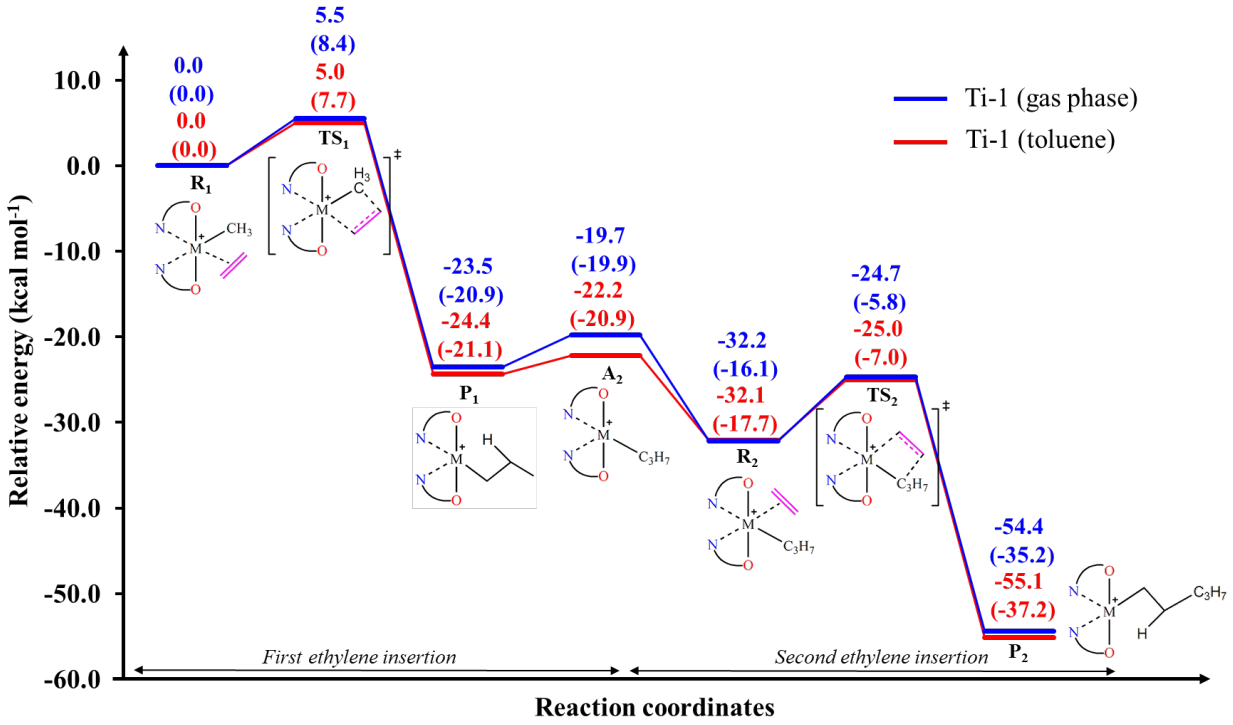


Fig. S1 Relative energy profiles for ethylene polymerization catalyzed by (Ti-1)-FI catalyst in gas phase (blue line) and toluene (red line). The energies relative to R_1 are given in kcal mol^{-1}. The relative Gibbs free energy ($\Delta G^{\ddagger}$) at 298.15 K are shown in parenthesis.

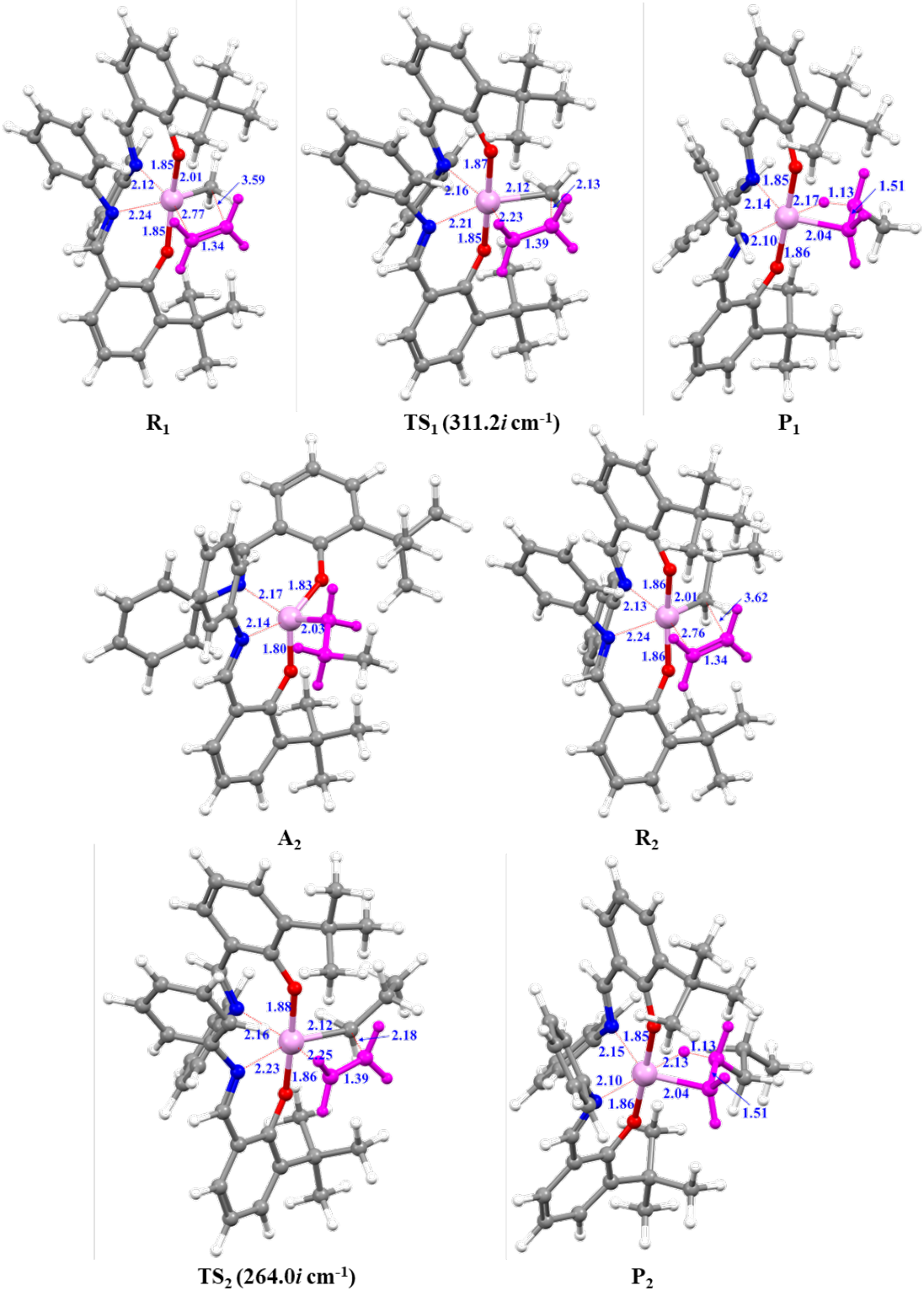


Fig. S2 Optimized structures of intermediates and transition states for ethylene polymerization catalyzed by (Ti-1)-FI catalyst in gas phase. Bond distances are displayed in blue color. Bond distances are given in Å.

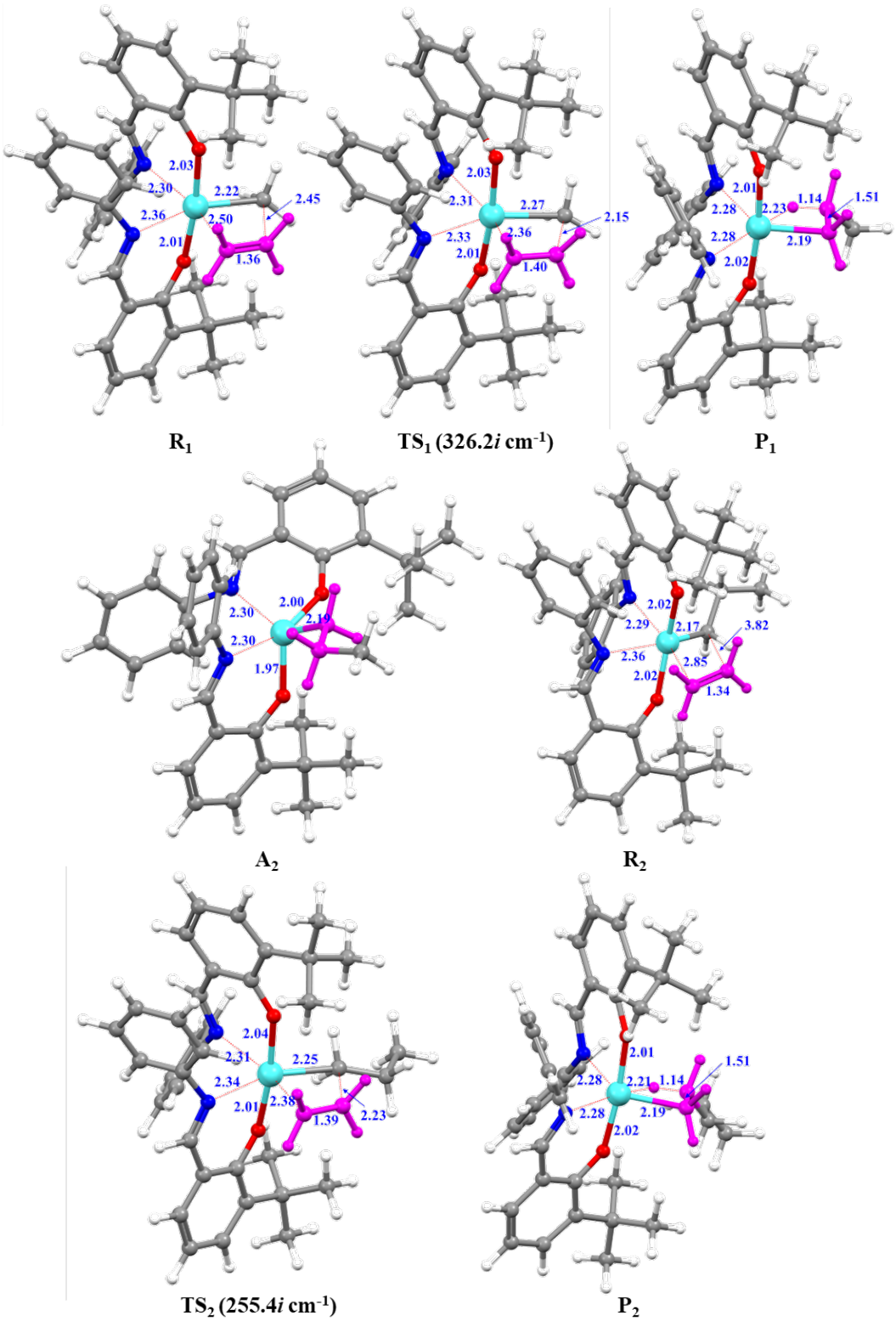


Fig. S3 Optimized structures of intermediates and transition states for ethylene polymerization catalyzed by (Zr-1)-FI catalyst in gas phase. Bond distances are displayed in blue color. Bond distances are given in Å.

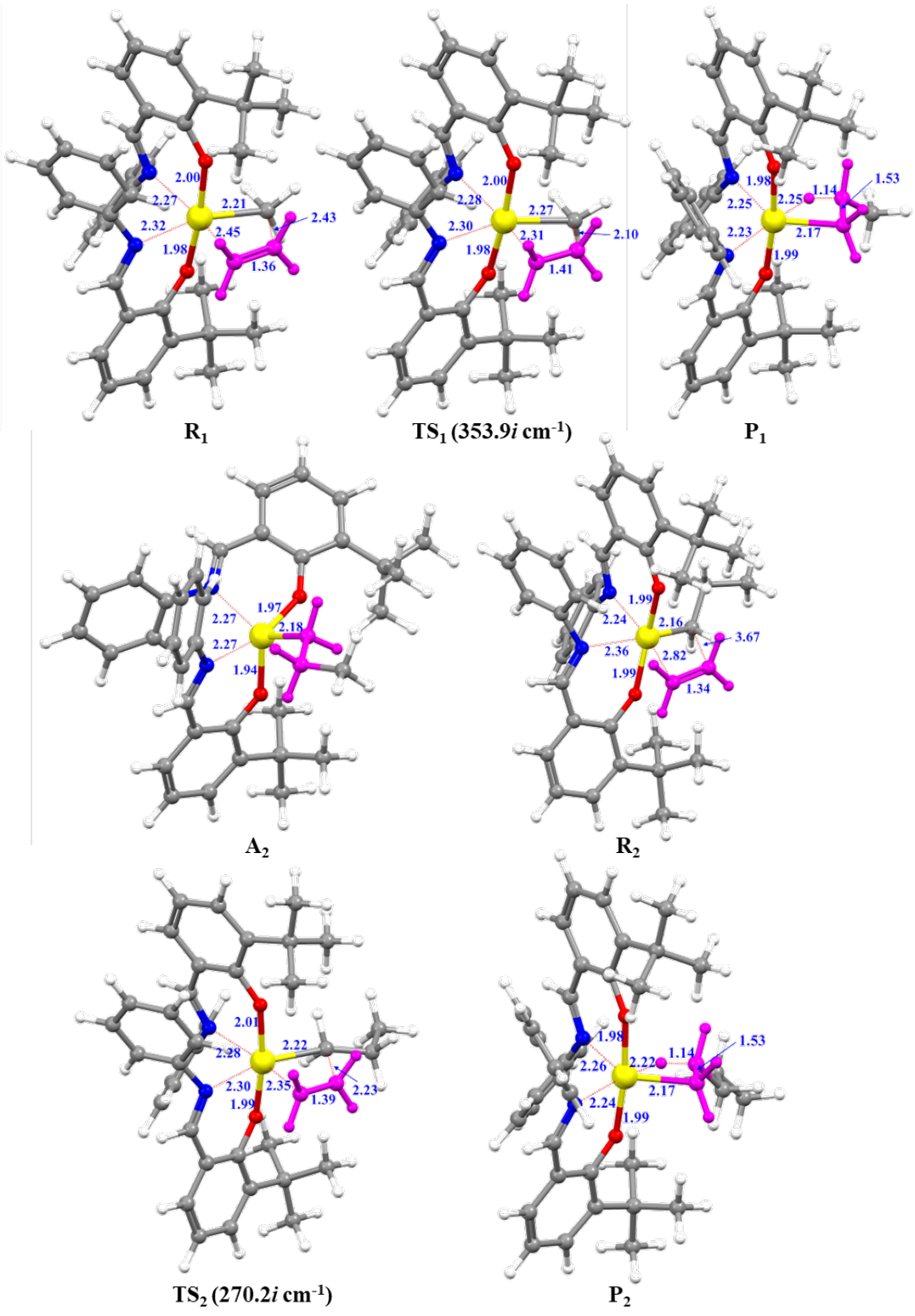


Fig. S4 Optimized structures of intermediates and transition states for ethylene polymerization catalyzed by (Hf-1)-FI catalyst in gas phase. Bond distances are displayed in blue color. Bond distances are given in Å.

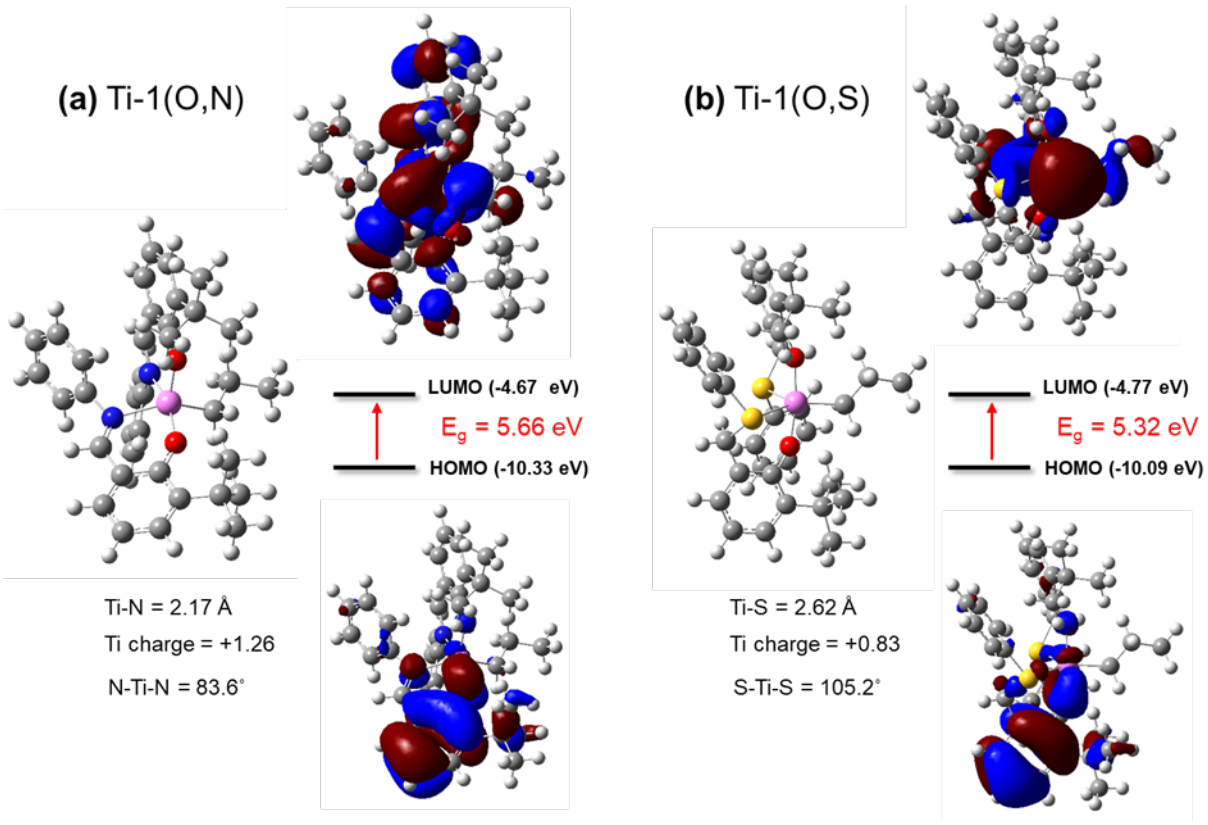


Fig. S5. The HOMO and LUMO of active cation species of (a) Ti-1(O, N) complex and (b) Ti-1(O, S) complex.

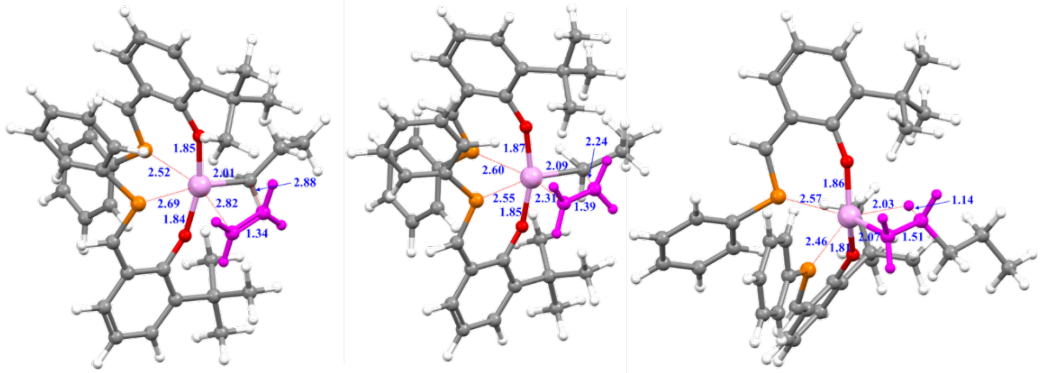
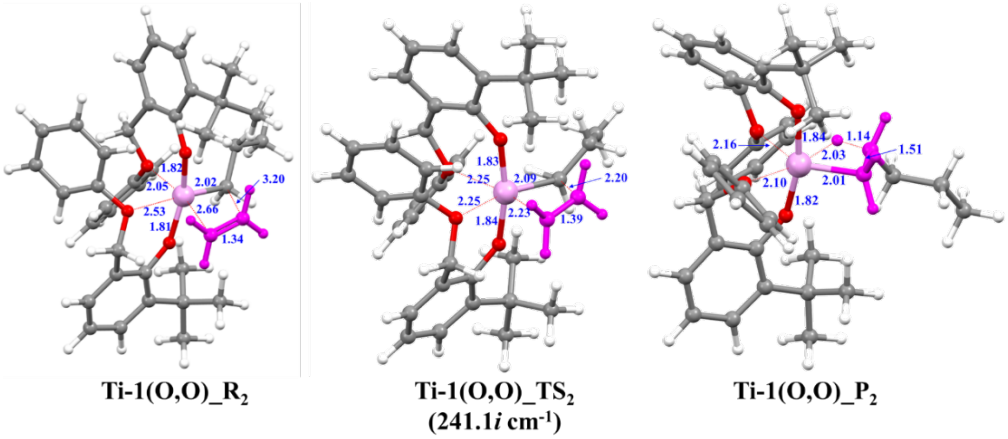
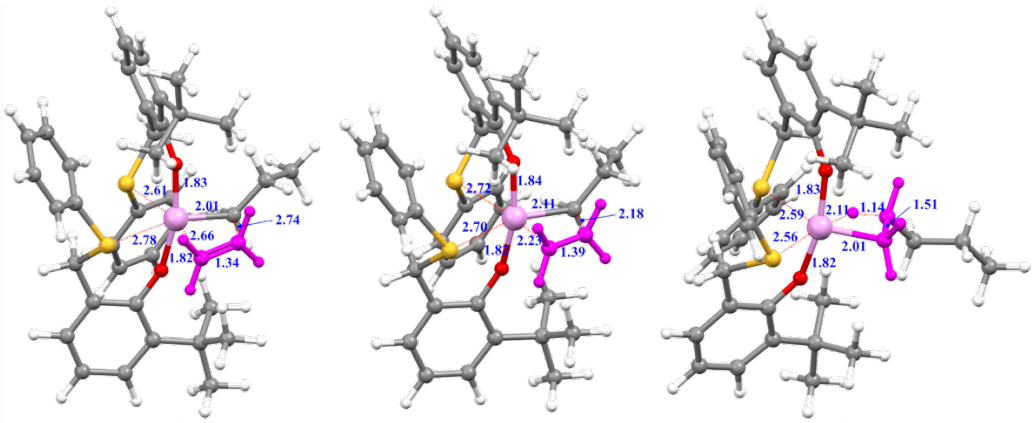


Fig. S6 Optimized structures of reactant π-complex (R_2), transition state (TS_2), β-agostic product (P_2) for ethylene polymerization catalyzed by Ti-1(O, P) complex in gas phase. Bond distances are displayed in blue color. Bond distances are given in Å.



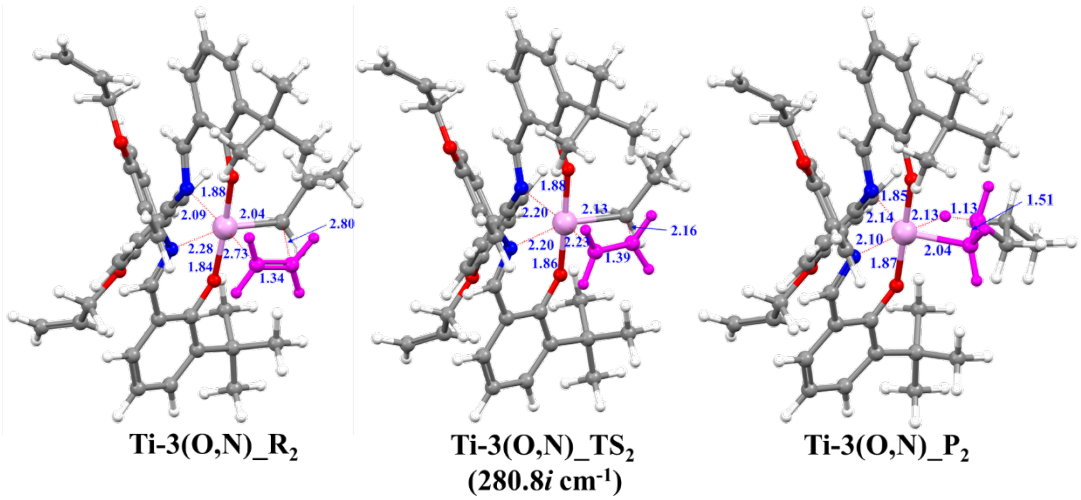
Ti-1(O,O)_R$_2$ **Ti-1(O,O)_TS$_2$ (241.1*i* cm^{-1})** **Ti-1(O,O)_P$_2$**

Fig. S7 Optimized structures of reactant π-complex (R_2), transition state (TS_2), β-agostic product (P_2) for ethylene polymerization catalyzed by Ti-1(O, O) complex in gas phase. Bond distances are displayed in blue color. Bond distances are given in Å.



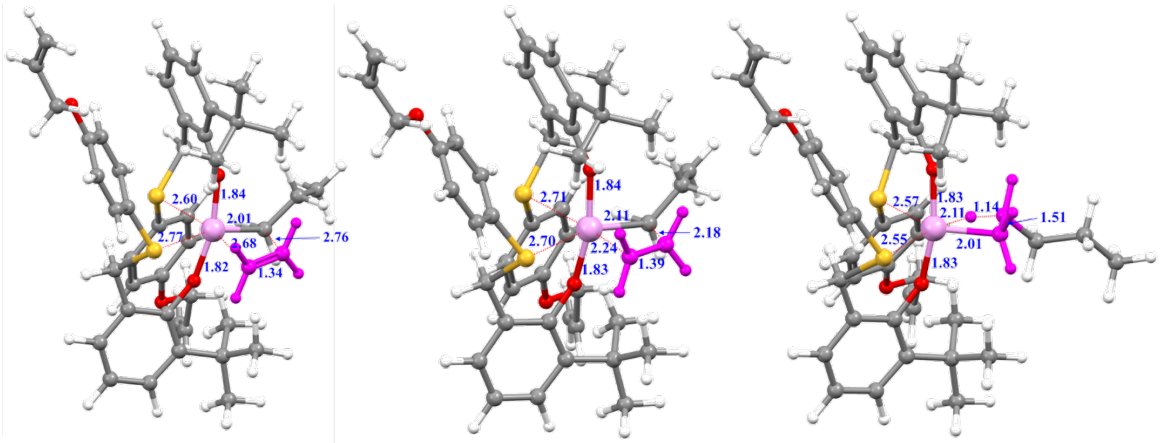
Ti-1(O,S)_R$_2$ **Ti-1(O,S)_TS$_2$ (245.1*i* cm^{-1})** **Ti-1(O,S)_P$_2$**

Fig. S8 Optimized structures of reactant π-complex (R_2), transition state (TS_2), β-agostic product (P_2) for ethylene polymerization catalyzed by Ti-1(O, S) complex in gas phase. Bond distances are displayed in blue color. Bond distances are given in Å.



Ti-3(O,N)_R$_2$ **Ti-3(O,N)_TS$_2$ (280.8*i* cm^{-1})** **Ti-3(O,N)_P$_2$**

Fig. S9 Optimized structures of reactant π-complex (R_2), transition state (TS_2), β-agostic product (P_2) for ethylene polymerization catalyzed by Ti-3(O, N) complex in gas phase. Bond distances are displayed in blue color. Bond distances are given in Å.



Ti-3(O,S)_R$_2$ **Ti-3(O,S)_TS$_2$ (246.7*i* cm^{-1})** **Ti-3(O,S)_P$_2$**

Fig. S10 Optimized structures of reactant π-complex (R_2), transition state (TS_2), β-agostic product (P_2) for ethylene polymerization catalyzed by Ti-3(O, S) complex in gas phase. Bond distances are displayed in blue color. Bond distances are given in Å.

Atomic coordinates of the optimized FI catalysts

Pre-reaction (isomer A)

C	-1.118800	1.492100	1.716200
C	-2.491400	1.105900	1.468600
C	-2.810800	-0.078800	0.769500
H	-3.253800	2.836700	2.512300
H	-0.995400	2.416300	2.302700
C	-3.515900	1.917000	1.984800
C	-4.153600	-0.531300	0.682800
C	-5.129700	0.316200	1.204000
C	-4.833500	1.538200	1.826900
H	-6.175600	0.018700	1.139800
H	-5.640700	2.161400	2.210200
O	-1.831400	-0.762900	0.207100
N	-0.046800	0.861900	1.363100
C	1.118800	1.492300	-1.716200
C	2.491400	1.106100	-1.468500
C	2.810800	-0.078600	-0.769500
H	3.253800	2.837000	-2.512000
H	0.995400	2.416600	-2.302600
C	3.515800	1.917300	-1.984500
C	4.153600	-0.531000	-0.682800
C	5.129700	0.316600	-1.203700
C	4.833500	1.538600	-1.826500
H	6.175600	0.019200	-1.139400
H	5.640700	2.162000	-2.209700
O	1.831400	-0.762800	-0.207200
N	0.046800	0.862200	-1.363100
Ti	-0.000000	-0.945800	-0.000100
C	-1.196300	1.483800	-1.698400
C	-1.442000	2.811600	-1.335500
C	-2.188200	0.740300	-2.342800
C	-2.682200	3.390500	-1.597200
H	-0.664400	3.379900	-0.822900
C	-3.419200	1.331100	-2.611600
H	-1.980800	-0.294400	-2.617400
C	-3.676000	2.649100	-2.230500
H	-2.871900	4.421200	-1.295000
H	-4.190000	0.753600	-3.123000
H	-4.650700	3.096200	-2.427400
C	1.196300	1.483400	1.698700
C	2.187900	0.739700	2.343200
C	1.442300	2.811100	1.335900
C	3.418900	1.330200	2.612200
H	1.980300	-0.295000	2.617700
C	2.682500	3.389800	1.597800
H	0.664900	3.379600	0.823100
C	3.676000	2.648200	2.231200
H	4.189600	0.752500	3.123700
H	2.872500	4.420500	1.295700
H	4.650900	3.095100	2.428300
C	4.482700	-1.917900	-0.118100
C	4.047500	-2.047200	1.349900
C	3.753600	-2.980200	-0.962000
C	5.986300	-2.203600	-0.191000
H	4.537900	-1.280800	1.969800
H	2.959400	-1.960600	1.457200
H	4.348400	-3.036000	1.730300
H	4.077200	-2.928900	-2.013100
H	3.994100	-3.983500	-0.576700
H	2.663900	-2.851500	-0.924700
H	6.175600	-3.214000	0.199300
H	6.360800	-2.167900	-1.225000
H	6.569200	-1.495300	0.418000
C	-4.482600	-1.918000	0.117900
C	-4.047500	-2.047000	-1.350100
C	-3.753600	-2.980500	0.961700
C	-5.986200	-2.203800	0.190800
H	-4.537900	-1.280500	-1.969800
H	-2.959400	-1.960500	-1.457400
H	-4.348400	-3.035700	-1.730700
H	-4.077200	-2.929500	2.012700
H	-3.993900	-3.983700	0.576000
H	-2.663800	-2.851700	0.924500
H	-6.175500	-3.214100	-0.199600
H	-6.360800	-2.168200	1.224900
H	-6.569200	-1.495400	-0.418000
Cl	0.228600	-2.323500	1.774600
Cl	-0.228600	-2.322500	-1.775700

Pre-reaction (isomer B)

C	-0.924800	0.350600	2.388700
C	-2.314000	-0.007600	2.167000
C	-2.771600	-0.491400	0.923700
H	-2.858700	0.549400	4.180100
H	-0.715900	0.831000	3.357400
C	-3.222100	0.168400	3.223600
C	-4.134000	-0.815800	0.716800
C	-4.989400	-0.631800	1.802600
C	-4.554900	-0.146100	3.043700
H	-6.045500	-0.872500	1.688900
H	-5.269600	-0.020000	3.856200
O	-1.899900	-0.608400	-0.071000
N	0.065800	0.157100	1.588400
C	2.856600	0.215700	-0.966500
C	2.407200	1.588800	-1.056200
C	1.036400	1.919300	-1.091800
H	4.432700	2.336500	-1.081100
H	3.939100	0.084500	-1.110600
C	3.374600	2.605300	-1.107800
C	0.610300	3.268700	-1.199400
C	1.611100	4.238600	-1.222100
C	2.978600	3.926900	-1.172500
H	1.329700	5.289000	-1.289000
H	3.717700	4.727100	-1.200600
O	0.148900	0.944900	-1.030400
N	2.147900	-0.844400	-0.744400
Ti	-0.136200	-0.795500	-0.475800
C	2.906000	-2.065800	-0.685100
C	2.499100	-3.179800	-1.424000
C	4.058200	-2.139300	0.104100
C	3.254400	-4.347600	-1.379600
H	1.594500	-3.123400	-2.026900
C	4.801400	-3.317300	0.151300
H	4.357300	-1.275400	0.698500
C	4.403600	-4.424900	-0.592700
H	2.934200	-5.209700	-1.965500
H	5.692800	-3.365000	0.778100
H	4.983800	-5.347400	-0.556900
C	1.330600	0.650300	2.037800
C	2.345700	-0.252800	2.357700
C	1.544600	2.027600	2.140100
C	3.576800	0.235600	2.791200
H	2.154500	-1.323300	2.255700
C	2.785400	2.504300	2.557900
H	0.745100	2.712400	1.852400
C	3.803300	1.610000	2.885300
H	4.366700	-0.467500	3.061700
H	2.955100	3.579800	2.620200
H	4.772200	1.982200	3.219600
C	-0.881100	3.608300	-1.293800
C	-1.483900	2.935300	-2.540700
C	-1.623700	3.128900	-0.033400
C	-1.100800	5.119400	-1.419900
H	-0.977300	3.289900	-3.451400
H	-1.395600	1.842200	-2.495700
H	-2.551400	3.194400	-2.618900
H	-1.224400	3.625800	0.866400
H	-2.690900	3.390500	-0.112200
H	-1.550000	2.041400	0.092800
H	-2.179400	5.320600	-1.493100
H	-0.717600	5.664700	-0.543500
H	-0.622400	5.527700	-2.322800
C	-4.613300	-1.356600	-0.634100
C	-4.324400	-0.333700	-1.747500
C	-3.898000	-2.684800	-0.940600
C	-6.122100	-1.623800	-0.618600
H	-4.805800	0.631300	-1.522800
H	-3.247500	-0.171400	-1.880400
H	-4.732200	-0.706300	-2.699900
H	-4.105700	-3.425700	-0.153400
H	-4.267600	-3.085800	-1.897200
H	-2.811500	-2.557900	-1.024400
H	-6.426800	-2.010900	-1.601600
H	-6.396300	-2.377000	0.135800
H	-6.700100	-0.706900	-0.425300
Cl	0.140100	-2.724200	0.723700
Cl	-0.465400	-1.667100	-2.536000

Pre-reaction (isomer C)

C	1.812300	0.254700	2.388200
C	0.641400	-0.343600	2.979100
C	-0.446500	-0.775500	2.180400
H	1.514100	-0.273100	4.955000
H	2.685000	0.334600	3.052900
C	0.658500	-0.603300	4.362400
C	-1.517800	-1.504200	2.770800
C	-1.462200	-1.706100	4.146400
C	-0.399200	-1.262100	4.949500
H	-2.276900	-2.239700	4.634100
H	-0.411200	-1.454200	6.021600
O	-0.417800	-0.529400	0.885500
N	1.961500	0.659500	1.165900
C	-2.090900	0.084600	-2.006400
C	-1.497700	-1.221400	-2.192600
C	-0.131500	-1.455900	-1.914200
H	-3.350800	-2.042000	-2.937500
H	-3.078700	0.222200	-2.470100
C	-2.301300	-2.248000	-2.716700
C	0.442000	-2.731800	-2.157200
C	-0.405600	-3.721700	-2.650600
C	-1.762100	-3.500200	-2.930900
H	-0.002200	-4.717400	-2.831100
H	-2.376200	-4.311400	-3.320100
O	0.593100	-0.454700	-1.440300
N	-1.584400	1.090100	-1.369900
Ti	0.263100	0.882200	-0.185500
C	-2.392900	2.278500	-1.347100
C	-1.856600	3.483600	-1.800500
C	-3.702500	2.220200	-0.867200
C	-2.650400	4.627300	-1.791900
H	-0.823800	3.512600	-2.145500
C	-4.484100	3.373500	-0.854400
H	-4.091900	1.279200	-0.475400
C	-3.962000	4.578200	-1.320000
H	-2.234000	5.568300	-2.152800
H	-5.503100	3.327600	-0.468600
H	-4.573700	5.480800	-1.307600
C	3.272200	1.133300	0.824200
C	3.965700	0.492800	-0.201400
C	3.830900	2.223000	1.489900
C	5.238400	0.933600	-0.547300

H	3.490000	-0.335900	-0.724200
C	5.104900	2.661800	1.131800
H	3.249800	2.741600	2.254400
C	5.812000	2.017500	0.118100
H	5.781000	0.431000	-1.348900
H	5.541000	3.521300	1.642100
H	6.806100	2.367000	-0.162000
C	1.918600	-2.991600	-1.853500
C	2.789800	-2.037300	-2.691000
C	2.166400	-2.803200	-0.344900
C	2.327800	-4.423900	-2.212400
H	2.662500	-2.253100	-3.762900
H	2.529800	-0.984700	-2.523800
H	3.852600	-2.186200	-2.439500
H	1.605100	-3.559500	0.226100
H	3.238000	-2.931100	-0.121500
H	1.850400	-1.814000	0.008600
H	3.396700	-4.556700	-1.990200
H	1.770100	-5.169400	-1.625700
H	2.179100	-4.635300	-3.282100
C	-2.666800	-2.040400	1.912900
C	-3.368100	-0.871500	1.200200
C	-2.109100	-3.047600	0.890600
C	-3.717300	-2.768000	2.758100
H	-3.852100	-0.209000	1.934900
H	-2.655500	-0.270500	0.624200
H	-4.144500	-1.260700	0.519600
H	-1.656200	-3.905700	1.411800
H	-2.924700	-3.425000	0.253100
H	-1.348600	-2.592700	0.243500
H	-4.518200	-3.131400	2.097200
H	-3.292500	-3.640100	3.278000
H	-4.174800	-2.102000	3.505200
Cl	-0.711300	2.361700	1.273700
Cl	1.474300	2.438200	-1.323100

Pre-reaction (isomer D)

C	-1.150800	-2.794100	-0.715700
C	0.123600	-3.414900	-0.407400
C	1.301300	-2.673200	-0.175300
H	-0.770600	-5.372500	-0.552300
H	-1.938400	-3.504500	-1.009200
C	0.148000	-4.817300	-0.353200
C	2.507300	-3.330800	0.174700
C	2.472200	-4.725100	0.227200
C	1.321400	-5.473800	-0.040000
H	3.380800	-5.264400	0.488700
H	1.355000	-6.561600	0.009900
O	1.245000	-1.346800	-0.313100
N	-1.468500	-1.544900	-0.675900
C	-1.153100	2.793400	0.715400
C	0.120900	3.415100	0.406800
C	1.299200	2.674100	0.175300
H	-0.774900	5.372000	0.550300
H	-1.941200	3.503300	1.008700
C	0.144200	4.817400	0.351600
C	2.504700	3.332300	-0.175000
C	2.468500	4.726600	-0.228500
C	1.317000	5.474600	0.038100
H	3.376700	5.266500	-0.490200
H	1.349900	6.562400	-0.012700
O	1.243900	1.347700	0.314100
N	-1.469900	1.543900	0.675800
Ti	0.049800	0.000000	0.000200
C	-2.850600	1.306500	1.006400
C	-3.204800	0.769900	2.244500
C	-3.833300	1.705000	0.096200
C	-4.555200	0.645700	2.570200
H	-2.424000	0.474700	2.942600
C	-5.177600	1.576800	0.434400
H	-3.526900	2.100500	-0.874000
C	-5.542100	1.050500	1.673300
H	-4.834000	0.241300	3.544400
H	-5.942400	1.886100	-0.279400
H	-6.596000	0.956300	1.938700
C	-2.849300	-1.308200	-1.006400
C	-3.831800	-1.707300	-0.096200
C	-3.203800	-0.771700	-2.244400
C	-5.176100	-1.579800	-0.434400
H	-3.525200	-2.102700	0.874000
C	-4.554200	-0.648200	-2.570100
H	-2.423100	-0.475900	-2.942400
C	-5.541000	-1.053700	-1.673300
H	-5.940800	-1.889600	0.279400
H	-4.833200	-0.243800	-3.544300
H	-6.594900	-0.960000	-1.938800
C	3.770900	2.549600	-0.529200
C	4.197400	1.670200	0.656200
C	3.487700	1.694300	-1.776400
C	4.941100	3.483000	-0.859700
H	4.380000	2.289600	1.548400
H	3.434800	0.922900	0.899600
H	5.132700	1.144000	0.408300
H	3.235700	2.339600	-2.631700
H	4.381400	1.105800	-2.036700
H	2.649100	1.003500	-1.620500
H	5.820600	2.872700	-1.111100
H	4.723900	4.125000	-1.726400
H	5.209700	4.123000	-0.005500
C	3.772900	-2.547400	0.529600
C	4.199200	-1.667200	-0.655200
C	3.489100	-1.693000	1.777300
C	4.943600	-3.480400	0.859900
H	4.382300	-2.286000	-1.547700
H	3.436300	-0.920100	-0.898400
H	5.134200	-1.140700	-0.406800
H	3.237300	-2.338900	2.632200
H	4.382600	-1.104200	2.038200
H	2.650300	-1.002500	1.621800
H	5.822700	-2.869700	1.111800
H	4.726500	-4.123000	1.726200
H	5.212800	-4.119700	0.005300
Cl	-0.330200	0.889000	-2.102000
Cl	-0.330200	-0.889300	2.102400

Pre-reaction (isomer E)

C	-0.125100	3.028700	-0.034500
C	1.235100	3.053300	-0.514500
C	2.112100	1.947000	-0.388500
H	0.992300	5.108900	-1.129200
H	-0.625900	4.008000	-0.034300
C	1.685100	4.267700	-1.064100
C	3.447700	2.051300	-0.864500
C	3.834000	3.272300	-1.414200
C	2.981600	4.379600	-1.516200
H	4.851400	3.379200	-1.786900
H	3.345100	5.310700	-1.949500
O	1.652800	0.856700	0.210900
N	-0.811600	2.023100	0.407200
C	0.128500	-3.026800	-0.037200
C	-1.231500	-3.053200	-0.517500
C	-2.110400	-1.948800	-0.389500
H	-0.986100	-5.107900	-1.134500
H	0.630400	-4.005500	-0.037300
C	-1.680300	-4.267900	-1.067600
C	-3.446800	-2.055000	-0.862800
C	-3.831700	-3.276200	-1.412900
C	-2.977300	-4.381700	-1.517700
H	-4.849700	-3.384700	-1.783800
H	-3.339900	-5.313000	-1.951300
O	-1.651700	-0.858300	0.209700
N	0.813400	-2.020800	0.406500
Ti	-0.000800	0.001000	0.359700
C	2.143500	-2.359600	0.843500
C	2.521600	-2.169200	2.173800
C	3.030500	-2.949900	-0.061000
C	3.788300	-2.574800	2.589500
H	1.819000	-1.721600	2.873100
C	4.294500	-3.351400	0.365500
H	2.727800	-3.072100	-1.102500
C	4.676400	-3.167400	1.693100
H	4.076000	-2.432200	3.631700
H	4.983400	-3.805300	-0.348400
H	5.665000	-3.483500	2.027700
C	-2.142500	2.362600	0.841500
C	-3.028900	2.947100	-0.067300
C	-2.522000	2.178400	2.172300
C	-4.294300	3.348500	0.355400
H	-2.724400	3.065000	-1.108700
C	-3.790100	2.583700	2.584000
H	-1.819500	1.735800	2.874800
C	-4.677900	3.170100	1.683200
H	-4.982800	3.798000	-0.361500
H	-4.079200	2.445900	3.626500
H	-5.667700	3.485900	2.014800
C	-4.400700	-0.861800	-0.824600
C	-4.575700	-0.363100	0.618200
C	-3.820200	0.237100	-1.729400
C	-5.790700	-1.220900	-1.361200
H	-5.032100	-1.150300	1.239000
H	-3.620000	-0.075500	1.070900
H	-5.242200	0.513400	0.629500
H	-3.744500	-0.126900	-2.765800
H	-4.479100	1.119500	-1.714800
H	-2.816000	0.539200	-1.405500
H	-6.433000	-0.329900	-1.302800
H	-5.759600	-1.538300	-2.414400
H	-6.267100	-2.016300	-0.767800
C	4.400100	0.856800	-0.828800
C	4.578900	0.359900	0.614200
C	3.815600	-0.242400	-1.730600
C	5.788800	1.213400	-1.370100
H	5.039200	1.147100	1.232000
H	3.624000	0.075400	1.070400
H	5.243400	-0.518100	0.624800
H	3.737000	0.120700	-2.767100
H	4.473800	-1.125300	-1.717300
H	2.812200	-0.543500	-1.403400
H	6.429700	0.321300	-1.313700
H	5.754600	1.530600	-2.423400
H	6.268600	2.008200	-0.778700
Cl	-0.004700	0.001400	2.668500
Cl	-0.001600	0.003700	-1.971100

Ti-1_R_1

C	-1.110300	0.099900	2.406800
C	-2.445900	-0.381500	2.122000
C	-2.847700	-0.754900	0.816000
H	-3.055800	-0.123100	4.182000
H	-0.943700	0.440400	3.440400
C	-3.374500	-0.415500	3.179600
C	-4.185900	-1.128400	0.543000
C	-5.059300	-1.154200	1.630900
C	-4.672600	-0.813400	2.935400
H	-6.095300	-1.447500	1.467600
H	-5.401400	-0.854300	3.743900
O	-1.932300	-0.730100	-0.148700

N	-0.120400	0.196800	1.576400
C	1.485300	2.001800	-0.879100
C	2.745200	1.297200	-0.772500
C	2.835700	-0.114600	-0.701800
H	3.829900	3.164600	-0.819600
H	1.567000	3.088800	-1.021300
C	3.914500	2.076900	-0.779100
C	4.094600	-0.758900	-0.723200
C	5.222800	0.066100	-0.726700
C	5.150800	1.463300	-0.734300
H	6.210700	-0.392200	-0.727100
H	6.064700	2.055600	-0.730300
O	1.701300	-0.820400	-0.599400
N	0.290800	1.503300	-0.853400
Ti	-0.129600	-0.553600	-0.539200
C	-0.802600	2.385200	-1.147600
C	-1.910700	2.434000	-0.298200
C	-0.771400	3.165600	-2.307500
C	-2.972000	3.283900	-0.598800
H	-1.939300	1.817100	0.598100
C	-1.840300	4.009400	-2.601700
H	0.077400	3.088700	-2.989400
C	-2.940700	4.072900	-1.748200
H	-3.830300	3.325800	0.072400
H	-1.815000	4.613100	-3.509000
H	-3.776600	4.732100	-1.982400
C	1.068000	0.827400	2.079100
C	1.074900	2.207800	2.293700
C	2.221600	0.073500	2.294400
C	2.247900	2.833000	2.715500
H	0.167400	2.785900	2.104600
C	3.387100	0.704600	2.721900
H	2.208800	-1.000300	2.106400
C	3.405000	2.084400	2.926900
H	2.253700	3.910800	2.880600
H	4.288100	0.113700	2.891800
H	4.321400	2.575900	3.254600
C	4.211000	-2.287000	-0.770600
C	3.581200	-2.911100	0.485100
C	3.511100	-2.804300	-2.040600
C	5.672500	-2.744300	-0.828200
H	4.091000	-2.553700	1.393900
H	2.515900	-2.663200	0.560200
H	3.682600	-4.006700	0.450400
H	4.041200	-2.454200	-2.938800
H	3.517800	-3.905500	-2.051700
H	2.471100	-2.456700	-2.106800
H	5.702600	-3.841600	-0.887700
H	6.190600	-2.349400	-1.714200
H	6.233200	-2.444300	0.069500
C	-4.642000	-1.450500	-0.883700
C	-4.462400	-0.198200	-1.760500
C	-3.828400	-2.622500	-1.461400
C	-6.121500	-1.848600	-0.922000
H	-5.105000	0.619700	-1.400300
H	-3.422400	0.156000	-1.754900
H	-4.750400	-0.425600	-2.798600
H	-3.871200	-3.497400	-0.793700
H	-4.249500	-2.918600	-2.434000
H	-2.779200	-2.342600	-1.619000
H	-6.408700	-2.056500	-1.962300
H	-6.317800	-2.757000	-0.332700
H	-6.773500	-1.042900	-0.553800
C	-0.461100	-0.435200	-2.525900
H	-0.527600	-1.553100	-2.564600
H	-1.412200	-0.000600	-2.858300
H	0.389100	-0.100200	-3.134700
C	-0.055600	-3.319200	-0.415800
H	-0.926900	-3.547200	-1.036500
H	0.937400	-3.454200	-0.853400
C	-0.208500	-2.945100	0.863400
H	0.653600	-2.765800	1.512300
H	-1.201000	-2.846800	1.312000

Ti-1_TS$_1$

C	1.074300	-0.831700	2.332500
C	2.434000	-0.369200	2.132800
C	2.826700	0.363700	0.984600
H	3.090400	-1.362900	3.937600
H	0.942500	-1.569700	3.137900
C	3.402500	-0.785600	3.065100
C	4.187300	0.688100	0.763100
C	5.101300	0.257700	1.725900
C	4.730300	-0.467300	2.866100
H	6.156400	0.490000	1.590700
H	5.489300	-0.780800	3.581800
O	1.883200	0.727400	0.113400
N	0.027600	-0.508900	1.644300
C	-1.235400	-1.650500	-1.462800
C	-2.578600	-1.193500	-1.197900
C	-2.837400	0.124100	-0.748900
H	-3.428400	-3.079500	-1.828300
H	-1.157700	-2.609400	-1.996900
C	-3.644200	-2.065100	-1.487000
C	-4.165600	0.613500	-0.671900
C	-5.182600	-0.299000	-0.954200
C	-4.943500	-1.627300	-1.334800
H	-6.218700	0.030000	-0.887600
H	-5.781800	-2.291600	-1.540800
O	-1.797300	0.884200	-0.415500
N	-0.126300	-1.041200	-1.172700
Ti	0.049900	0.834100	-0.113700
C	1.076100	-1.623000	-1.707700
C	2.012700	-2.214600	-0.858700
C	1.307300	-1.565700	-3.083200
C	3.175500	-2.762200	-1.392600
H	1.824900	-2.250200	0.213700
C	2.478000	-2.112300	-3.609900
H	0.572100	-1.088200	-3.734100
C	3.411000	-2.712800	-2.767700
H	3.902200	-3.229900	-0.727300
H	2.656100	-2.068400	-4.684500
H	4.324400	-3.140600	-3.181500
C	-1.157200	-1.283700	1.876600
C	-1.107000	-2.674100	1.727400
C	-2.367200	-0.658900	2.181100
C	-2.266100	-3.432000	1.880600
H	-0.163300	-3.155200	1.461000
C	-3.520900	-1.423000	2.335100
H	-2.410000	0.424100	2.285100
C	-3.476100	-2.808400	2.180300
H	-2.221400	-4.514600	1.758300
H	-4.463700	-0.928500	2.572800
H	-4.384700	-3.400600	2.291800
C	-4.463500	2.078600	-0.328800
C	-3.954600	2.422100	1.079600
C	-3.780200	2.989300	-1.364000
C	-5.967100	2.372200	-0.364200
H	-4.423300	1.773200	1.836200
H	-2.865100	2.309300	1.141600
H	-4.209000	3.464600	1.325100
H	-4.167700	2.788100	-2.373900
H	-3.982800	4.044900	-1.125300
H	-2.693100	2.832200	-1.374500
H	-6.130800	3.435100	-0.137200
H	-6.400700	2.172200	-1.354900
H	-6.517000	1.784000	0.385400
C	4.617700	1.506000	-0.459100
C	4.212500	0.785800	-1.757300
C	3.968200	2.898800	-0.371300
C	6.136600	1.707600	-0.500800
H	4.728400	-0.183300	-1.830500
H	3.132600	0.596500	-1.817100
H	4.511200	1.394900	-2.624400
H	4.363400	3.452600	0.493800
H	4.192600	3.479100	-1.279700
H	2.879300	2.822500	-0.258800
H	6.395000	2.298700	-1.390700
H	6.504700	2.255800	0.378900
H	6.673900	0.750000	-0.569300
C	0.312100	2.490000	-1.414600
H	1.295900	2.951600	-1.537600
H	0.343700	1.508900	-1.982700
H	-0.482800	3.080900	-1.879900
C	-0.105600	3.224400	0.547600
H	0.776500	3.847200	0.395400
H	-1.057900	3.640000	0.211300
C	-0.115100	2.286900	1.579100
H	-1.059800	2.027000	2.056200
H	0.795700	2.112600	2.157800

Ti-1_P$_1$

C	-0.826800	2.663800	-0.417100
C	-2.225600	2.422900	-0.220300
C	-2.697800	1.219300	0.362800
H	-2.760000	4.330600	-1.102500
H	-0.578300	3.630500	-0.877900
C	-3.137700	3.409900	-0.653800
C	-4.084100	1.006100	0.568300
C	-4.936400	2.006200	0.104000
C	-4.488300	3.190900	-0.507200
H	-6.011100	1.876500	0.224900
H	-5.211500	3.931800	-0.845200
O	-1.788700	0.321900	0.707100
N	0.183400	1.869600	-0.161000
C	0.960900	-1.906400	-1.654100
C	2.351500	-1.816700	-1.287000
C	2.778000	-1.080000	-0.155400
H	2.958700	-3.029100	-2.977200
H	0.751600	-2.491100	-2.561500
C	3.296800	-2.467100	-2.104400
C	4.144600	-1.022300	0.206500
C	5.036500	-1.675100	-0.645200
C	4.636400	-2.382000	-1.790000
H	6.100300	-1.646800	-0.414100
H	5.384700	-2.870600	-2.412700
O	1.839000	-0.455400	0.547400
N	-0.065300	-1.363500	-1.064000
Ti	0.033800	-0.064700	0.643600
C	4.598800	-0.334900	1.498600
C	4.150700	1.135600	1.531000
C	3.993200	-1.097000	2.690200
C	6.124000	-0.364600	1.641300
H	4.483300	1.668300	0.627400
H	3.060300	1.229200	1.602300
H	4.596000	1.633300	2.406100
H	4.373500	-2.128900	2.727200
H	4.264800	-0.596700	3.632400
H	2.897200	-1.134300	2.620800
H	6.404800	0.126700	2.583500
H	6.515100	-1.392000	1.675200
H	6.621100	0.174900	0.821100
C	-4.599200	-0.218100	1.332300
C	-4.119100	-1.529300	0.688900
C	-4.085400	-0.118900	2.779300
C	-6.130500	-0.251700	1.371800
H	-4.441000	-1.594300	-0.361300
H	-3.026900	-1.625900	0.718200

H	-4.556200	-2.381200	1.232900
H	-4.486000	0.778500	3.274300
H	-4.407700	-1.000200	3.355700
H	-2.988200	-0.066400	2.805700
H	-6.454100	-1.140100	1.932400
H	-6.551200	0.628800	1.878900
H	-6.562600	-0.317300	0.361700
C	0.038400	-0.537800	2.629100
H	1.004800	-0.313800	3.095800
H	-0.799700	-0.061600	3.153800
C	3.901100	3.402000	-1.458800
C	3.384700	2.232000	-2.018500
C	3.204400	4.053000	-0.442000
C	2.169100	1.722100	-1.571900
H	3.923600	1.716900	-2.814300
C	1.987000	3.546400	0.014200
H	3.608400	4.962400	0.003300
C	1.471900	2.385500	-0.561900
H	1.742300	0.821800	-2.017500
H	1.441400	4.044100	0.818000
C	-3.754900	-2.103400	-2.977900
C	-3.262700	-0.800600	-2.879500
C	-3.043000	-3.160800	-2.414400
C	-2.056000	-0.555300	-2.230300
H	-3.815300	0.030400	-3.319600
C	-1.832000	-2.924300	-1.763700
H	-3.428200	-4.178500	-2.481300
C	-1.338900	-1.621400	-1.685700
H	-1.649700	0.455900	-2.164700
H	-1.269700	-3.744800	-1.313100
C	-0.196600	-1.987700	2.272800
H	-0.581500	-2.070300	1.209500
H	0.756100	-2.536900	2.242400
C	-1.237000	-2.709600	3.130100
H	-0.897500	-2.747300	4.173900
H	-2.198900	-2.180600	3.099700
H	4.849900	3.804400	-1.814300
H	-4.697600	-2.293100	-3.491400
H	-1.394400	-3.738100	2.778000

Ti-1_A_2

C	-1.329600	-1.366500	-2.195700
C	-2.699100	-1.053200	-1.876200
C	-3.034300	-0.238700	-0.768600
H	-3.431800	-2.111800	-3.616400
H	-1.169200	-1.859700	-3.165700
C	-3.704600	-1.496400	-2.757300
C	-4.370900	0.156400	-0.530400
C	-5.326800	-0.326100	-1.426100
C	-5.016300	-1.142600	-2.523600
H	-6.370500	-0.055000	-1.274700
H	-5.809700	-1.481100	-3.188500
O	-2.042300	0.162800	0.030700
N	-0.271800	-1.096700	-1.489800
C	2.721600	-0.608900	0.588900
C	3.031800	0.775900	0.308600
C	2.050200	1.786800	0.166500
H	5.150500	0.341500	0.305800
H	3.602900	-1.254700	0.688300
C	4.392800	1.119600	0.198500
C	2.398000	3.133800	-0.068200
C	3.763800	3.412300	-0.163900
C	4.755100	2.430200	-0.037700
H	4.080400	4.438000	-0.346000
H	5.805400	2.706600	-0.121400
O	0.757200	1.431800	0.240700
N	1.550300	-1.150000	0.735600
Ti	-0.257400	-0.048500	0.412000
C	1.446500	-2.516700	1.145900
C	0.231000	-3.176500	0.928300
C	2.474200	-3.190000	1.818600
C	0.058100	-4.497400	1.332200
H	-0.597800	-2.671500	0.422800
C	2.298600	-4.512400	2.214600
H	3.402200	-2.680800	2.077200
C	1.096500	-5.174600	1.968400
H	-0.894900	-4.994900	1.151900
H	3.105700	-5.022700	2.740300
H	0.963300	-6.207600	2.289200
C	0.993800	-1.402100	-2.105600
C	1.423700	-2.722700	-2.239300
C	1.796900	-0.341800	-2.528800
C	2.679000	-2.978200	-2.789100
H	0.786700	-3.539800	-1.896800
C	3.048600	-0.608600	-3.080400
H	1.436600	0.684100	-2.420600
C	3.494100	-1.924700	-3.204300
H	3.020100	-4.008500	-2.893500
H	3.676300	0.218800	-3.413300
H	4.474200	-2.130100	-3.635400
C	1.324500	4.219500	-0.212800
C	0.421800	3.905100	-1.420000
C	0.489800	4.303500	1.078000
C	1.956200	5.596000	-0.449800
H	1.018300	3.852300	-2.344000
H	-0.122300	2.959500	-1.296600
H	-0.319600	4.708800	-1.543600
H	1.129700	4.559100	1.935800
H	-0.268800	5.093600	0.972900
H	-0.027600	3.360900	1.297300
H	1.157300	6.345100	-0.540000
H	2.603100	5.899200	0.386700
H	2.544400	5.624400	-1.379100
C	-4.740400	1.057400	0.653100
C	-4.382900	0.348500	1.970300
C	-3.994700	2.399600	0.545100
C	-6.242400	1.361300	0.678000
H	-4.942400	-0.594500	2.065600
H	-3.310800	0.124200	2.033300
H	-4.651700	0.991100	2.822300
H	-4.261700	2.916800	-0.388900
H	-4.284100	3.047400	1.386400
H	-2.905300	2.270100	0.570800
H	-6.460300	2.012600	1.536100
H	-6.569500	1.888000	-0.230900
H	-6.845600	0.448500	0.793400
C	-0.547800	-0.262800	2.417900
C	0.609900	-0.173800	3.401000
H	1.314600	0.613000	3.079100
H	1.167500	-1.123800	3.395200
C	0.129100	0.124100	4.821500
H	0.974700	0.168600	5.522200
H	-0.399400	1.088000	4.865700
H	-0.562800	-0.656100	5.171500
H	-1.154000	0.674500	2.447000
H	-1.235300	-1.098500	2.637800

Ti-1_R_2

C	1.197300	0.574800	-2.526200
C	2.525400	0.041700	-2.305500
C	2.902900	-0.560300	-1.079400
H	3.167200	0.653200	-4.278800
H	1.054500	1.097000	-3.484700
C	3.469700	0.184900	-3.340000
C	4.235300	-0.989100	-0.861000
C	5.123500	-0.835800	-1.925800
C	4.760000	-0.266000	-3.154700
H	6.153900	-1.166300	-1.804400
H	5.500300	-0.170900	-3.947900
O	1.975300	-0.692300	-0.135500
N	0.188400	0.520200	-1.716300
C	-1.491700	1.877700	0.963500
C	-2.743700	1.196100	0.713100
C	-2.823500	-0.186100	0.415700
H	-3.840900	3.029400	1.033700
H	-1.590100	2.927800	1.272700
C	-3.917700	1.961700	0.819400
C	-4.079300	-0.829900	0.315200
C	-5.212600	-0.020100	0.427300
C	-5.149200	1.359200	0.654700
H	-6.197200	-0.476300	0.336300
H	-6.066900	1.941800	0.724100
O	-1.683700	-0.861000	0.227400
N	-0.290600	1.397500	0.893100
Ti	0.154000	-0.583700	0.234000
C	0.779100	2.233100	1.358000
C	1.947600	2.360000	0.601700
C	0.667300	2.898000	2.584800
C	2.989300	3.157900	1.067800
H	2.038100	1.849000	-0.354900
C	1.716400	3.690900	3.044000
H	-0.234100	2.778900	3.188700
C	2.879900	3.822600	2.288500
H	3.894500	3.257400	0.467600
H	1.623400	4.199900	4.003700
H	3.701400	4.440300	2.651500
C	-0.993500	1.223200	-2.129400
C	-1.009700	2.619600	-2.105800
C	-2.135600	0.509900	-2.495200
C	-2.179900	3.300100	-2.441600
H	-0.112000	3.162800	-1.801600
C	-3.298200	1.197100	-2.835200
H	-2.115900	-0.580100	-2.492800
C	-3.325200	2.591600	-2.803400
H	-2.193000	4.390300	-2.421100
H	-4.189500	0.637200	-3.120900
H	-4.238800	3.126700	-3.062500
C	-4.185900	-2.346300	0.116700
C	-3.549300	-2.752100	-1.222100
C	-3.484900	-3.060600	1.286900
C	-5.644600	-2.815600	0.094600
H	-4.058100	-2.249000	-2.059400
H	-2.484800	-2.490600	-1.250500
H	-3.645700	-3.838800	-1.371100
H	-4.002700	-2.844000	2.233600
H	-3.508700	-4.150200	1.129700
H	-2.438200	-2.743500	1.392400
H	-5.667800	-3.908200	-0.023900
H	-6.168800	-2.570600	1.029900
H	-6.203500	-2.378400	-0.746200
C	4.672700	-1.555300	0.494400
C	4.499300	-0.465200	1.567700
C	3.839300	-2.796300	0.860600
C	6.146800	-1.974400	0.477400
H	5.166200	0.386100	1.362300
H	3.467200	-0.089400	1.602200
H	4.760700	-0.870600	2.557600
H	3.887400	-3.550600	0.059400
H	4.241900	-3.251200	1.778100
H	2.789800	-2.534700	1.044600
H	6.422200	-2.358900	1.469600
H	6.337200	-2.772300	-0.256000
H	6.811300	-1.126600	0.255300
C	0.450600	-0.813200	2.210600
C	-0.596900	-0.551100	3.268000
H	-1.604700	-0.711000	2.852500
H	-0.531500	0.512000	3.550800
C	-0.402000	-1.419900	4.512300

H	-1.157500	-1.185400	5.274900
H	-0.493600	-2.488100	4.264100
H	0.592100	-1.259100	4.954500
H	0.436100	-1.863900	1.885500
H	1.477000	-0.578400	2.531600
C	0.101600	-3.289600	-0.411300
H	0.978700	-3.628800	0.147000
H	-0.887200	-3.526200	-0.007900
C	0.240500	-2.659600	-1.587300
H	-0.629100	-2.368000	-2.181800
H	1.228600	-2.462100	-2.012600

Ti-1_TS_2

C	-1.011300	-2.022200	-1.757200
C	-2.383900	-1.560800	-1.814100
C	-2.814200	-0.396400	-1.133400
H	-2.975900	-3.280600	-2.983400
H	-0.841800	-3.041900	-2.134900
C	-3.320100	-2.378500	-2.473400
C	-4.184700	-0.035600	-1.114300
C	-5.067400	-0.879300	-1.789400
C	-4.656900	-2.036600	-2.464800
H	-6.128500	-0.634100	-1.797300
H	-5.392400	-2.658300	-2.973400
O	-1.899600	0.341700	-0.504100
N	0.007700	-1.388600	-1.273900
C	1.228000	-0.947800	2.050000
C	2.568200	-0.663100	1.596300
C	2.831100	0.274700	0.565500
H	3.398000	-2.030200	3.051400
H	1.157800	-1.541400	2.973800
C	3.625100	-1.310400	2.262400
C	4.171200	0.621100	0.242100
C	5.176500	-0.067200	0.923100
C	4.927400	-1.033400	1.906900
H	6.216200	0.156400	0.690200
H	5.759000	-1.534400	2.400400
O	1.788900	0.812500	-0.069000
N	0.114500	-0.570000	1.502000
C	-1.089900	-0.860100	2.231900
C	-2.018500	-1.766400	1.717000
C	-1.335500	-0.208400	3.441900
C	-3.186000	-2.032900	2.425300
H	-1.821100	-2.259200	0.765700
C	-2.512200	-0.475800	4.142700
H	-0.608000	0.509700	3.825900
C	-3.435800	-1.388700	3.638500
H	-3.905200	-2.748400	2.025300
H	-2.702600	0.032200	5.088400
H	-4.352600	-1.598700	4.189800
C	1.208100	-2.158000	-1.117900
C	1.193400	-3.294400	-0.301800
C	2.392600	-1.752700	-1.730200
C	2.367300	-4.016400	-0.097200
H	0.265700	-3.589500	0.193600
C	3.562200	-2.478500	-1.521000
H	2.398300	-0.869000	-2.365500
C	3.555400	-3.606800	-0.700800
H	2.352500	-4.899700	0.541900
H	4.486800	-2.159500	-2.004200
H	4.475700	-4.167000	-0.534200
C	4.516100	1.713700	-0.780400
C	3.979100	1.352800	-2.172700
C	3.892700	3.042600	-0.329500
C	6.029500	1.920700	-0.904300
H	4.406800	0.403000	-2.529700
H	2.885600	1.268700	-2.155500
H	4.253600	2.138600	-2.893100
H	4.264200	3.336800	0.663800
H	4.149400	3.840700	-1.043100
H	2.800900	2.953600	-0.282000
H	6.221500	2.721600	-1.632100
H	6.481400	2.222600	0.051800
H	6.540900	1.015300	-1.263900
C	-4.651800	1.253900	-0.432000
C	-4.254700	1.259900	1.055500
C	-4.029000	2.445100	-1.183800
C	-6.174700	1.413600	-0.497200
H	-4.753200	0.433200	1.584000
H	-3.173300	1.150000	1.207200
H	-4.583400	2.203300	1.519000
H	-4.465900	2.532200	-2.189900
H	-4.225300	3.384700	-0.643600
H	-2.944500	2.320600	-1.302300
H	-6.457400	2.352700	-0.000300
H	-6.540000	1.463800	-1.533200
H	-6.693200	0.592700	0.019800
C	-0.500500	2.632300	0.196100
H	-1.576200	2.788500	0.045700
H	-0.413400	1.963100	1.064800
C	0.214500	3.914100	0.558800
H	0.148600	4.618800	-0.284800
H	1.279800	3.716100	0.740600
C	-0.417000	4.552700	1.798800
H	-0.349800	3.883200	2.669500
H	0.098900	5.488200	2.053100
H	-1.478800	4.782600	1.627500
Ti	-0.074100	0.611900	-0.295200
C	0.087300	2.469100	-1.904300
H	-0.784800	3.112100	-2.034900
H	1.038100	2.972100	-1.710800
C	0.101500	1.196600	-2.461600
H	1.049800	0.746400	-2.752900
H	-0.802600	0.793300	-2.925200

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C	-1.001700	-1.205000	2.191700
C	-2.381300	-1.345700	1.799000
C	-2.820400	-1.022400	0.492600
H	-2.947900	-2.070000	3.760200
H	-0.776000	-1.496500	3.227600
C	-3.297300	-1.826500	2.755000
C	-4.165400	-1.227900	0.103000
C	-5.029900	-1.697500	1.093000
C	-4.621200	-1.985900	2.404200
H	-6.077200	-1.860400	0.842800
H	-5.346900	-2.352500	3.128900
O	-1.912900	-0.532200	-0.346400
N	-0.002700	-0.770500	1.479500
C	0.402500	2.979000	-0.168800
C	1.827400	2.839000	-0.239000
C	2.434000	1.588500	-0.517600
H	2.142600	4.939600	0.198100
H	0.040000	4.000600	0.014600
C	2.623700	3.983300	-0.015800
C	3.842400	1.474100	-0.636600
C	4.577400	2.631000	-0.385400
C	3.994400	3.871000	-0.067900
H	5.664000	2.585300	-0.446700
H	4.630600	4.736200	0.114100
O	1.628400	0.550600	-0.669000
N	-0.515100	2.049600	-0.266200
Ti	-0.148100	-0.005600	-0.523100
C	-1.868900	2.530800	-0.115600
C	-2.602600	2.148400	1.007400
C	-2.412400	3.400400	-1.060700
C	-3.885500	2.657000	1.193500
H	-2.154600	1.473600	1.739300
C	-3.698200	3.904800	-0.866500
H	-1.831100	3.674900	-1.942700
C	-4.432300	3.540400	0.260800
H	-4.455800	2.368900	2.077200
H	-4.123800	4.588800	-1.601000
H	-5.434200	3.943000	0.411800
C	1.274000	-0.769300	2.145300
C	1.863300	-1.975200	2.527200
C	1.899600	0.447600	2.418100
C	3.082500	-1.957100	3.204800
H	1.365700	-2.918900	2.294200
C	3.115700	0.456100	3.096100
H	1.417500	1.380100	2.118300
C	3.705800	-0.744600	3.494600
H	3.542700	-2.897400	3.510000
H	3.599300	1.407700	3.320100
H	4.654800	-0.734200	4.031200
C	4.499700	0.170800	-1.100700
C	4.120600	-1.006700	-0.187700
C	4.037200	-0.097300	-2.543700
C	6.027700	0.282100	-1.105400
H	4.453800	-0.822200	0.844500
H	3.038200	-1.185600	-0.170800
H	4.616800	-1.922500	-0.547500
H	4.375800	0.706100	-3.214900
H	4.459900	-1.047500	-2.906900
H	2.941900	-0.158100	-2.604700
H	6.455200	-0.672300	-1.444100
H	6.383400	1.064400	-1.791900
H	6.424300	0.488800	-0.099900
C	-4.619700	-1.009800	-1.344000
C	-4.343900	0.432700	-1.797000
C	-3.862000	-2.001800	-2.243900
C	-6.120100	-1.273900	-1.506900
H	-4.830500	1.153800	-1.123300
H	-3.270500	0.656100	-1.821500
H	-4.751000	0.581600	-2.808900
H	-4.123200	-3.039300	-1.986700
H	-4.129500	-1.831400	-3.298000
H	-2.774900	-1.883000	-2.138100
H	-6.399400	-1.110300	-2.557400
H	-6.386900	-2.309800	-1.251100
H	-6.724500	-0.591800	-0.890300
C	-0.009700	-1.006300	-2.298500
H	0.782700	-0.587000	-2.931100
C	0.397400	-2.237900	-1.530200
H	-0.461300	-2.908300	-1.370300
C	1.610800	-3.001000	-2.068700
H	1.335200	-3.446200	-3.038300
H	2.423800	-2.285200	-2.267400
H	-0.977000	-1.054200	-2.810900
C	2.102600	-4.080200	-1.111200
H	1.272000	-4.766000	-0.872500
H	2.400500	-3.602400	-0.159900
C	3.277900	-4.866800	-1.680100
H	4.122700	-4.199300	-1.910800
H	3.633300	-5.627800	-0.972400
H	2.994700	-5.378800	-2.611700
H	0.701100	-1.958100	-0.469800

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C	-1.172100	0.512400	2.453500
C	-2.538000	0.106700	2.195300
C	-2.959900	-0.441500	0.955100
H	-3.156800	0.812200	4.145400
H	-1.036700	1.136700	3.350400
C	-3.489500	0.381400	3.198800
C	-4.330300	-0.701200	0.704100
C	-5.220500	-0.426700	1.742100

C	-4.821200	0.102200	2.978700
H	-6.280700	-0.626500	1.593900
H	-5.564500	0.296000	3.750800
O	-2.037300	-0.693400	0.032000
N	-0.113500	0.262900	1.743500
C	1.357700	1.916400	-1.211600
C	2.689800	1.420600	-0.965100
C	2.969100	0.047300	-0.738600
H	3.513600	3.406900	-1.204100
H	1.306600	2.963800	-1.546000
C	3.743800	2.353500	-1.032700
C	4.308700	-0.411600	-0.663400
C	5.307800	0.560200	-0.719900
C	5.046100	1.928900	-0.880600
H	6.349000	0.249500	-0.645700
H	5.871200	2.638900	-0.916900
O	1.940800	-0.786000	-0.612000
N	0.226200	1.279900	-1.110700
C	-0.947800	1.981700	-1.559300
C	-1.946400	2.327100	-0.646400
C	-1.096400	2.275500	-2.916000
C	-3.090500	2.980300	-1.094500
H	-1.822200	2.084500	0.408800
C	-2.250000	2.923500	-3.357100
H	-0.315600	1.981600	-3.619900
C	-3.246100	3.276700	-2.449700
H	-3.867000	3.254800	-0.379500
H	-2.367700	3.149600	-4.417100
H	-4.147200	3.782100	-2.798000
C	1.080000	0.980600	2.090300
C	1.060800	2.378700	2.161100
C	2.275200	0.288600	2.288900
C	2.235700	3.074300	2.441000
H	0.130200	2.917400	1.968700
C	3.444600	0.990500	2.569300
H	2.292900	-0.798600	2.218700
C	3.429300	2.382900	2.644700
H	2.216400	4.163300	2.493700
H	4.374400	0.443700	2.730100
H	4.348500	2.928300	2.858700
C	4.640200	-1.905400	-0.551500
C	4.059500	-2.496200	0.743000
C	4.060600	-2.648900	-1.767500
C	6.153900	-2.146200	-0.534000
H	4.449500	-1.968400	1.627700
H	2.964000	-2.435200	0.744100
H	4.345100	-3.555500	0.829800
H	4.483900	-2.252400	-2.702300
H	4.313700	-3.718500	-1.705600
H	2.967800	-2.551200	-1.812100
H	6.344800	-3.226700	-0.470900
H	6.637000	-1.775500	-1.450000
H	6.636800	-1.672000	0.333500
C	-4.794300	-1.273300	-0.641600
C	-4.442000	-0.295800	-1.776900
C	-4.130800	-2.641100	-0.885300
C	-6.312100	-1.486400	-0.666400
H	-4.990000	0.650600	-1.651500
H	-3.368300	-0.064700	-1.810200
H	-4.737600	-0.732300	-2.743700
H	-4.374200	-3.339700	-0.069900
H	-4.509200	-3.071100	-1.825300
H	-3.039700	-2.551200	-0.962200
H	-6.601200	-1.886200	-1.648800
H	-6.639300	-2.208400	0.096500
H	-6.860100	-0.544200	-0.517500
C	-0.350500	-2.404200	-1.908500
H	-0.800200	-1.494600	-2.414600
H	0.631200	-2.588000	-2.376100
H	-1.030600	-3.233500	-2.130900
Zr	-0.066500	-0.861300	-0.329000
C	-0.142500	-3.541000	0.251800
H	-1.154600	-3.884300	0.031900
H	0.674000	-4.026600	-0.286300
C	0.095600	-2.732000	1.321400
H	1.114600	-2.573100	1.683300
H	-0.726400	-2.425300	1.974600

Zr-1_TS$_1$

C	-1.171800	0.573000	2.436900
C	-2.538600	0.163100	2.187600
C	-2.961500	-0.415300	0.962000
H	-3.154900	0.913400	4.121300
H	-1.031100	1.198700	3.331700
C	-3.488900	0.460700	3.185400
C	-4.332000	-0.680900	0.719600
C	-5.222100	-0.380400	1.750500
C	-4.821300	0.177900	2.973300
H	-6.282400	-0.582700	1.607600
H	-5.563700	0.390900	3.741300
O	-2.041900	-0.691200	0.041700
N	-0.118700	0.326200	1.719800
C	1.362300	1.892400	-1.260300
C	2.693200	1.397400	-0.998700
C	2.969600	0.028600	-0.743800
H	3.519900	3.375600	-1.282900
H	1.317000	2.924900	-1.639500
C	3.748500	2.326000	-1.087200
C	4.308900	-0.429500	-0.654200
C	5.309800	0.539100	-0.730600
C	5.050300	1.903600	-0.924000
H	6.350300	0.228800	-0.646700
H	5.876400	2.611500	-0.975900
O	1.940800	-0.803500	-0.605500
N	0.230800	1.266000	-1.125000
C	-0.943200	1.948200	-1.600300
C	-1.946400	2.314600	-0.700500
C	-1.090600	2.205600	-2.965100
C	-3.089600	2.955300	-1.167600
H	-1.824500	2.099600	0.361000
C	-2.244000	2.840900	-3.425700
H	-0.307600	1.895400	-3.659800
C	-3.242200	3.217700	-2.530100
H	-3.867800	3.247500	-0.461400
H	-2.359400	3.039400	-4.491500
H	-4.142300	3.714300	-2.893200
C	1.079300	1.038900	2.060800
C	1.064900	2.437600	2.102100
C	2.269400	0.343800	2.279200
C	2.241700	3.134400	2.368200
H	0.136100	2.974300	1.896400
C	3.441100	1.048000	2.545900
H	2.278500	-0.745000	2.234400
C	3.431900	2.441900	2.588400
H	2.227100	4.224300	2.396900
H	4.368600	0.501700	2.721600
H	4.353300	2.988000	2.790800
C	4.639200	-1.920500	-0.504500
C	4.056900	-2.477400	0.804000
C	4.061000	-2.694800	-1.701800
C	6.152600	-2.162600	-0.480300
H	4.452100	-1.931100	1.675000
H	2.962200	-2.408200	0.806500
H	4.336400	-3.536200	0.915600
H	4.482400	-2.320300	-2.646500
H	4.315700	-3.762200	-1.614000
H	2.968000	-2.600600	-1.747400
H	6.342200	-3.241400	-0.389500
H	6.636900	-1.815500	-1.404900
H	6.635200	-1.667300	0.375400
C	-4.795900	-1.284900	-0.612100
C	-4.442900	-0.335400	-1.770900
C	-4.135600	-2.659700	-0.822500
C	-6.313800	-1.497200	-0.632400
H	-4.991300	0.613400	-1.668700
H	-3.369700	-0.102600	-1.808800
H	-4.738300	-0.794800	-2.727200
H	-4.382000	-3.338500	0.008600
H	-4.512500	-3.110900	-1.753100
H	-3.043800	-2.576100	-0.896700
H	-6.603500	-1.920300	-1.604800
H	-6.641900	-2.199800	0.148000
H	-6.860500	-0.551000	-0.506400
C	-0.346000	-2.580200	-1.754300
H	-0.965700	-1.727000	-2.158600
H	0.658900	-2.545800	-2.209300
H	-0.866300	-3.480400	-2.091600
Zr	-0.065000	-0.871900	-0.282700
C	-0.173200	-3.469600	0.197700
H	-1.176100	-3.886100	0.090300
H	0.634800	-4.064600	-0.234500
C	0.095900	-2.626000	1.284600
H	1.111600	-2.588700	1.684700
H	-0.714600	-2.404200	1.984800

Zr-1_P$_1$

C	-0.945100	2.728800	-0.475400
C	-2.346600	2.448200	-0.314200
C	-2.828800	1.261400	0.299100
H	-2.873400	4.314000	-1.283600
H	-0.720400	3.690500	-0.960300
C	-3.256600	3.406400	-0.813200
C	-4.220500	1.043100	0.459600
C	-5.068300	2.017900	-0.064400
C	-4.610300	3.183200	-0.702000
H	-6.145100	1.882400	0.029000
H	-5.326700	3.906700	-1.088300
O	-1.933000	0.381400	0.721400
N	0.084700	1.986400	-0.162000
C	1.137000	-1.888300	-1.742100
C	2.521100	-1.745800	-1.366900
C	2.937300	-1.046800	-0.202500
H	3.149500	-2.866700	-3.111900
H	0.962300	-2.454900	-2.669000
C	3.480600	-2.333900	-2.218300
C	4.309200	-0.966000	0.142900
C	5.209400	-1.562000	-0.740400
C	4.819200	-2.230500	-1.911700
H	6.273800	-1.518200	-0.514100
H	5.573500	-2.674300	-2.559900
O	1.994600	-0.487900	0.547500
N	0.077000	-1.417900	-1.146400
C	4.766600	-0.293900	1.443100
C	4.393300	1.197200	1.432300
C	4.111300	-1.004200	2.641100
C	6.285600	-0.393300	1.620800
H	4.923700	1.720900	0.623500
H	3.315500	1.351200	1.290400
H	4.688900	1.658200	2.387600
H	4.382400	-2.070800	2.654100
H	4.468000	-0.551700	3.578700
H	3.017700	-0.921700	2.611800
H	6.566600	0.093400	2.565500
H	6.625300	-1.438600	1.669400
H	6.828600	0.116500	0.811200
C	-4.748900	-0.173700	1.227600
C	-4.311800	-1.484300	0.551700
C	-4.224400	-0.104000	2.673000

C	-6.280200	-0.177100	1.289500
H	-4.760000	-1.569300	-0.449200
H	-3.221100	-1.558300	0.443600
H	-4.659900	-2.340000	1.151700
H	-4.588200	0.807300	3.171200
H	-4.589100	-0.971700	3.244900
H	-3.127000	-0.099700	2.705500
H	-6.612700	-1.060800	1.852500
H	-6.673000	0.711800	1.804800
H	-6.730800	-0.231900	0.287100
C	-0.059900	-0.871200	2.795900
H	0.881100	-0.839900	3.359600
H	-0.880000	-0.426200	3.380200
C	3.845700	3.523100	-1.318500
C	3.358600	2.343300	-1.883900
C	3.098600	4.191900	-0.350900
C	2.122500	1.841200	-1.490000
H	3.938200	1.812800	-2.640100
C	1.858100	3.694900	0.050800
H	3.480400	5.109400	0.097500
C	1.372900	2.522900	-0.529500
H	1.722800	0.929100	-1.938800
H	1.271700	4.207400	0.815600
C	-3.635700	-2.196800	-2.993900
C	-3.173400	-0.885900	-2.866400
C	-2.879000	-3.255200	-2.494500
C	-1.950900	-0.633400	-2.251200
H	-3.763700	-0.053300	-3.251100
C	-1.651600	-3.012400	-1.877800
H	-3.242800	-4.279000	-2.584100
C	-1.189000	-1.700300	-1.770000
H	-1.571400	0.387000	-2.159300
H	-1.054300	-3.833100	-1.475300
C	-0.406900	-2.242500	2.244700
H	0.481100	-2.892300	2.226400
C	-1.595700	-2.943400	2.901200
H	-1.364100	-3.149200	3.954900
H	-2.488200	-2.304200	2.862900
H	4.812700	3.918500	-1.630500
H	-4.592600	-2.392100	-3.478500
H	-1.826600	-3.894600	2.401700
Zr	0.026300	-0.117900	0.732700
H	-0.692000	-2.188900	1.137400

Zr-1_A_2

C	-1.334000	-1.393600	-2.332600
C	-2.713000	-1.233000	-1.955900
C	-3.106900	-0.513700	-0.796100
H	-3.370300	-2.255000	-3.749200
H	-1.165800	-1.777200	-3.350300
C	-3.687900	-1.717100	-2.853900
C	-4.475000	-0.262900	-0.531500
C	-5.392200	-0.784200	-1.445100
C	-5.022600	-1.506000	-2.590600
H	-6.454600	-0.621600	-1.271100
H	-5.789000	-1.880900	-3.267300
O	-2.153700	-0.067800	0.020900
N	-0.271200	-1.089500	-1.640900
C	3.013200	-0.101800	0.400100
C	3.012100	1.327800	0.197200
C	1.855700	2.145800	0.298200
H	5.147300	1.290600	-0.149200
H	4.012100	-0.560200	0.400600
C	4.259500	1.922700	-0.085900
C	1.928700	3.544300	0.101100
C	3.189500	4.069700	-0.186400
C	4.347300	3.284100	-0.279500
H	3.288800	5.142400	-0.344200
H	5.305600	3.753700	-0.497500
O	0.682500	1.567700	0.587300
N	1.991400	-0.890500	0.568800
C	2.216500	-2.262300	0.896700
C	1.222100	-3.186600	0.559600
C	3.329200	-2.688200	1.629900
C	1.344100	-4.523100	0.927900
H	0.345300	-2.873900	-0.017900
C	3.454400	-4.029100	1.983300
H	4.073100	-1.969500	1.975100
C	2.467200	-4.950200	1.634800
H	0.560000	-5.231700	0.660100
H	4.321300	-4.349600	2.561500
H	2.564900	-5.995500	1.927400
C	0.993200	-1.153000	-2.327400
C	1.579200	-2.373200	-2.664500
C	1.644600	0.052200	-2.600300
C	2.837000	-2.381500	-3.265200
H	1.060700	-3.307200	-2.442400
C	2.901300	0.033200	-3.201600
H	1.162100	1.000300	-2.344400
C	3.501400	-1.183100	-3.527400
H	3.300600	-3.332700	-3.527900
H	3.409000	0.974300	-3.416600
H	4.484700	-1.198400	-3.998200
C	0.676300	4.427000	0.184800
C	-0.338200	3.995300	-0.890000
C	0.052400	4.331500	1.588300
C	1.015700	5.900200	-0.070900
H	0.104600	4.079500	-1.894700
H	-0.688100	2.964700	-0.744100
H	-1.217300	4.656300	-0.853500
H	0.765800	4.679300	2.350400
H	-0.837800	4.976800	1.637200
H	-0.250500	3.307500	1.837800
H	0.094700	6.495700	-0.000700
H	1.723200	6.293600	0.673800
H	1.437100	6.057600	-1.075000
C	-4.917800	0.533000	0.702000
C	-4.480500	-0.203900	1.979600
C	-4.311200	1.947000	0.661800
C	-6.442500	0.684900	0.750700
H	-4.946600	-1.199700	2.030700
H	-3.391600	-0.327800	2.028800
H	-4.802300	0.367400	2.863700
H	-4.630100	2.479200	-0.247300
H	-4.662800	2.521500	1.532200
H	-3.214600	1.925600	0.685700
H	-6.715500	1.262200	1.645000
H	-6.828800	1.226800	-0.125700
H	-6.951500	-0.288200	0.816300
C	-0.584600	-0.975700	2.495100
C	0.525100	-1.213500	3.522100
H	1.292000	-0.422000	3.444200
H	1.034300	-2.161400	3.285700
C	-0.004400	-1.266700	4.954100
H	0.804100	-1.463000	5.672700
H	-0.482700	-0.315600	5.233000
H	-0.755700	-2.063300	5.061000
H	-1.194500	-0.090400	2.811400
H	-1.301800	-1.819200	2.478200
Zr	-0.206000	-0.196700	0.479200

Zr-1_R_2

C	1.313400	0.379200	-2.563100
C	2.660600	-0.070600	-2.295400
C	3.064200	-0.601500	-1.042400
H	3.274800	0.465300	-4.300300
H	1.161300	0.805800	-3.566200
C	3.598300	0.055900	-3.341200
C	4.409600	-0.992200	-0.821800
C	5.288500	-0.849300	-1.894500
C	4.903600	-0.337600	-3.143500
H	6.328900	-1.144000	-1.765700
H	5.638000	-0.249300	-3.942800
O	2.151600	-0.709400	-0.084300
N	0.283600	0.350500	-1.771300
C	-1.741000	2.010000	0.688400
C	-2.941900	1.234300	0.466500
C	-2.963200	-0.181700	0.373800
H	-4.112200	3.050600	0.432500
H	-1.915600	3.086300	0.830000
C	-4.143700	1.961100	0.369200
C	-4.192300	-0.875000	0.250900
C	-5.349500	-0.100500	0.150700
C	-5.340800	1.299300	0.191900
H	-6.310700	-0.600000	0.039300
H	-6.275400	1.852200	0.107100
O	-1.802600	-0.839400	0.398600
N	-0.510000	1.602400	0.744000
C	0.496700	2.558000	1.099500
C	1.728600	2.529500	0.436600
C	0.286100	3.479900	2.131600
C	2.731700	3.427200	0.792800
H	1.905000	1.818700	-0.370500
C	1.293800	4.376600	2.477900
H	-0.654900	3.475700	2.684200
C	2.518100	4.354500	1.811200
H	3.685100	3.399100	0.264500
H	1.123300	5.088900	3.285400
H	3.306300	5.053700	2.090400
C	-0.920900	0.940100	-2.290900
C	-0.995300	2.322800	-2.476300
C	-2.025100	0.131400	-2.561200
C	-2.184200	2.893300	-2.929300
H	-0.128400	2.944100	-2.239500
C	-3.207100	0.708400	-3.019900
H	-1.959700	-0.945800	-2.401800
C	-3.290900	2.088500	-3.200600
H	-2.242600	3.972900	-3.071700
H	-4.068000	0.074100	-3.235200
H	-4.219600	2.536700	-3.554600
C	-4.244500	-2.407900	0.248600
C	-3.467300	-2.966600	-0.954900
C	-3.653800	-2.939600	1.567400
C	-5.682800	-2.927300	0.144700
H	-3.899300	-2.599300	-1.899300
H	-2.410200	-2.675100	-0.919100
H	-3.525900	-4.066100	-0.963100
H	-4.279200	-2.631900	2.418600
H	-3.626200	-4.040500	1.549300
H	-2.637600	-2.561400	1.743100
H	-5.670200	-4.026200	0.169900
H	-6.303600	-2.582100	0.984200
H	-6.162600	-2.621100	-0.796700
C	4.864800	-1.521900	0.542800
C	4.653400	-0.430600	1.607700
C	4.075900	-2.790600	0.912800
C	6.352700	-1.889700	0.534100
H	5.269100	0.452400	1.378000
H	3.603300	-0.115100	1.663700
H	4.959400	-0.809700	2.594900
H	4.202500	-3.566000	0.141400
H	4.452600	-3.195100	1.864400
H	3.005800	-2.578000	1.032500
H	6.638000	-2.254900	1.530800
H	6.573800	-2.687800	-0.190500
H	6.987700	-1.021400	0.304800
C	0.584300	-0.381900	2.548100
C	-0.513800	0.033000	3.517400

H	-1.497900	-0.298500	3.142100
H	-0.544100	1.135500	3.534400
C	-0.300800	-0.489800	4.937700
H	-1.099400	-0.148300	5.611500
H	-0.291300	-1.590200	4.955100
H	0.660300	-0.138700	5.341600
H	0.643200	-1.479100	2.496000
H	1.581800	-0.045800	2.875900
Zr	0.197800	-0.551600	0.414900
C	0.071400	-3.424500	0.291500
H	0.846200	-3.705500	1.011600
H	-0.973900	-3.518000	0.603300
C	0.394000	-3.049000	-0.957500
H	-0.380300	-2.833500	-1.701600
H	1.436400	-2.992400	-1.284400

Zr-1_TS$_2$

C	-1.044000	-1.932100	-1.930100
C	-2.430900	-1.515600	-1.915700
C	-2.900000	-0.430500	-1.132100
H	-2.981100	-3.142200	-3.233800
H	-0.858900	-2.903200	-2.413900
C	-3.348700	-2.301900	-2.641200
C	-4.282900	-0.128800	-1.061200
C	-5.140900	-0.932500	-1.811400
C	-4.694500	-2.005700	-2.597100
H	-6.210100	-0.726500	-1.791700
H	-5.411900	-2.600700	-3.160600
O	-2.014200	0.293200	-0.457500
N	-0.017400	-1.326400	-1.415500
C	1.440400	-1.246400	1.953800
C	2.761700	-0.893300	1.490900
C	3.003200	0.198200	0.616100
H	3.639100	-2.468400	2.684700
H	1.416000	-1.978300	2.776100
C	3.841900	-1.629800	2.015400
C	4.330800	0.610400	0.332500
C	5.357900	-0.168100	0.865200
C	5.134100	-1.288000	1.679400
H	6.390900	0.103200	0.652000
H	5.979300	-1.856900	2.064800
O	1.958100	0.826800	0.088600
N	0.296600	-0.788200	1.539900
C	-0.868100	-1.192400	2.280500
C	-1.840500	-1.988500	1.671100
C	-1.040500	-0.748200	3.593400
C	-2.978200	-2.352900	2.385300
H	-1.700600	-2.322100	0.642700
C	-2.187800	-1.111600	4.298800
H	-0.280600	-0.112000	4.051100
C	-3.155400	-1.914400	3.698500
H	-3.732100	-2.981300	1.909500
H	-2.321800	-0.763100	5.323100
H	-4.049900	-2.197300	4.253700
C	1.206900	-2.074800	-1.369800
C	1.228000	-3.323100	-0.737600
C	2.384000	-1.533600	-1.888600
C	2.425700	-4.026600	-0.630600
H	0.308300	-3.725600	-0.307400
C	3.577600	-2.243200	-1.777000
H	2.366100	-0.557700	-2.373500
C	3.603100	-3.486900	-1.147000
H	2.437800	-4.997400	-0.133900
H	4.495600	-1.818000	-2.184300
H	4.542000	-4.033400	-1.056400
C	4.617400	1.867200	-0.499900
C	4.059700	1.714300	-1.923400
C	3.977100	3.091000	0.179900
C	6.122400	2.134200	-0.615800
H	4.498100	0.837700	-2.426200
H	2.968500	1.605500	-1.905200
H	4.309900	2.604700	-2.520100
H	4.382200	3.226200	1.193900
H	4.203700	3.998400	-0.400700
H	2.885900	2.985900	0.250700
H	6.280800	3.052400	-1.199000
H	6.589100	2.280000	0.369300
H	6.645500	1.317300	-1.134600
C	-4.790700	1.038500	-0.205200
C	-4.442400	0.797000	1.274700
C	-4.166900	2.357700	-0.696600
C	-6.312900	1.186200	-0.305600
H	-4.965200	-0.096300	1.648900
H	-3.365200	0.648200	1.433300
H	-4.771600	1.657900	1.877500
H	-4.439300	2.548100	-1.746200
H	-4.545200	3.195500	-0.089800
H	-3.072000	2.338500	-0.619700
H	-6.634200	2.028700	0.323100
H	-6.637800	1.395000	-1.335800
H	-6.835100	0.286400	0.051600
C	-0.454400	2.828300	0.363400
H	-1.249400	2.221700	0.882000
H	0.503600	2.718800	0.921000
Zr	-0.053300	0.686000	-0.209800
C	-0.896800	4.276400	0.384000
H	-1.811400	4.386500	-0.219500
H	-0.121000	4.896400	-0.091500
C	-1.158600	4.773800	1.805700
H	-0.255900	4.690400	2.428500
H	-1.466500	5.827800	1.794000
H	-1.959900	4.191300	2.284700
C	-0.146300	2.731800	-1.846200
H	-1.145600	3.163500	-1.928100
H	0.666800	3.443900	-1.686400
C	0.123000	1.498300	-2.437700
H	1.142700	1.264600	-2.749800
H	-0.683400	0.964000	-2.947900

Zr-1_P$_2$

C	-1.148600	-1.342400	2.180000
C	-2.527800	-1.435100	1.771900
C	-2.975100	-1.071200	0.474100
H	-3.090600	-2.201800	3.718500
H	-0.946400	-1.667500	3.211600
C	-3.446100	-1.927000	2.723600
C	-4.332600	-1.238100	0.102500
C	-5.192100	-1.726100	1.087000
C	-4.774300	-2.060600	2.384600
H	-6.244200	-1.866100	0.843400
H	-5.496800	-2.438600	3.106500
O	-2.073400	-0.588700	-0.374200
N	-0.122800	-0.917000	1.498400
C	0.480500	3.057000	-0.013000
C	1.909100	2.895800	-0.057600
C	2.531300	1.674300	-0.426400
H	2.208100	4.950900	0.563700
H	0.138600	4.071300	0.242000
C	2.698300	4.016500	0.283400
C	3.943600	1.572800	-0.499700
C	4.668800	2.705900	-0.135100
C	4.071000	3.914600	0.261500
H	5.756900	2.665700	-0.166300
H	4.695300	4.765400	0.530500
O	1.745800	0.646000	-0.706800
N	-0.455800	2.164300	-0.204900
C	-1.807300	2.646700	-0.056200
C	-2.577900	2.178100	1.009400
C	-2.328900	3.572000	-0.960500
C	-3.872800	2.658600	1.182000
H	-2.151800	1.456300	1.710100
C	-3.629600	4.043600	-0.782400
H	-1.719200	3.912800	-1.799200
C	-4.398200	3.595000	0.289300
H	-4.471400	2.303900	2.021700
H	-4.039600	4.767700	-1.486600
H	-5.411900	3.971600	0.427400
C	1.149100	-0.937500	2.171700
C	1.741400	-2.149000	2.530500
C	1.785400	0.275600	2.441800
C	2.973200	-2.139000	3.185400
H	1.239800	-3.089300	2.293000
C	3.014100	0.275500	3.096100
H	1.303700	1.214000	2.157500
C	3.605900	-0.930900	3.473500
H	3.437500	-3.082900	3.472400
H	3.506600	1.223900	3.314100
H	4.566000	-0.929100	3.990200
C	4.618300	0.298100	-1.017500
C	4.260000	-0.911500	-0.136800
C	4.170000	0.067900	-2.472000
C	6.145000	0.430900	-1.017300
H	4.663300	-0.779900	0.877800
H	3.175400	-1.067500	-0.055200
H	4.709600	-1.822400	-0.563900
H	4.487700	0.906800	-3.109300
H	4.631300	-0.851900	-2.865200
H	3.079200	-0.029300	-2.549000
H	6.585500	-0.502300	-1.396400
H	6.486800	1.247900	-1.669600
H	6.541600	0.599300	-0.004800
C	-4.813600	-0.937200	-1.322000
C	-4.622700	0.553500	-1.645500
C	-4.031300	-1.809700	-2.319600
C	-6.301600	-1.262400	-1.492000
H	-5.260700	1.171300	-0.996900
H	-3.582300	0.877700	-1.509400
H	-4.913300	0.744300	-2.690200
H	-4.175000	-2.877500	-2.095200
H	-4.401100	-1.624400	-3.339500
H	-2.957200	-1.588400	-2.295800
H	-6.598400	-1.039300	-2.526600
H	-6.513900	-2.325600	-1.305300
H	-6.933800	-0.654700	-0.827800
C	0.091900	-1.226700	-2.471800
H	0.861500	-0.814500	-3.142100
C	0.601700	-2.377900	-1.627800
H	-0.179000	-3.140400	-1.478700
C	1.917000	-3.020700	-2.071700
H	1.747500	-3.496100	-3.051300
H	2.665600	-2.227600	-2.229800
H	-0.831400	-1.445900	-3.022600
C	2.454700	-4.041300	-1.075200
H	1.682200	-4.804200	-0.878800
H	2.649200	-3.533700	-0.112500
C	3.729700	-4.714000	-1.571400
H	4.516800	-3.969200	-1.766900
H	4.119500	-5.432300	-0.837800
H	3.546400	-5.256600	-2.510700
Zr	-0.147800	-0.061900	-0.622900
H	0.820300	-2.050500	-0.549100

Hf-1_R$_1$

C	-1.169400	0.919100	2.385200
C	-2.534800	0.500500	2.160600
C	-2.937700	-0.241500	1.018800
H	-3.187100	1.549100	3.939200

H	-1.041000	1.666100	3.182900
C	-3.505000	0.969000	3.070600
C	-4.306400	-0.515000	0.776500
C	-5.216900	-0.035500	1.718600
C	-4.838000	0.694100	2.855600
H	-6.278100	-0.230800	1.571200
H	-5.596400	1.044600	3.554100
O	-1.993700	-0.658700	0.180700
N	-0.098400	0.563300	1.736900
C	1.290700	1.810000	-1.423600
C	2.636800	1.381800	-1.137300
C	2.942800	0.058200	-0.730300
H	3.423800	3.326400	-1.669600
H	1.206800	2.797200	-1.902500
C	3.674400	2.309200	-1.361900
C	4.288600	-0.374200	-0.636200
C	5.272200	0.591000	-0.853600
C	4.986100	1.923100	-1.189800
H	6.319600	0.304300	-0.768800
H	5.799200	2.630800	-1.345100
O	1.932000	-0.758600	-0.449300
N	0.175900	1.166400	-1.215200
C	-1.017400	1.773400	-1.750400
C	-1.986800	2.291400	-0.890100
C	-1.208600	1.802800	-3.132500
C	-3.146600	2.851000	-1.418600
H	-1.829000	2.255400	0.187500
C	-2.376600	2.359500	-3.653400
H	-0.448500	1.380200	-3.792300
C	-3.344400	2.884900	-2.799900
H	-3.900000	3.259800	-0.744400
H	-2.527100	2.380500	-4.732900
H	-4.256300	3.318800	-3.210500
C	1.089100	1.333800	1.983100
C	1.054300	2.729400	1.870800
C	2.296100	0.688400	2.255900
C	2.223600	3.468600	2.040700
H	0.116100	3.230700	1.622400
C	3.460100	1.433400	2.423200
H	2.329300	-0.397800	2.332500
C	3.428800	2.823300	2.314100
H	2.190900	4.554700	1.950100
H	4.399000	0.921800	2.637900
H	4.344300	3.401900	2.438200
C	4.637600	-1.837800	-0.337600
C	4.099000	-2.256300	1.039800
C	4.030200	-2.737800	-1.428600
C	6.153300	-2.064200	-0.330900
H	4.506300	-1.612200	1.835100
H	3.003500	-2.203800	1.066300
H	4.399800	-3.292200	1.258500
H	4.443300	-2.482300	-2.415900
H	4.274900	-3.791000	-1.220600
H	2.937400	-2.632900	-1.474700
H	6.357100	-3.126800	-0.137400
H	6.609700	-1.808600	-1.298400
H	6.652200	-1.481200	0.457700
C	-4.749600	-1.326700	-0.446700
C	-4.309900	-0.623700	-1.743600
C	-4.148500	-2.740500	-0.356500
C	-6.274500	-1.476500	-0.501600
H	-4.793200	0.361400	-1.826400
H	-3.223200	-0.473600	-1.794800
H	-4.619200	-1.226900	-2.611000
H	-4.551300	-3.273000	0.518500
H	-4.411400	-3.317100	-1.256700
H	-3.054900	-2.707700	-0.269000
H	-6.544200	-2.062600	-1.391600
H	-6.668500	-2.008400	0.377000
H	-6.779300	-0.502000	-0.579400
C	-0.364500	-2.465200	-1.571300
H	-1.368200	-2.908700	-1.638400
H	-0.386000	-1.562000	-2.261700
H	0.375500	-3.142500	-2.017000
Hf	-0.040800	-0.814900	-0.129900
C	0.249000	-3.400000	0.588600
H	-0.632300	-3.981300	0.317200
H	1.196400	-3.699700	0.133300
C	0.227400	-2.512200	1.623300
H	1.163600	-2.144900	2.050300
H	-0.690000	-2.340600	2.194800

Hf-1_TS$_1$

C	1.168000	0.963500	-2.362800
C	2.534700	0.541600	-2.143500
C	2.939000	-0.220900	-1.016100
H	3.182900	1.620400	-3.904400
H	1.035400	1.704400	-3.165300
C	3.503000	1.025600	-3.046600
C	4.307700	-0.497500	-0.783000
C	5.218300	0.000400	-1.716200
C	4.837600	0.749900	-2.838400
H	6.279600	-0.196300	-1.572500
H	5.594400	1.114600	-3.531500
O	1.997700	-0.654600	-0.178600
N	0.103700	0.617000	-1.702600
C	-1.296400	1.791100	1.461200
C	-2.640700	1.361900	1.162300
C	-2.942600	0.043400	0.736000
H	-3.431700	3.295000	1.725600
H	-1.219600	2.761600	1.974600
C	-3.680200	2.282600	1.400800
C	-4.288100	-0.388500	0.628900
C	-5.274000	0.571400	0.859700
C	-4.991000	1.897400	1.220200
H	-6.320600	0.284700	0.766600
H	-5.805500	2.601000	1.386200
O	-1.929700	-0.769900	0.450300
N	-0.181500	1.161100	1.225700
C	1.011900	1.748300	1.778800
C	1.985700	2.279700	0.931500
C	1.202800	1.748400	3.161800
C	3.145200	2.827200	1.472600
H	1.829100	2.266300	-0.146600
C	2.371200	2.292600	3.695800
H	0.440300	1.315900	3.812600
C	3.340700	2.834500	2.854800
H	3.900100	3.248300	0.807600
H	2.519800	2.292100	4.775800
H	4.251900	3.260200	3.275400
C	-1.088300	1.378600	-1.951300
C	-1.058500	2.771700	-1.819300
C	-2.289400	0.729000	-2.239900
C	-2.230100	3.508200	-1.979800
H	-0.122100	3.271400	-1.561600
C	-3.456000	1.472800	-2.398800
H	-2.310600	-0.356500	-2.332300
C	-3.431400	2.860900	-2.265800
H	-2.202800	4.592900	-1.872200
H	-4.392400	0.961500	-2.625100
H	-4.349500	3.437100	-2.382200
C	-4.635900	-1.846400	0.301500
C	-4.094400	-2.237000	-1.082700
C	-4.030200	-2.767500	1.375500
C	-6.151400	-2.074400	0.288700
H	-4.504900	-1.580100	-1.865900
H	-2.999500	-2.176900	-1.107600
H	-4.390300	-3.270100	-1.321000
H	-4.443600	-2.530800	2.367300
H	-4.274800	-3.816500	1.147000
H	-2.937400	-2.663900	1.423300
H	-6.353600	-3.133200	0.074000
H	-6.609800	-1.837800	1.260100
H	-6.649500	-1.476800	-0.489400
C	4.751600	-1.330700	0.424900
C	4.311900	-0.652000	1.734800
C	4.154100	-2.744100	0.306800
C	6.276500	-1.480200	0.478100
H	4.796100	0.330900	1.835600
H	3.225800	-0.498600	1.789200
H	4.621300	-1.270800	2.591300
H	4.567600	-3.262500	-0.571500
H	4.406600	-3.334900	1.200900
H	3.062200	-2.712600	0.200300
H	6.546900	-2.083000	1.356700
H	6.671500	-1.994200	-0.410700
H	6.779800	-0.506700	0.574800
C	0.340400	-2.637500	1.420600
H	1.402000	-2.910700	1.491400
H	0.209700	-1.743400	2.047900
H	-0.275800	-3.389000	1.925000
C	-0.214700	-3.335900	-0.487300
H	0.625000	-4.021700	-0.359800
H	-1.177900	-3.711800	-0.133000
C	-0.216800	-2.412800	-1.555600
H	-1.168800	-2.218300	-2.053900
H	0.677200	-2.344000	-2.183600
Hf	0.041400	-0.815700	0.095500

Hf-1_P$_1$

C	0.925700	2.725800	0.553000
C	2.324900	2.453800	0.390900
C	2.810500	1.262000	-0.211400
H	2.846800	4.336700	1.333200
H	0.694900	3.683500	1.041800
C	3.232500	3.427100	0.868700
C	4.200700	1.057900	-0.396400
C	5.044700	2.047300	0.105400
C	4.585300	3.214500	0.740800
H	6.121300	1.922700	-0.004200
H	5.301100	3.947400	1.110200
O	1.915900	0.367300	-0.600400
N	-0.107900	1.983700	0.232100
C	-1.083900	-1.923900	1.761000
C	-2.470500	-1.786500	1.401300
C	-2.901800	-1.048800	0.267100
H	-3.075000	-2.985000	3.104000
H	-0.896200	-2.511300	2.671700
C	-3.417200	-2.424400	2.231900
C	-4.273700	-0.985700	-0.078500
C	-5.160800	-1.631700	0.782800
C	-4.757300	-2.334500	1.929700
H	-6.225900	-1.601500	0.557500
H	-5.503300	-2.815800	2.560500
O	-1.968700	-0.438200	-0.454500
N	-0.028100	-1.434000	1.167200
C	-4.744000	-0.285800	-1.359200
C	-4.400000	1.211200	-1.309300
C	-4.072100	-0.950500	-2.574000
C	-6.260600	-0.410800	-1.540500
H	-4.931500	1.702000	-0.480800
H	-3.323800	1.381800	-1.176400
H	-4.714800	1.692400	-2.248300
H	-4.326400	-2.020400	-2.619300
H	-4.431600	-0.476300	-3.499800
H	-2.980100	-0.850400	-2.537300
H	-6.550800	0.093600	-2.473000
H	-6.580200	-1.460900	-1.615200

H	-6.813400	0.068300	-0.718700
C	4.729500	-0.154300	-1.171500
C	4.314400	-1.470500	-0.494200
C	4.177900	-0.091400	-2.606800
C	6.259600	-0.140200	-1.257200
H	4.758900	-1.546500	0.509100
H	3.224800	-1.563100	-0.394500
H	4.680600	-2.320000	-1.092100
H	4.515500	0.825900	-3.112300
H	4.546400	-0.953100	-3.185300
H	3.080100	-0.108500	-2.616600
H	6.593400	-1.020200	-1.825100
H	6.634200	0.752800	-1.779000
H	6.726300	-0.189400	-0.261800
C	0.044700	-0.706100	-2.718500
H	-0.872800	-0.664600	-3.319400
H	0.882200	-0.278500	-3.291900
C	-3.848200	3.540600	1.433100
C	-3.356100	2.364700	2.002000
C	-3.115200	4.197200	0.446700
C	-2.128600	1.853600	1.592700
H	-3.924900	1.844400	2.773300
C	-1.883200	3.691300	0.029400
H	-3.501000	5.111500	-0.004600
C	-1.393900	2.523500	0.613000
H	-1.726000	0.943600	2.043600
H	-1.307500	4.193900	-0.749900
C	3.665000	-2.262500	3.036900
C	3.195800	-0.950100	2.956000
C	2.925000	-3.303300	2.479700
C	1.983300	-0.679100	2.328800
H	3.772400	-0.132100	3.389400
C	1.706500	-3.041900	1.852500
H	3.293500	-4.327900	2.532900
C	1.237700	-1.729700	1.791000
H	1.600200	0.342700	2.270700
H	1.121600	-3.848600	1.406100
C	0.364600	-2.123100	-2.234600
H	-0.555500	-2.725900	-2.175700
C	1.450600	-2.861900	-3.015700
H	1.126900	-2.991700	-4.057400
H	2.384100	-2.282600	-3.016000
H	-4.808300	3.942800	1.757600
H	4.613600	-2.472100	3.531700
H	1.653900	-3.853300	-2.586900
Hf	-0.027300	-0.077500	-0.634800
H	0.742900	-2.130800	-1.158300

Hf-1_A_2

C	-1.132000	-1.578900	-2.321400
C	-2.520700	-1.519300	-1.960600
C	-2.980200	-0.793400	-0.830100
H	-3.081400	-2.652700	-3.721300
H	-0.924000	-1.984800	-3.322600
C	-3.447200	-2.110700	-2.847100
C	-4.364500	-0.640300	-0.581100
C	-5.229900	-1.262800	-1.481100
C	-4.795700	-1.994400	-2.598300
H	-6.303500	-1.176400	-1.320000
H	-5.526000	-2.449500	-3.265600
O	-2.068000	-0.248900	-0.027100
N	-0.098300	-1.162700	-1.637400
C	2.993300	0.282300	0.338700
C	2.806700	1.693900	0.102200
C	1.555700	2.357700	0.206800
H	4.924000	1.926600	-0.282400
H	4.042200	-0.043500	0.344000
C	3.962900	2.439600	-0.211200
C	1.444100	3.751000	0.001800
C	2.622500	4.429200	-0.316900
C	3.869300	3.797300	-0.427000
H	2.581400	5.503800	-0.486700
H	4.753600	4.382700	-0.674500
O	0.468900	1.630100	0.505300
N	2.082000	-0.628000	0.537000
C	2.486900	-1.948400	0.907400
C	1.630700	-3.009100	0.593300
C	3.640700	-2.195200	1.657900
C	1.933600	-4.305200	0.999100
H	0.719900	-2.834400	0.010600
C	3.946600	-3.495600	2.050300
H	4.274600	-1.370800	1.985600
C	3.098900	-4.553200	1.722500
H	1.256700	-5.122400	0.749900
H	4.844500	-3.679100	2.640900
H	3.338000	-5.566600	2.044400
C	1.163400	-1.150500	-2.337100
C	1.839800	-2.332600	-2.636800
C	1.710800	0.089900	-2.671900
C	3.085300	-2.267000	-3.259900
H	1.401100	-3.295500	-2.369800
C	2.955600	0.145400	-3.295500
H	1.156900	1.006400	-2.449000
C	3.646800	-1.032000	-3.582700
H	3.619200	-3.188500	-3.492400
H	3.381400	1.113700	-3.561700
H	4.620600	-0.987100	-4.071100
C	0.093100	4.470300	0.112400
C	-0.879900	3.921100	-0.947000
C	-0.489900	4.287800	1.525200
C	0.245200	5.975400	-0.136000
H	-0.471200	4.063900	-1.959300
H	-1.094400	2.854500	-0.800000
H	-1.833900	4.466600	-0.887800
H	0.195100	4.700300	2.281000
H	-1.443800	4.831400	1.599200
H	-0.676600	3.233400	1.762600
H	-0.738900	6.454800	-0.039400
H	0.917800	6.444700	0.597200
H	0.621600	6.189700	-1.147500
C	-4.874700	0.157500	0.624400
C	-4.404700	-0.517800	1.924200
C	-4.361900	1.607300	0.555500
C	-6.406300	0.208600	0.651000
H	-4.815800	-1.535700	2.001400
H	-3.310800	-0.579800	1.981400
H	-4.762500	0.059200	2.790700
H	-4.691500	2.090500	-0.377000
H	-4.775300	2.181000	1.398900
H	-3.267400	1.661700	0.608300
H	-6.728000	0.792300	1.524900
H	-6.816200	0.696600	-0.245900
H	-6.850000	-0.794000	0.741400
C	-0.476900	-0.970200	2.455800
C	0.642000	-1.111000	3.495800
H	1.337100	-0.254400	3.425300
H	1.238300	-2.007900	3.264700
C	0.111300	-1.213700	4.923800
H	0.927700	-1.334800	5.650200
H	-0.456700	-0.312100	5.198800
H	-0.564100	-2.076900	5.024100
H	-1.168100	-0.155300	2.789200
H	-1.118300	-1.874100	2.455500
Hf	-0.146600	-0.216300	0.431100

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C	1.266300	0.655500	-2.583700
C	2.612000	0.180300	-2.357700
C	3.012500	-0.446300	-1.150100
H	3.230200	0.869000	-4.314800
H	1.112200	1.170600	-3.544200
C	3.550400	0.383900	-3.390500
C	4.355300	-0.854700	-0.956000
C	5.235100	-0.637300	-2.015900
C	4.853400	-0.031300	-3.222800
H	6.274000	-0.946400	-1.909900
H	5.589000	0.111900	-4.012900
O	2.095900	-0.629800	-0.205600
N	0.240200	0.555600	-1.792100
C	-1.672600	1.991400	0.856600
C	-2.891600	1.270800	0.567700
C	-2.945100	-0.126700	0.326600
H	-4.022000	3.104100	0.750500
H	-1.819200	3.045600	1.132300
C	-4.078500	2.028200	0.573900
C	-4.190100	-0.780300	0.168600
C	-5.332500	0.023700	0.176700
C	-5.293100	1.411700	0.357100
H	-6.306800	-0.443700	0.042400
H	-6.216700	1.988700	0.351300
O	-1.795600	-0.804000	0.249500
N	-0.447400	1.556400	0.846000
C	0.579100	2.439900	1.320000
C	1.789100	2.526800	0.624200
C	0.395900	3.173800	2.497000
C	2.802700	3.355100	1.100800
H	1.937500	1.964200	-0.298000
C	1.414200	4.001000	2.963300
H	-0.532400	3.073500	3.062100
C	2.619400	4.093400	2.268600
H	3.740900	3.422200	0.549400
H	1.267100	4.564600	3.884900
H	3.416700	4.736900	2.640700
C	-0.964100	1.198700	-2.244400
C	-1.035200	2.593400	-2.281000
C	-2.073500	0.426400	-2.589400
C	-2.226500	3.212100	-2.658500
H	-0.163200	3.184600	-1.992000
C	-3.258300	1.051900	-2.970700
H	-2.010900	-0.661800	-2.546100
C	-3.339300	2.443900	-3.000700
H	-2.282400	4.300800	-2.685600
H	-4.124200	0.446300	-3.240900
H	-4.270100	2.930700	-3.292700
C	-4.276700	-2.304600	0.022700
C	-3.537700	-2.764300	-1.244800
C	-3.672600	-2.966700	1.274500
C	-5.728200	-2.782100	-0.097300
H	-3.984200	-2.303900	-2.140500
H	-2.474600	-2.496100	-1.208800
H	-3.618300	-3.857100	-1.351800
H	-4.272000	-2.720600	2.163500
H	-3.673500	-4.061900	1.158400
H	-2.643700	-2.630200	1.461400
H	-5.740200	-3.878500	-0.176000
H	-6.324500	-2.505400	0.784100
H	-6.219700	-2.378900	-0.995400
C	4.807300	-1.478800	0.369200
C	4.598000	-0.460500	1.504400
C	4.015500	-2.767700	0.653800
C	6.294100	-1.849300	0.335200
H	5.223400	0.430200	1.339000
H	3.550500	-0.139400	1.577000
H	4.894000	-0.909000	2.465200
H	4.138500	-3.490500	-0.167800
H	4.394000	-3.235400	1.575200
H	2.946500	-2.561600	0.792600
H	6.578800	-2.281200	1.305100

H	6.512500	-2.598100	-0.441100
H	6.931900	-0.969500	0.164300
C	0.535100	-0.744100	2.431800
C	-0.542500	-0.362400	3.445900
H	-1.546300	-0.552600	3.024600
H	-0.481400	0.728000	3.603700
C	-0.408500	-1.075400	4.789500
H	-1.177900	-0.743100	5.501300
H	-0.509800	-2.164800	4.666800
H	0.577700	-0.880500	5.237100
H	0.525900	-1.835900	2.297900
H	1.546000	-0.523400	2.814400
Hf	0.176000	-0.526100	0.306000
C	0.015000	-3.370600	-0.083800
H	0.788400	-3.761700	0.583900
H	-1.028400	-3.463000	0.234800
C	0.334900	-2.852800	-1.281700
H	-0.440900	-2.515100	-1.978100
H	1.374100	-2.795800	-1.618600

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C	-0.998500	-2.088300	-1.810800
C	-2.387100	-1.684000	-1.818900
C	-2.860900	-0.558100	-1.098900
H	-2.926200	-3.385800	-3.043800
H	-0.802100	-3.084000	-2.236100
C	-3.299200	-2.514700	-2.501200
C	-4.244000	-0.255800	-1.051400
C	-5.096400	-1.103500	-1.758500
C	-4.645500	-2.219800	-2.479200
H	-6.166100	-0.898800	-1.755700
H	-5.359900	-2.847400	-3.010200
O	-1.977100	0.202700	-0.462100
N	0.024000	-1.440000	-1.337800
C	1.368600	-1.156900	2.050900
C	2.704100	-0.856100	1.596900
C	2.975500	0.151500	0.635200
H	3.541500	-2.315100	2.959200
H	1.313200	-1.826700	2.922500
C	3.765900	-1.539200	2.224300
C	4.310700	0.550300	0.371300
C	5.318600	-0.173200	1.007900
C	5.068000	-1.221600	1.906200
H	6.357900	0.087100	0.812400
H	5.899500	-1.748700	2.371800
O	1.947800	0.721200	0.014600
N	0.239500	-0.711400	1.580000
C	-0.946000	-1.060300	2.320500
C	-1.868300	-1.958500	1.779700
C	-1.181700	-0.465000	3.560800
C	-3.018600	-2.276600	2.496100
H	-1.681400	-2.405300	0.802700
C	-2.341900	-0.782900	4.268000
H	-0.459000	0.247400	3.963100
C	-3.258000	-1.690100	3.740000
H	-3.733400	-2.985700	2.077200
H	-2.524200	-0.319600	5.238000
H	-4.161100	-1.939900	4.297000
C	1.257900	-2.172500	-1.257000
C	1.308200	-3.348400	-0.501400
C	2.409600	-1.684200	-1.873800
C	2.515000	-4.030300	-0.359300
H	0.404200	-3.709100	-0.005300
C	3.612600	-2.370400	-1.724600
H	2.362300	-0.772600	-2.469100
C	3.670700	-3.538200	-0.963500
H	2.550300	-4.944500	0.233900
H	4.512300	-1.990600	-2.210200
H	4.617500	-4.065400	-0.845500
C	4.623400	1.744300	-0.540300
C	4.122600	1.486000	-1.969300
C	3.949300	3.007200	0.025600
C	6.130300	2.014400	-0.616000
H	4.591800	0.584600	-2.393200
H	3.033400	1.359300	-1.983900
H	4.383200	2.338600	-2.614800
H	4.308100	3.214400	1.045000
H	4.196600	3.874800	-0.605200
H	2.856300	2.899100	0.055000
H	6.307200	2.890100	-1.256600
H	6.557800	2.232400	0.373600
H	6.677300	1.166700	-1.055300
C	-4.759000	0.957800	-0.267200
C	-4.423300	0.798400	1.226300
C	-4.129600	2.247800	-0.823800
C	-6.280100	1.099800	-0.389900
H	-4.954600	-0.068700	1.646700
H	-3.348000	0.650800	1.400100
H	-4.749800	1.694500	1.777200
H	-4.375600	2.371700	-1.889800
H	-4.527900	3.118600	-0.279600
H	-3.037300	2.240700	-0.716200
H	-6.606200	1.975700	0.188600
H	-6.594800	1.251300	-1.433200
H	-6.806400	0.221400	0.011900
C	-0.421100	2.716700	0.307300
H	-1.197300	2.107500	0.856500
H	0.543900	2.627700	0.856700
Hf	-0.037500	0.599000	-0.266200
C	-0.886300	4.158900	0.338200
H	-0.127500	4.788000	-0.153100
H	-1.811400	4.255300	-0.251500
C	-1.131000	4.661000	1.760600
H	-0.216700	4.592300	2.368200
H	-1.453300	5.710800	1.750800
H	-1.915900	4.069700	2.256100
C	-0.137200	2.608800	-1.904300
H	-1.138200	3.037600	-1.982000
H	0.670900	3.328800	-1.755200
C	0.135700	1.367600	-2.483800
H	1.155200	1.145800	-2.806000
H	-0.670800	0.835700	-2.997000

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C	-1.072400	-1.335000	2.235700
C	-2.456300	-1.433400	1.850900
C	-2.924400	-1.067100	0.561800
H	-2.985000	-2.217000	3.801400
H	-0.852900	-1.658200	3.263900
C	-3.356300	-1.941600	2.812400
C	-4.280600	-1.258500	0.201200
C	-5.121700	-1.761400	1.194300
C	-4.686000	-2.091300	2.487600
H	-6.173800	-1.918200	0.961200
H	-5.396100	-2.480600	3.215700
O	-2.038800	-0.558500	-0.288700
N	-0.053400	-0.912600	1.537100
C	0.454700	3.043200	0.021400
C	1.881700	2.892900	-0.002900
C	2.514000	1.669600	-0.349200
H	2.164500	4.959200	0.593400
H	0.101000	4.054800	0.268500
C	2.662000	4.024500	0.327700
C	3.925800	1.578900	-0.429500
C	4.641000	2.721300	-0.074700
C	4.034500	3.930000	0.312000
H	5.729400	2.689400	-0.106300
H	4.653500	4.786700	0.574200
O	1.733600	0.631800	-0.603700
N	-0.479400	2.145500	-0.186000
C	-1.832800	2.634000	-0.046900
C	-2.597200	2.204000	1.038800
C	-2.353400	3.534500	-0.975400
C	-3.887300	2.699100	1.206300
H	-2.171600	1.499800	1.757600
C	-3.649400	4.021000	-0.801900
H	-1.747200	3.845600	-1.827900
C	-4.412700	3.611500	0.289200
H	-4.481700	2.375400	2.061200
H	-4.059400	4.727200	-1.524000
H	-5.422200	4.000500	0.423700
C	1.222700	-0.940100	2.207900
C	1.820000	-2.157500	2.535100
C	1.847300	0.268300	2.519900
C	3.046600	-2.159300	3.199900
H	1.325400	-3.093500	2.267300
C	3.070700	0.256700	3.184200
H	1.361100	1.212200	2.263200
C	3.668300	-0.956300	3.529800
H	3.514900	-3.108400	3.462000
H	3.554100	1.200900	3.437700
H	4.623600	-0.963500	4.055200
C	4.608400	0.312700	-0.957900
C	4.254100	-0.914300	-0.100300
C	4.159900	0.103600	-2.415600
C	6.134000	0.454200	-0.952800
H	4.635700	-0.792300	0.923800
H	3.171500	-1.089700	-0.044000
H	4.726400	-1.811000	-0.533100
H	4.477800	0.950600	-3.041800
H	4.618600	-0.811900	-2.821600
H	3.068500	0.008600	-2.492100
H	6.580700	-0.471700	-1.342100
H	6.473000	1.280600	-1.594800
H	6.527100	0.612900	0.062700
C	-4.778000	-0.974900	-1.221300
C	-4.615400	0.515300	-1.560100
C	-3.985600	-1.841100	-2.216500
C	-6.261000	-1.328300	-1.377000
H	-5.250000	1.129500	-0.904700
H	-3.577000	0.854400	-1.449000
H	-4.929500	0.691700	-2.600500
H	-4.108000	-2.909700	-1.982600
H	-4.365100	-1.671200	-3.235400
H	-2.915800	-1.598700	-2.201800
H	-6.569500	-1.118400	-2.410900
H	-6.452900	-2.393700	-1.181000
H	-6.898900	-0.726800	-0.712500
C	0.076100	-1.125700	-2.419600
H	0.853200	-0.726600	-3.089500
C	0.590800	-2.314700	-1.608800
H	-0.198500	-3.070500	-1.468400
C	1.883300	-2.965600	-2.102100
H	1.683600	-3.408000	-3.091600
H	2.640300	-2.179300	-2.254800
H	-0.827000	-1.362000	-2.996200
C	2.431600	-4.023100	-1.150800
H	1.658900	-4.788900	-0.967100
H	2.645200	-3.549800	-0.174600
C	3.695900	-4.683200	-1.689700
H	4.482800	-3.934400	-1.870600
H	4.093700	-5.428000	-0.987500
H	3.496900	-5.191700	-2.644700
Hf	-0.142600	-0.039000	-0.544600
H	0.839400	-2.028500	-0.527100

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C	-1.062900	-1.421700	-2.262900
C	-2.416100	-0.908600	-2.154400
C	-2.786800	0.162500	-1.293900
H	-3.137500	-2.392000	-3.542700
H	-0.976200	-2.403200	-2.742300
C	-3.420900	-1.561800	-2.893900
C	-4.134800	0.584300	-1.189700
C	-5.078100	-0.093700	-1.966900
C	-4.738200	-1.155500	-2.808400
H	-6.122300	0.208800	-1.917700
H	-5.510900	-1.658800	-3.388700
O	-1.844400	0.754400	-0.533600
C	1.454300	-1.643600	1.727000
C	2.694000	-1.013400	1.352300
C	2.763300	0.294100	0.790400
H	3.814300	-2.754600	1.962000
H	1.551100	-2.650800	2.145500
C	3.881100	-1.751800	1.536800
C	4.014300	0.860500	0.430500
C	5.149400	0.076200	0.643500
C	5.099400	-1.213100	1.184700
H	6.125900	0.479800	0.381900
H	6.019600	-1.778500	1.328200
O	1.617100	0.971700	0.616000
C	-1.352100	-2.216500	2.075700
C	-2.593700	-2.153300	1.427800
C	-1.136900	-3.158500	3.091600
C	-3.605500	-3.043500	1.777900
H	-2.767300	-1.412800	0.644700
C	-2.153700	-4.044900	3.432900
H	-0.187200	-3.189900	3.628700
C	-3.385400	-3.990600	2.776900
H	-4.566900	-2.994200	1.265500
H	-1.988700	-4.777300	4.223500
H	-4.178800	-4.685500	3.053700
C	1.691300	-1.890900	-1.844700
C	1.470400	-3.224900	-1.469900
C	2.992000	-1.462900	-2.144500
C	2.537200	-4.119500	-1.423900
H	0.468200	-3.558500	-1.192100
C	4.054100	-2.361600	-2.096400
H	3.174500	-0.421200	-2.414500
C	3.827200	-3.690300	-1.737800
H	2.360300	-5.156700	-1.136200
H	5.062500	-2.022200	-2.335700
H	4.659700	-4.393600	-1.696900
C	4.133300	2.259600	-0.189900
C	3.446700	2.255500	-1.565800
C	3.494100	3.309500	0.731400
C	5.593100	2.674400	-0.406300
H	4.032400	1.661200	-2.284100
H	2.437900	1.826200	-1.503000
H	3.374000	3.280000	-1.965300
H	3.984900	3.308500	1.716700
H	3.616800	4.312700	0.293600
H	2.427100	3.120000	0.884000
H	5.613800	3.680300	-0.849800
H	6.151600	2.714100	0.540300
H	6.118600	1.999600	-1.097500
C	-4.545200	1.738900	-0.267300
C	-4.235800	1.374100	1.195400
C	-3.814500	3.023800	-0.697400
C	-6.048900	2.028400	-0.350500
H	-4.833400	0.502200	1.503100
H	-3.178200	1.130200	1.352300
H	-4.500100	2.214100	1.856700
H	-4.142900	3.328700	-1.702700
H	-4.052200	3.843900	-0.001500
H	-2.726300	2.887000	-0.722700
H	-6.288700	2.865900	0.320100
H	-6.355700	2.317100	-1.366400
H	-6.651500	1.165100	-0.032900
C	-0.718900	2.587700	1.415500
H	-1.674400	3.058700	1.136500
H	-0.981000	1.685000	1.986900
C	0.175400	3.485600	2.243100
H	0.508700	4.327000	1.612700
H	1.079400	2.935700	2.544000
C	-0.545200	4.030100	3.478700
H	-0.869200	3.210700	4.137400
H	0.118400	4.687100	4.057600
H	-1.435600	4.609400	3.193700
Ti	-0.186700	1.092800	0.185700
P	0.360300	-0.656700	-1.792200
P	-0.100500	-1.028200	1.547400
C	0.150600	3.507500	-1.171800
H	-0.674700	4.063700	-0.724300
H	1.163500	3.756000	-0.842400
C	-0.060900	2.634000	-2.172300
H	0.769700	2.165300	-2.701000
H	-1.069300	2.418000	-2.537100

Ti-1(O,P)_TS_2

C	-1.221400	-1.638800	-2.249500
C	-2.553800	-1.088300	-2.069600
C	-2.822400	0.081100	-1.305400
H	-3.428100	-2.688600	-3.218800
H	-1.175000	-2.597000	-2.776800
C	-3.635300	-1.792400	-2.631700
C	-4.149200	0.530900	-1.099600
C	-5.176900	-0.214600	-1.682800
C	-4.934400	-1.361700	-2.442700
H	-6.208400	0.104800	-1.546300
H	-5.767000	-1.910100	-2.882400
O	-1.798900	0.755800	-0.749300
C	1.279900	-1.576800	1.781200
C	2.580500	-1.061700	1.425500
C	2.778900	0.208000	0.811500
H	3.532800	-2.836400	2.199200
H	1.293400	-2.543400	2.296400
C	3.698800	-1.856300	1.748900
C	4.090800	0.727000	0.651500
C	5.154600	-0.110100	0.996800
C	4.977200	-1.397300	1.513200
H	6.172800	0.252600	0.869600
H	5.843200	-2.010900	1.759200
O	1.703500	0.902500	0.397700
C	-1.500200	-1.933400	2.229300
C	-2.742900	-2.004700	1.585700
C	-1.285800	-2.653500	3.413400
C	-3.750600	-2.813200	2.107200
H	-2.923800	-1.436600	0.671000
C	-2.297500	-3.458600	3.927500
H	-0.336200	-2.570500	3.945100
C	-3.528600	-3.541600	3.274900
H	-4.711900	-2.872700	1.595400
H	-2.127900	-4.015200	4.849800
H	-4.319300	-4.170900	3.684700
C	1.618700	-2.069000	-1.898600
C	1.499500	-3.464100	-1.837100
C	2.888800	-1.478300	-1.974500
C	2.644600	-4.255400	-1.871300
H	0.517900	-3.930800	-1.739000
C	4.029300	-2.275500	-2.001700
H	2.986600	-0.390300	-1.997600
C	3.906400	-3.663800	-1.951300
H	2.552200	-5.340900	-1.822800
H	5.014400	-1.810700	-2.056600
H	4.798900	-4.290200	-1.967500
C	4.353300	2.150000	0.139800
C	3.905800	2.263100	-1.322900
C	3.588600	3.158300	1.012700
C	5.838600	2.523100	0.201400
H	4.492300	1.586600	-1.964200
H	2.846400	2.004100	-1.416600
H	4.051300	3.290100	-1.693400
H	3.960100	3.131100	2.048200
H	3.736600	4.179000	0.624800
H	2.514800	2.935000	1.029000
H	5.957900	3.562600	-0.136600
H	6.235200	2.454700	1.224800
H	6.452000	1.890400	-0.456200
C	-4.442400	1.785100	-0.267500
C	-3.950400	1.580600	1.178300
C	-3.784200	3.007100	-0.937500
C	-5.945300	2.079700	-0.184400
H	-4.532800	0.783500	1.665400
H	-2.892200	1.295000	1.235200
H	-4.096800	2.504900	1.759700
H	-4.302300	3.242400	-1.879100
H	-3.859600	3.889400	-0.281500
H	-2.728900	2.829200	-1.180400
H	-6.098400	2.991600	0.411100
H	-6.385700	2.252300	-1.176900
H	-6.495100	1.264700	0.308200
C	-0.462800	2.954600	0.637600
H	-1.547000	2.893800	0.456500
H	-0.191600	2.209300	1.446200
C	-0.064200	4.335500	1.105400
H	-0.389500	5.073400	0.356000
H	1.028700	4.415500	1.189800
C	-0.716400	4.660600	2.452200
H	-0.380300	3.964400	3.234300
H	-0.450300	5.678100	2.767800
H	-1.812700	4.598500	2.386100
Ti	-0.059200	1.081000	-0.207400
P	0.212200	-0.952900	-1.724300
P	-0.221800	-0.861900	1.521600
C	0.340300	3.179400	-1.448300
H	-0.532400	3.831000	-1.506600
H	1.259200	3.623200	-1.054700
C	0.411300	2.056500	-2.254700
H	1.378100	1.655300	-2.557100
H	-0.449400	1.772900	-2.864100

Ti-1(O,P)_P_2

C	-0.658700	-1.873500	-2.389400
C	-2.088900	-1.752500	-2.342400
C	-2.764300	-0.936200	-1.392000
H	-2.319500	-3.095900	-4.020000
H	-0.271400	-2.566800	-3.144200
C	-2.844800	-2.468900	-3.297900
C	-4.178500	-0.802700	-1.421800
C	-4.860700	-1.529400	-2.395000
C	-4.215900	-2.361600	-3.321800
H	-5.945200	-1.453900	-2.446900
H	-4.802300	-2.908700	-4.059200
O	-2.034700	-0.311700	-0.459100
C	2.683300	-0.419900	1.552800
C	3.090100	0.767800	0.823100
C	2.172700	1.684100	0.240200
H	5.181200	0.292200	1.074100
H	3.488500	-0.979700	2.037600
C	4.467400	0.986200	0.627900
C	2.599800	2.775300	-0.547600
C	3.978800	2.915200	-0.727800
C	4.905900	2.043700	-0.145300
H	4.355500	3.733600	-1.338400

H	5.972000	2.202900	-0.305000
O	0.856900	1.478800	0.451500
Ti	-0.540200	0.323500	0.446000
C	0.976800	-2.582300	2.549800
C	-0.146400	-3.363700	2.241700
C	1.884100	-3.006100	3.530400
C	-0.351500	-4.573200	2.899800
H	-0.855900	-3.028800	1.479200
C	1.670000	-4.216400	4.182300
H	2.744300	-2.389600	3.795200
C	0.556600	-4.999100	3.867700
H	-1.221600	-5.182700	2.655600
H	2.371800	-4.549000	4.947400
H	0.394900	-5.944700	4.385800
C	2.128300	-1.651800	-1.940200
C	2.369100	-3.027200	-2.075500
C	3.174700	-0.739300	-2.134300
C	3.639600	-3.479200	-2.421700
H	1.565900	-3.745600	-1.900100
C	4.444000	-1.200500	-2.476900
H	3.001300	0.334500	-2.025700
C	4.676600	-2.567300	-2.623000
H	3.822400	-4.548900	-2.528200
H	5.250800	-0.483700	-2.633200
H	5.670600	-2.925300	-2.893300
C	1.596200	3.750100	-1.181100
C	0.638700	3.007700	-2.133100
C	0.802000	4.463100	-0.073500
C	2.312700	4.823800	-2.008600
H	1.197700	2.402900	-2.864400
H	-0.058800	2.344200	-1.602100
H	0.034700	3.738500	-2.691800
H	1.478000	5.046400	0.570000
H	0.074500	5.158100	-0.521400
H	0.255900	3.749300	0.557200
H	1.566100	5.514200	-2.424900
H	3.007600	5.416300	-1.396200
H	2.870000	4.386500	-2.850600
C	-4.924500	0.107300	-0.439800
C	-4.700100	-0.392500	0.997400
C	-4.443400	1.558200	-0.621200
C	-6.437300	0.102700	-0.689000
H	-5.137500	-1.394400	1.123000
H	-3.634900	-0.454200	1.247500
H	-5.194500	0.283200	1.713600
H	-4.745500	1.933600	-1.610500
H	-4.902100	2.208400	0.140900
H	-3.353100	1.650800	-0.549100
H	-6.917800	0.780000	0.031600
H	-6.687300	0.459600	-1.698700
H	-6.874900	-0.896500	-0.549600
C	-1.290500	0.385500	2.375900
H	-1.994300	-0.442400	2.537900
P	1.133700	-1.046400	1.630300
P	0.487400	-1.017200	-1.491100
C	-1.916300	1.692300	1.955800
H	-3.014300	1.625400	1.935900
C	-1.419500	2.924700	2.706500
H	-0.320700	2.981000	2.609900
H	-1.634500	2.789300	3.778600
H	-0.601100	0.489100	3.220700
C	-2.063000	4.213300	2.203200
H	-3.149700	4.167900	2.385400
H	-1.937700	4.279500	1.107900
C	-1.473800	5.453900	2.863600
H	-0.397100	5.537000	2.649400
H	-1.962200	6.369300	2.503800
H	-1.595700	5.413700	3.956400
H	-1.719000	1.933800	0.855400

Ti-1(O,O)_R_2

C	-1.081600	-1.950200	-2.285600
C	-2.448600	-1.613300	-1.746700
C	-2.730100	-0.340600	-1.213800
H	-3.275600	-3.510400	-2.343400
H	-1.009500	-3.026400	-2.495500
C	-3.491000	-2.518300	-1.940100
C	-4.056000	0.098400	-1.001500
C	-5.066300	-0.847800	-1.218000
C	-4.798300	-2.144900	-1.649300
H	-6.103900	-0.564000	-1.053200
H	-5.615800	-2.850900	-1.793400
O	-1.676900	0.458700	-0.907800
C	1.198300	-0.808900	2.000500
C	2.578100	-0.372200	1.594800
C	2.892700	0.216400	0.360300
H	3.355700	-1.151800	3.448400
H	1.070200	-0.665000	3.081500
C	3.602800	-0.700000	2.485200
C	4.233900	0.463400	-0.014900
C	5.224800	0.095400	0.900600
C	4.925700	-0.474900	2.136600
H	6.270200	0.264900	0.651200
H	5.728600	-0.735600	2.825500
O	1.869400	0.539100	-0.474300
C	-1.082700	-0.104100	2.152500
C	-2.025100	-1.089700	1.901000
C	-1.232200	0.841800	3.159800
C	-3.167500	-1.129500	2.701100
H	-1.862400	-1.798800	1.089900
C	-2.378800	0.788100	3.950300
H	-0.462800	1.599400	3.317500
C	-3.339400	-0.199300	3.725900
H	-3.923600	-1.893500	2.519800
H	-2.518700	1.520300	4.745400
H	-4.231800	-0.237800	4.350800
C	0.647400	-2.588500	-0.749200
C	-0.089800	-3.552400	-0.058800
C	2.039000	-2.590600	-0.725900
C	0.590600	-4.502000	0.703700
H	-1.180000	-3.564300	-0.117700
C	2.704900	-3.534700	0.053200
H	2.578900	-1.839800	-1.302000
C	1.984200	-4.485500	0.776100
H	0.023600	-5.258600	1.247000
H	3.795000	-3.525500	0.088600
H	2.507700	-5.226800	1.379800
C	4.591100	1.130400	-1.349400
C	4.003500	0.340100	-2.531700
C	4.056700	2.571800	-1.336400
C	6.107400	1.200200	-1.564400
H	4.415900	-0.681000	-2.553800
H	2.909300	0.270400	-2.480600
H	4.276800	0.830200	-3.478900
H	4.573900	3.164500	-0.566800
H	4.226900	3.054600	-2.311900
H	2.983100	2.596500	-1.109400
H	6.310000	1.673300	-2.536000
H	6.605400	1.803500	-0.792100
H	6.563800	0.199300	-1.577000
C	-4.381800	1.546700	-0.610700
C	-3.911600	1.824900	0.823800
C	-3.707200	2.518200	-1.597600
C	-5.889800	1.819100	-0.668800
H	-4.513700	1.249800	1.542300
H	-2.861400	1.541800	0.966600
H	-4.026800	2.894900	1.059100
H	-4.022000	2.300000	-2.629900
H	-4.009800	3.549800	-1.362200
H	-2.611900	2.463800	-1.546700
H	-6.071500	2.872600	-0.412500
H	-6.300100	1.640900	-1.673800
H	-6.447900	1.205100	0.052500
C	-0.080600	2.633900	0.292700
H	-0.252700	3.377300	-0.505600
H	-1.042000	2.540200	0.837900
C	1.057000	3.043200	1.224200
H	1.972800	3.219100	0.640200
H	1.301700	2.213200	1.909700
C	0.706200	4.292400	2.032200
H	-0.185000	4.121600	2.656700
H	1.535700	4.582900	2.691900
H	0.486500	5.140900	1.367700
Ti	0.061400	0.779600	-0.503400
O	0.028900	-1.566000	-1.455200
O	0.096700	-0.064200	1.370600
H	-0.926200	-1.420200	-3.237600
H	1.024200	-1.870100	1.759800
C	0.611300	2.261800	-2.812100
H	-0.030900	3.145500	-2.812400
H	1.667800	2.398800	-2.570700
C	0.127400	1.057900	-3.153900
H	0.782200	0.180100	-3.198800
H	-0.921700	0.933100	-3.433400

Ti-1(O,O)_TS_2

C	-0.727300	-1.662600	-2.410200
C	-2.092900	-1.671100	-1.786200
C	-2.596200	-0.480200	-1.232500
H	-2.526500	-3.719500	-2.300400
H	-0.437600	-2.666900	-2.744900
C	-2.919700	-2.788600	-1.886200
C	-3.967000	-0.319200	-0.945700
C	-4.760200	-1.468100	-1.061400
C	-4.248300	-2.695500	-1.483200
H	-5.821100	-1.407900	-0.824000
H	-4.903500	-3.564200	-1.544200
O	-1.705700	0.511700	-1.000600
C	0.920200	-0.847600	2.133300
C	2.330600	-0.724800	1.621300
C	2.755500	0.210200	0.665900
H	2.933400	-2.274500	2.988500
H	0.838500	-0.271500	3.068200
C	3.270900	-1.529100	2.264800
C	4.131500	0.421200	0.405900
C	5.035300	-0.396600	1.092600
C	4.622800	-1.373900	1.994900
H	6.102400	-0.272800	0.921100
H	5.360300	-2.001400	2.495100
O	1.794300	0.873800	-0.031800
C	-1.362300	-0.400100	1.989000
C	-2.278200	-1.421800	1.776800
C	-1.565100	0.568900	2.970400
C	-3.417900	-1.478000	2.582800
H	-2.109700	-2.158700	0.991300
C	-2.700300	0.498200	3.772900
H	-0.820600	1.353600	3.121500
C	-3.622000	-0.533600	3.587200
H	-4.143700	-2.275900	2.423900
H	-2.860300	1.246800	4.548900
H	-4.505800	-0.594200	4.222600
C	1.166000	-2.157600	-1.022000
C	0.644600	-3.162200	-0.212900
C	2.513900	-2.110900	-1.355000
C	1.509100	-4.137200	0.285500
H	-0.422400	-3.181000	0.012700
C	3.369700	-3.081000	-0.838100
H	2.878800	-1.306300	-1.993700

C	2.869300	-4.093100	-0.019400
H	1.114100	-4.934300	0.916400
H	4.432600	-3.044300	-1.078700
H	3.541900	-4.853400	0.378100
C	4.631200	1.505300	-0.559300
C	4.183200	1.185400	-1.992000
C	4.077600	2.872900	-0.130000
C	6.160700	1.609200	-0.565500
H	4.629900	0.240700	-2.339500
H	3.091500	1.098600	-2.045200
H	4.504800	1.983200	-2.679400
H	4.416100	3.127400	0.885800
H	4.434300	3.656600	-0.816400
H	2.981100	2.871400	-0.135100
H	6.460900	2.417000	-1.248200
H	6.558800	1.847700	0.431500
H	6.634900	0.682600	-0.920200
C	-4.564000	1.058800	-0.632100
C	-3.999000	1.637900	0.671500
C	-4.244100	2.003600	-1.805500
C	-6.087700	0.988100	-0.488400
H	-4.266300	1.002800	1.526900
H	-2.906300	1.723700	0.639800
H	-4.424500	2.639200	0.844200
H	-4.671900	1.618100	-2.743100
H	-4.679300	2.996700	-1.614500
H	-3.159000	2.117900	-1.943900
H	-6.478900	1.998100	-0.299800
H	-6.568300	0.607900	-1.401700
H	-6.387000	0.351900	0.357800
C	-0.384800	2.847400	-0.118700
H	-1.409200	3.073600	-0.450300
H	-0.498800	2.156500	0.729600
C	0.343400	4.065300	0.407000
H	0.451500	4.805800	-0.400500
H	1.355600	3.784700	0.732700
C	-0.426200	4.695900	1.570200
H	-0.532100	3.988100	2.406300
H	0.102200	5.582500	1.945300
H	-1.434400	5.004200	1.257400
Ti	0.054300	0.860300	-0.602000
O	0.327400	-1.163400	-1.541300
O	-0.151600	-0.375900	1.264300
H	-0.716500	-0.992200	-3.282000
H	0.698200	-1.900100	2.364000
C	0.549100	2.734900	-2.114900
H	-0.218300	3.481200	-2.322700
H	1.510500	3.107300	-1.750600
C	0.478100	1.480500	-2.709400
H	1.381400	0.893200	-2.881100
H	-0.411100	1.221100	-3.285800

Ti-1(O,O)_P_2

C	0.324500	-2.089100	1.181400
C	-1.013400	-2.605200	0.742000
C	-1.898300	-1.755300	0.053800
H	-0.720000	-4.560600	1.600700
H	0.244400	-1.390100	2.026400
C	-1.412900	-3.897400	1.079300
C	-3.205800	-2.165100	-0.283200
C	-3.566500	-3.464600	0.092000
C	-2.694500	-4.325700	0.756500
H	-4.564700	-3.827200	-0.147400
H	-3.018800	-5.332500	1.017800
O	-1.430900	-0.529700	-0.294500
C	0.827600	1.558900	2.507800
C	2.197000	1.051900	2.145000
C	2.647000	1.136000	0.814800
H	2.756100	0.610500	4.182700
H	0.780500	2.652100	2.376400
C	3.095900	0.688500	3.148000
C	4.009700	1.026300	0.473000
C	4.875100	0.671600	1.516100
C	4.431500	0.467900	2.823400
H	5.937100	0.551300	1.309100
H	5.141700	0.179300	3.598100
O	1.698300	1.321100	-0.133300
Ti	0.075800	0.498000	-0.394300
C	-1.536400	1.228100	2.198000
C	-2.098900	2.494800	2.077200
C	-2.214900	0.175100	2.799000
C	-3.387300	2.705600	2.568300
H	-1.536500	3.307300	1.612900
C	-3.499900	0.401600	3.289100
H	-1.752500	-0.809800	2.870100
C	-4.086000	1.661700	3.173600
H	-3.841700	3.692600	2.479900
H	-4.045000	-0.416300	3.760900
H	-5.091800	1.831300	3.558400
C	2.039400	-1.978900	-0.533300
C	3.229000	-2.214700	0.147700
C	1.833400	-2.382700	-1.845000
C	4.245000	-2.896700	-0.518100
H	3.350500	-1.855600	1.172200
C	2.869100	-3.046700	-2.505300
H	0.871500	-2.194100	-2.327700
C	4.065800	-3.310600	-1.840300
H	5.185700	-3.095700	-0.004100
H	2.730500	-3.372500	-3.536200
H	4.866300	-3.841300	-2.355800
C	4.516700	1.387500	-0.931000
C	3.925300	0.485900	-2.026000
C	4.132800	2.852000	-1.212500
C	6.042300	1.268700	-1.013800
H	4.209300	-0.564700	-1.872700
H	2.830700	0.550300	-2.067800
H	4.319800	0.804400	-3.003300
H	4.570800	3.522100	-0.457700
H	4.513700	3.153600	-2.200300
H	3.041600	2.984700	-1.206700
H	6.371900	1.556600	-2.022100
H	6.545500	1.932500	-0.295600
H	6.379400	0.236000	-0.834900
C	-4.175000	-1.233800	-1.018500
C	-4.425300	0.025500	-0.169400
C	-3.593300	-0.871100	-2.395500
C	-5.533800	-1.901300	-1.258100
H	-4.956300	-0.244000	0.756200
H	-3.493700	0.536000	0.111700
H	-5.058200	0.733300	-0.728900
H	-3.491900	-1.773600	-3.017400
H	-4.267800	-0.173300	-2.916900
H	-2.606300	-0.402000	-2.306600
H	-6.194200	-1.191200	-1.776600
H	-5.446600	-2.797500	-1.889700
H	-6.023800	-2.182700	-0.314400
C	-0.923100	2.481700	-1.442100
C	-0.253800	1.358200	-2.188400
H	0.698300	1.608700	-2.671900
H	-0.919500	0.760400	-2.824700
H	0.586300	1.313900	3.551100
H	0.994500	-2.910500	1.462900
C	-2.392000	2.730500	-1.786200
H	-2.946700	1.784700	-1.682100
H	-2.824000	3.432200	-1.053800
H	-0.320100	3.400500	-1.480500
C	-2.573300	3.285900	-3.196200
H	-1.997500	4.221200	-3.296100
H	-2.145100	2.577700	-3.925200
C	-4.041100	3.538800	-3.520700
H	-4.163500	3.934200	-4.537700
H	-4.625400	2.608600	-3.446900
H	-4.479600	4.266200	-2.821200
O	-0.244100	0.990300	1.686400
O	0.998000	-1.317400	0.135700
H	-0.922000	2.263300	-0.318200

Ti-1(O,S)_R_2

C	-0.718700	2.632900	-0.959800
C	-2.150200	2.538400	-0.503600
C	-2.619600	1.450600	0.258600
H	-2.685800	4.388800	-1.466200
H	-0.476300	1.905100	-1.749100
C	-3.045900	3.540900	-0.880800
C	-3.969700	1.356500	0.668700
C	-4.826100	2.378900	0.248400
C	-4.383300	3.454900	-0.519100
H	-5.875700	2.346900	0.534500
H	-5.083700	4.233400	-0.820800
O	-1.730000	0.493500	0.617400
C	0.875500	-2.241400	-1.811400
C	2.304900	-1.872500	-1.526200
C	2.640100	-1.285100	-0.289800
H	3.041300	-2.619200	-3.408100
H	0.491800	-2.923500	-1.036800
C	3.307300	-2.176200	-2.446600
C	3.987100	-1.096800	0.090500
C	4.957300	-1.425300	-0.863400
C	4.636000	-1.935100	-2.120500
H	6.008500	-1.282200	-0.620200
H	5.427900	-2.168500	-2.831800
O	1.612000	-0.910900	0.512000
Ti	-0.110900	-0.325600	0.763200
C	-1.839100	-1.336000	-2.157500
C	-2.772300	-0.370000	-2.543800
C	-2.199400	-2.679800	-2.052700
C	-4.079300	-0.758900	-2.824000
H	-2.482500	0.678600	-2.632500
C	-3.511400	-3.055300	-2.344900
H	-1.475900	-3.441900	-1.762000
C	-4.449400	-2.100500	-2.730400
H	-4.807300	-0.005100	-3.125900
H	-3.794000	-4.106100	-2.275500
H	-5.471100	-2.402300	-2.962200
C	2.034900	2.669600	-0.427700
C	2.510800	1.793300	-1.404600
C	2.786000	3.781800	-0.041400
C	3.752200	2.024300	-1.991300
H	1.925600	0.922700	-1.697600
C	4.028800	4.006200	-0.633800
H	2.402000	4.462200	0.719400
C	4.513500	3.127800	-1.602700
H	4.126800	1.329900	-2.744300
H	4.619300	4.872700	-0.335500
H	5.487500	3.304900	-2.059800
C	4.372100	-0.598800	1.488400
C	3.847600	0.826800	1.707700
C	3.788600	-1.559700	2.539000
C	5.891600	-0.563500	1.683500
H	4.300700	1.521700	0.984100
H	2.758800	0.874400	1.581900
H	4.104100	1.168500	2.723400
H	4.238800	-2.558800	2.438700
H	4.006100	-1.187300	3.552500
H	2.701500	-1.664500	2.424600
H	6.111900	-0.226600	2.706700
H	6.346100	-1.556200	1.552800
H	6.375400	0.140200	0.990200

C	-4.464700	0.200400	1.545800
C	-4.300900	-1.133400	0.797000
C	-3.684000	0.188100	2.872400
C	-5.949300	0.349600	1.897600
H	-4.992900	-1.176700	-0.057000
H	-3.283700	-1.270600	0.406700
H	-4.539800	-1.974300	1.468100
H	-3.834500	1.134300	3.414500
H	-4.046800	-0.631300	3.512800
H	-2.607700	0.053500	2.707600
H	-6.257200	-0.503900	2.518600
H	-6.145600	1.268400	2.469600
H	-6.584100	0.352900	0.999800
C	-0.791600	-2.067000	1.519800
H	-1.769800	-1.999400	2.020000
H	-1.025200	-2.157900	0.448700
S	-0.182700	-0.741400	-1.815900
S	0.483900	2.368600	0.413700
H	0.773700	-2.714100	-2.796100
H	-0.513400	3.637700	-1.349700
C	0.048000	-3.242200	1.980600
H	0.222900	-3.153700	3.064700
H	1.037500	-3.214000	1.496100
C	-0.641700	-4.578000	1.692900
H	-0.033800	-5.418600	2.054900
H	-1.625300	-4.630100	2.182200
H	-0.798000	-4.718000	0.611400
C	0.141300	-0.392200	3.481300
H	-0.806000	-0.834900	3.793900
H	1.042100	-1.004300	3.572800
C	0.223800	0.898600	3.107900
H	1.194600	1.365000	2.927800
H	-0.659700	1.542900	3.071800

Ti-1(O,S)_TS_2

C	-0.704100	2.700200	-0.809600
C	-2.136300	2.570600	-0.360600
C	-2.610700	1.445600	0.342800
H	-2.667700	4.464200	-1.236900
H	-0.460900	2.042800	-1.657800
C	-3.032500	3.587400	-0.698600
C	-3.967000	1.328900	0.727100
C	-4.822500	2.366900	0.346700
C	-4.374100	3.481300	-0.360000
H	-5.875700	2.316300	0.617100
H	-5.072600	4.272600	-0.631000
O	-1.725300	0.473900	0.672000
C	0.862800	-2.118900	-1.875700
C	2.297500	-1.797800	-1.565000
C	2.636900	-1.286400	-0.296500
H	3.025800	-2.445000	-3.485400
H	0.455200	-2.804300	-1.116700
C	3.297100	-2.061400	-2.500300
C	3.985800	-1.120900	0.090000
C	4.952900	-1.410300	-0.880300
C	4.628100	-1.854200	-2.160900
H	6.005400	-1.287700	-0.632000
H	5.418400	-2.058800	-2.882700
O	1.609900	-0.956300	0.526600
Ti	-0.078600	-0.292500	0.837100
C	-1.816200	-1.166300	-2.213000
C	-2.181100	-2.513000	-2.175400
C	-2.754100	-0.184300	-2.546900
C	-3.494500	-2.873800	-2.482300
H	-1.457200	-3.291400	-1.935100
C	-4.060900	-0.557800	-2.845600
H	-2.465600	0.867900	-2.581500
C	-4.432900	-1.902400	-2.820300
H	-3.776000	-3.927100	-2.465800
H	-4.788700	0.211100	-3.107500
H	-5.454500	-2.192000	-3.067300
C	2.056800	2.665700	-0.322800
C	2.532100	1.826500	-1.331500
C	2.801600	3.770700	0.095100
C	3.767400	2.087000	-1.918700
H	1.952800	0.962400	-1.650800
C	4.036200	4.027000	-0.501400
H	2.420500	4.420200	0.884200
C	4.521100	3.184800	-1.501800
H	4.141500	1.418900	-2.695500
H	4.621400	4.888900	-0.179700
H	5.490000	3.385400	-1.960200
C	4.383600	-0.655800	1.496300
C	3.925400	0.793300	1.710700
C	3.752300	-1.582200	2.549600
C	5.902100	-0.695400	1.701600
H	4.424400	1.469700	0.999200
H	2.844500	0.895900	1.555400
H	4.171100	1.121200	2.733600
H	4.092000	-2.619300	2.406000
H	4.053000	-1.261600	3.558900
H	2.656600	-1.567800	2.488600
H	6.131300	-0.385900	2.731300
H	6.309500	-1.706600	1.556000
H	6.425100	-0.004200	1.024800
C	-4.469800	0.129600	1.539500
C	-4.289400	-1.165100	0.728600
C	-3.709800	0.059800	2.876000
C	-5.960300	0.252100	1.875800
H	-4.977200	-1.171200	-0.129300
H	-3.270900	-1.274900	0.332300
H	-4.527000	-2.040300	1.355600
H	-3.910800	0.959000	3.478000
H	-4.043700	-0.816800	3.454200
H	-2.626700	-0.009000	2.719500
H	-6.270800	-0.631000	2.452900
H	-6.172100	1.142100	2.486300
H	-6.581600	0.291900	0.969600
C	-0.823000	-2.119800	1.587600
H	-1.864500	-2.113200	1.937000
H	-0.906200	-2.024100	0.494900
S	-0.154300	-0.592300	-1.870100
S	0.514100	2.326200	0.523900
H	0.764300	-2.579000	-2.866700
H	-0.500300	3.734600	-1.113500
C	-0.093700	-3.414500	1.883800
H	-0.117300	-3.602200	2.967800
H	0.964500	-3.317400	1.589300
C	-0.744900	-4.596100	1.162300
H	-0.234800	-5.533700	1.420700
H	-1.805300	-4.693900	1.437800
H	-0.691100	-4.478600	0.068700
C	-0.062300	-0.894600	3.229000
H	-1.025200	-1.117200	3.691200
H	0.736100	-1.619100	3.395800
C	0.277100	0.417400	2.925900
H	1.332800	0.696300	2.890700
H	-0.454600	1.217300	3.064200

Ti-1(O,S)_P_2

C	-0.168000	-2.942700	-0.508100
C	-1.656600	-2.824200	-0.688000
C	-2.293700	-1.581600	-0.861400
H	-1.939200	-4.952200	-0.485800
H	0.148400	-2.693900	0.516500
C	-2.429700	-3.985300	-0.611200
C	-3.698500	-1.475300	-0.978600
C	-4.425600	-2.664500	-0.870300
C	-3.813000	-3.903500	-0.685300
H	-5.510700	-2.632600	-0.946100
H	-4.420000	-4.806200	-0.619700
O	-1.504700	-0.482700	-0.935400
C	0.792500	1.063300	2.665900
C	2.249300	0.951400	2.300600
C	2.650900	1.050700	0.953900
H	2.909900	0.784900	4.344900
H	0.396700	2.039400	2.347500
C	3.217500	0.875200	3.301600
C	4.003200	1.235200	0.596000
C	4.936200	1.154500	1.636900
C	4.564000	0.946000	2.964200
H	5.995000	1.266900	1.411100
H	5.327200	0.880200	3.739300
O	1.683700	0.964600	0.009100
Ti	0.088400	0.362500	-0.660800
C	-1.859100	-0.051100	2.527800
C	-2.332600	1.162100	3.030000
C	-2.653700	-1.200200	2.549000
C	-3.613100	1.213400	3.578500
H	-1.717000	2.061900	3.009100
C	-3.935900	-1.130400	3.089700
H	-2.273200	-2.142800	2.149900
C	-4.412800	0.071100	3.613300
H	-3.985300	2.155100	3.982700
H	-4.557700	-2.025800	3.108300
H	-5.410900	0.119900	4.049200
C	2.487300	-2.346500	-1.053700
C	2.886100	-2.087900	0.258400
C	3.347300	-2.964800	-1.961700
C	4.172500	-2.437700	0.660700
H	2.207400	-1.605600	0.963800
C	4.632700	-3.313000	-1.547400
H	3.018200	-3.163700	-2.982400
C	5.045800	-3.045900	-0.242500
H	4.491400	-2.222000	1.681300
H	5.313300	-3.793300	-2.250900
H	6.053600	-3.316500	0.073700
C	4.417100	1.601000	-0.835700
C	4.074500	0.484000	-1.831200
C	3.698400	2.903200	-1.233100
C	5.926100	1.852200	-0.933900
H	4.564600	-0.457300	-1.540700
H	2.992200	0.308900	-1.894700
H	4.433600	0.763200	-2.833800
H	4.001500	3.729800	-0.573100
H	3.962300	3.175900	-2.266600
H	2.606700	2.794500	-1.168500
H	6.173200	2.149400	-1.962900
H	6.251700	2.661700	-0.264500
H	6.506500	0.947300	-0.699300
C	-4.389900	-0.130100	-1.230900
C	-4.114300	0.833100	-0.065600
C	-3.886400	0.461600	-2.558500
C	-5.910500	-0.288400	-1.342400
H	-4.513100	0.424400	0.874200
H	-3.040300	1.013400	0.072400
H	-4.607900	1.799600	-0.254500
H	-4.118600	-0.213600	-3.395600
H	-4.384400	1.425400	-2.750800
H	-2.801600	0.625200	-2.540800
H	-6.359500	0.698800	-1.523200
H	-6.195300	-0.942900	-2.178900
H	-6.349000	-0.688700	-0.416400
C	-0.712300	2.715400	-0.723900
C	-0.181300	1.924800	-1.895500
H	0.778600	2.260300	-2.308100
H	-0.929000	1.705100	-2.669900
S	-0.215300	-0.232600	1.847800

S	0.857600	-1.875500	-1.631100
H	0.646500	0.946400	3.747200
H	0.161900	-3.966100	-0.727300
C	-1.997100	3.497800	-1.011800
H	-2.741100	2.809100	-1.441200
H	-2.419700	3.875500	-0.066200
H	0.071800	3.361300	-0.300900
C	-1.752300	4.658500	-1.971700
H	-0.999200	5.338000	-1.538300
H	-1.317800	4.269000	-2.907700
C	-3.033200	5.426800	-2.276900
H	-2.844800	6.255900	-2.971900
H	-3.786700	4.767600	-2.734600
H	-3.469100	5.848600	-1.358900
H	-0.968000	2.011900	0.140300

Ti-3(O,N)_R_2

C	-0.395500	-1.809200	-1.959900
C	-1.780500	-1.543900	-2.291400
C	-2.430600	-0.343500	-1.922600
H	-1.974900	-3.470800	-3.251500
H	-0.026000	-2.798500	-2.271000
C	-2.488400	-2.546900	-2.978000
C	-3.788900	-0.120100	-2.256900
C	-4.441400	-1.149000	-2.939300
C	-3.817000	-2.351400	-3.296800
H	-5.486400	-1.016000	-3.215500
H	-4.378100	-3.118000	-3.829500
O	-1.721600	0.561300	-1.247000
N	0.431200	-1.033600	-1.334000
C	0.433300	0.476000	2.477700
C	1.802600	0.897300	2.414300
C	2.413600	1.283700	1.190100
H	2.052200	0.588500	4.544300
H	0.063100	0.200500	3.475700
C	2.542200	0.893100	3.617400
C	3.776100	1.691700	1.171200
C	4.451400	1.670100	2.389600
C	3.863300	1.273800	3.603200
H	5.494500	1.982300	2.414100
H	4.452800	1.280600	4.518800
O	1.671700	1.258600	0.093800
N	-0.411100	0.353100	1.490000
Ti	-0.107200	1.009500	-0.472600
C	4.465500	2.140700	-0.122200
C	4.541900	0.953300	-1.094100
C	3.681300	3.298900	-0.760300
C	5.892400	2.636000	0.134800
H	5.241400	0.190700	-0.719500
H	3.561600	0.475400	-1.222100
H	4.905400	1.292800	-2.077000
H	3.597900	4.145900	-0.061500
H	4.207400	3.648500	-1.661700
H	2.671000	2.981600	-1.043600
H	6.338100	2.947800	-0.820500
H	5.910600	3.503300	0.811800
H	6.533800	1.847300	0.554800
C	-4.491600	1.196600	-1.911800
C	-4.531500	1.388100	-0.387000
C	-3.743300	2.359500	-2.586500
C	-5.936900	1.219500	-2.421000
H	-5.178900	0.628000	0.077300
H	-3.534800	1.309500	0.067600
H	-4.950200	2.378300	-0.147800
H	-3.742300	2.234300	-3.680100
H	-4.243700	3.311400	-2.352300
H	-2.704400	2.416900	-2.239500
H	-6.396300	2.180000	-2.146900
H	-5.990700	1.124100	-3.515700
H	-6.543300	0.421300	-1.967600
C	-0.645400	2.968200	-0.270300
H	-1.273300	3.424400	-1.047900
H	-1.367500	2.509800	0.466100
C	6.254400	-2.998500	0.550200
H	6.186600	-2.008600	1.039100
H	5.727000	-3.735700	1.179500
C	7.683400	-3.394300	0.356800
H	8.259800	-2.773600	-0.335400
C	8.251400	-4.416500	0.990700
H	7.679800	-5.047900	1.676100
H	9.306100	-4.656100	0.849600
O	5.645300	-2.919500	-0.735600
C	4.365400	-2.498900	-0.803500
C	3.575700	-2.172600	0.306700
C	3.830100	-2.374300	-2.093500
C	2.281000	-1.697000	0.114800
H	3.954700	-2.276000	1.321800
C	2.537100	-1.906800	-2.274200
H	4.461300	-2.638400	-2.941500
C	1.757300	-1.551300	-1.166300
H	1.663200	-1.442100	0.976100
H	2.134300	-1.789900	-3.282600
C	-6.274600	-2.228300	2.034800
H	-6.207400	-2.106100	0.937800
H	-5.750000	-3.157000	2.316700
C	-7.703800	-2.270000	2.472200
H	-8.273200	-1.348500	2.319700
C	-8.279100	-3.350300	2.992900
H	-7.715200	-4.272200	3.157500
H	-9.334300	-3.352900	3.269500
O	-5.659700	-1.104500	2.662200
C	-4.374100	-0.836000	2.364000
C	-3.587500	-1.590600	1.482800
C	-3.829400	0.299500	2.982300
C	-2.281200	-1.192100	1.213700
H	-3.978000	-2.482900	0.997100
C	-2.527200	0.688600	2.711400
H	-4.463500	0.872100	3.658600
C	-1.748400	-0.058900	1.820300
H	-1.662400	-1.771900	0.527100
H	-2.116900	1.591400	3.169400
C	0.251800	3.977200	0.423700
H	0.874800	3.482000	1.186800
H	0.951700	4.404700	-0.312200
C	-0.552500	5.107500	1.069600
H	0.113200	5.832400	1.558700
H	-1.148300	5.645700	0.317700
H	-1.245400	4.715900	1.829900
C	0.481800	2.467500	-2.791400
H	-0.515800	2.689100	-3.177500
H	1.037400	3.288400	-2.334700
C	1.022600	1.249200	-2.949700
H	2.039100	1.024600	-2.613400
H	0.476200	0.469200	-3.483700

Ti-3(O,N)_TS_2

C	-0.457600	-1.809000	-1.934700
C	-1.846400	-1.520300	-2.229000
C	-2.465700	-0.305300	-1.850100
H	-2.100300	-3.453600	-3.161900
H	-0.098400	-2.792100	-2.274000
C	-2.591800	-2.520000	-2.880600
C	-3.831500	-0.068600	-2.147000
C	-4.523400	-1.096500	-2.789400
C	-3.928800	-2.312700	-3.152200
H	-5.575500	-0.951400	-3.030300
H	-4.518500	-3.078500	-3.654500
O	-1.728900	0.603500	-1.211000
N	0.382700	-1.055400	-1.302900
C	0.462200	0.339000	2.465600
C	1.838800	0.770600	2.421700
C	2.438100	1.252900	1.231600
H	2.102600	0.306900	4.518000
H	0.084000	0.067100	3.462600
C	2.586400	0.674600	3.610900
C	3.809100	1.625800	1.220100
C	4.501600	1.501500	2.425100
C	3.916300	1.036900	3.611700
H	5.552900	1.783300	2.456900
H	4.511900	0.971200	4.521300
O	1.674000	1.349700	0.146300
N	-0.351300	0.201900	1.463200
Ti	-0.025700	0.985300	-0.568400
C	4.504100	2.123200	-0.053300
C	4.512400	0.996600	-1.098900
C	3.775800	3.355600	-0.612200
C	5.957700	2.530600	0.211600
H	5.200300	0.193000	-0.795300
H	3.515300	0.552300	-1.226200
H	4.856700	1.385500	-2.070200
H	3.714000	4.154100	0.143800
H	4.325500	3.749300	-1.480600
H	2.760400	3.095700	-0.930900
H	6.408600	2.873000	-0.730800
H	6.028400	3.355300	0.936500
H	6.561500	1.687100	0.577200
C	-4.496300	1.270500	-1.813500
C	-4.455700	1.522900	-0.297500
C	-3.764300	2.387700	-2.579100
C	-5.966000	1.302000	-2.247000
H	-5.081900	0.786200	0.229000
H	-3.438600	1.453500	0.110000
H	-4.859700	2.523700	-0.077300
H	-3.892200	2.257000	-3.664300
H	-4.178100	3.369800	-2.301900
H	-2.689200	2.380700	-2.359300
H	-6.394300	2.280700	-1.986500
H	-6.080000	1.166500	-3.332700
H	-6.559400	0.532000	-1.731700
C	-0.603000	3.040800	-0.459000
H	-1.544100	3.346200	-0.932900
H	-0.926400	2.420800	0.390000
C	6.289600	-2.926400	0.400800
H	6.212000	-1.948400	0.911900
H	5.794200	-3.688000	1.026900
C	7.721600	-3.286500	0.163900
H	8.263200	-2.646200	-0.538600
C	8.331300	-4.300100	0.772100
H	7.794900	-4.950900	1.467800
H	9.386900	-4.513200	0.599200
O	5.647500	-2.834000	-0.868200
C	4.355900	-2.445900	-0.895700
C	3.586500	-2.164000	0.239700
C	3.787900	-2.304700	-2.170400
C	2.276000	-1.717000	0.089000
H	3.991700	-2.278600	1.243500
C	2.481400	-1.862400	-2.311400
H	4.406100	-2.534700	-3.037900
C	1.720500	-1.555200	-1.176200
H	1.671200	-1.500700	0.968700
H	2.051900	-1.727100	-3.306300
C	-6.295800	-2.200300	1.919400
H	-6.208100	-2.028800	0.830000
H	-5.817600	-3.165000	2.160500
C	-7.731300	-2.198700	2.338100
H	-8.252500	-1.242100	2.238500
C	-8.366800	-3.279600	2.782000
H	-7.851300	-4.237100	2.893700

H	-9.424700	-3.247400	3.045900
O	-5.640600	-1.137100	2.606200
C	-4.344700	-0.901600	2.317800
C	-3.580200	-1.655500	1.417800
C	-3.765700	0.199000	2.966100
C	-2.262800	-1.287200	1.157300
H	-3.996000	-2.523900	0.909800
C	-2.453400	0.557300	2.701000
H	-4.381800	0.772200	3.658400
C	-1.694900	-0.184000	1.785800
H	-1.660300	-1.871300	0.462100
H	-2.019100	1.436200	3.182700
C	0.180700	4.206000	0.109000
H	1.167700	3.861700	0.451900
H	0.345700	4.954800	-0.680900
C	-0.578200	4.851600	1.270600
H	-0.023800	5.715900	1.660600
H	-1.573200	5.198400	0.955000
H	-0.711100	4.136300	2.097100
C	0.383000	2.650000	-2.344600
H	-0.518300	3.028800	-2.829000
H	1.123000	3.396400	-2.056100
C	0.796600	1.347800	-2.617600
H	1.849400	1.079600	-2.499000
H	0.180000	0.724800	-3.268600

Ti-3(O,N)_P_2

C	0.054900	-2.276700	-1.581400
C	-1.354300	-2.273600	-1.848600
C	-2.118000	-1.081500	-1.773900
H	-1.367800	-4.405500	-2.240800
H	0.559300	-3.243300	-1.721600
C	-1.970500	-3.496600	-2.191500
C	-3.498100	-1.085300	-2.106800
C	-4.055700	-2.322900	-2.419300
C	-3.321600	-3.522500	-2.452000
H	-5.115400	-2.371800	-2.666600
H	-3.821800	-4.455600	-2.707400
O	-1.486200	0.017300	-1.396000
N	0.806300	-1.287200	-1.171300
C	0.443700	0.823800	2.336800
C	1.811500	1.275000	2.273400
C	2.458200	1.526800	1.038800
H	1.985900	1.271800	4.431700
H	0.042600	0.671400	3.349200
C	2.496700	1.472800	3.488100
C	3.779200	2.038800	1.003700
C	4.411000	2.208400	2.236600
C	3.799400	1.923100	3.466700
H	5.430100	2.591700	2.255000
H	4.348200	2.079600	4.394500
O	1.766100	1.275600	-0.068800
N	-0.363500	0.570400	1.349200
Ti	0.145200	0.655800	-0.730200
C	4.444800	2.452600	-0.312800
C	4.569200	1.251900	-1.263400
C	3.599000	3.565900	-0.955000
C	5.853200	3.011800	-0.085700
H	5.252800	0.499300	-0.842700
H	3.601600	0.770000	-1.452700
H	4.987400	1.586400	-2.225500
H	3.571000	4.453200	-0.304500
H	4.038600	3.862000	-1.919600
H	2.567900	3.233500	-1.129400
H	6.281900	3.299100	-1.056400
H	5.845700	3.907900	0.552200
H	6.523600	2.264200	0.364400
C	-4.297900	0.217300	-2.202300
C	-4.286900	0.980500	-0.867800
C	-3.673500	1.067400	-3.323000
C	-5.762100	-0.042900	-2.571700
H	-4.816700	0.407500	-0.092100
H	-3.269300	1.182200	-0.508400
H	-4.808700	1.943400	-0.990700
H	-3.755200	0.549900	-4.290500
H	-4.199800	2.031600	-3.404600
H	-2.611400	1.265200	-3.127700
H	-6.292900	0.918200	-2.627400
H	-5.861600	-0.533100	-3.551200
H	-6.270200	-0.660200	-1.815300
C	0.052200	2.246500	-2.011400
H	1.049300	2.600100	-2.294800
H	-0.573100	2.014000	-2.882200
C	6.839100	-2.478200	0.727200
H	6.715600	-1.456100	1.131400
H	6.371800	-3.190200	1.428600
C	8.287500	-2.798000	0.536400
H	8.802700	-2.223200	-0.238600
C	8.939400	-3.701000	1.263600
H	8.430100	-4.285900	2.034100
H	10.004900	-3.883500	1.118800
O	6.205900	-2.549400	-0.547500
C	4.893600	-2.251200	-0.620200
C	4.097600	-1.896800	0.477400
C	4.326800	-2.292000	-1.902500
C	2.756300	-1.576800	0.281100
H	4.505400	-1.863500	1.485900
C	2.990500	-1.974000	-2.089300
H	4.966500	-2.567100	-2.740700
C	2.201000	-1.611600	-0.993500
H	2.132200	-1.306500	1.134900
H	2.557200	-1.988300	-3.091300
C	-6.096900	-2.179200	2.316900
H	-6.005300	-2.273800	1.218500
H	-5.534700	-3.003900	2.787000
C	-7.533200	-2.214900	2.731900
H	-8.139700	-1.360600	2.417600
C	-8.071800	-3.218800	3.418400
H	-7.470500	-4.071900	3.743700
H	-9.131900	-3.226400	3.674600
O	-5.559500	-0.921100	2.715800
C	-4.285100	-0.640700	2.378700
C	-3.429100	-1.519500	1.702300
C	-3.828500	0.638100	2.731500
C	-2.140200	-1.106600	1.372600
H	-3.747500	-2.522600	1.424900
C	-2.544000	1.041500	2.399800
H	-4.513600	1.302300	3.258100
C	-1.695200	0.166200	1.713000
H	-1.466600	-1.791400	0.854000
H	-2.197700	2.043900	2.660300
C	-0.652400	3.029000	-0.932800
H	0.050000	3.683700	-0.393800
C	-1.911300	3.786800	-1.362700
H	-1.609100	4.605000	-2.036200
H	-2.549900	3.110200	-1.951600
C	-2.706300	4.337000	-0.184300
H	-2.054500	4.975000	0.436100
H	-3.022100	3.492600	0.455400
C	-3.930800	5.126800	-0.632500
H	-4.512100	5.489400	0.225900
H	-3.638700	5.999200	-1.235500
H	-4.594300	4.502800	-1.251100
H	-1.023700	2.328900	-0.116800

Ti-3(O,S)_R_2

C	0.154400	2.675500	-0.578300
C	-1.210200	3.069600	-0.080700
C	-2.001900	2.199100	0.694800
H	-1.103200	5.000200	-1.024600
H	0.115100	1.917200	-1.374700
C	-1.716600	4.323100	-0.427700
C	-3.289400	2.571400	1.147100
C	-3.752000	3.832500	0.758800
C	-2.989400	4.700000	-0.021500
H	-4.738400	4.160700	1.080300
H	-3.387300	5.676100	-0.298300
O	-1.486100	0.989300	1.021100
C	0.026600	-2.438800	-1.465500
C	1.501600	-2.567900	-1.204300
C	2.031600	-2.135800	0.028300
H	1.922900	-3.490700	-3.105200
H	-0.550500	-2.964300	-0.688400
C	2.334600	-3.170100	-2.146600
C	3.373200	-2.401300	0.382600
C	4.166700	-3.014300	-0.593600
C	3.675200	-3.376600	-1.846700
H	5.212200	-3.221500	-0.373600
H	4.336800	-3.843500	-2.575900
O	1.197200	-1.453400	0.850900
Ti	-0.226900	-0.324400	1.124900
C	-2.239900	-0.683100	-1.729700
C	-3.037700	-1.813300	-1.585500
C	-2.817100	0.543200	-2.089500
C	-4.418000	-1.727400	-1.780000
H	-2.609500	-2.782500	-1.327600
C	-4.184500	0.633000	-2.270700
H	-2.197200	1.432600	-2.219300
C	-5.000300	-0.498600	-2.107000
H	-5.020500	-2.627000	-1.670000
H	-4.657400	1.578500	-2.536100
C	2.776700	1.789700	-0.111900
C	2.946000	0.800400	-1.089900
C	3.853200	2.599400	0.244700
C	4.177800	0.623300	-1.693700
H	2.114800	0.157600	-1.377100
C	5.099600	2.427200	-0.358500
H	3.725400	3.369400	1.006500
C	5.268000	1.434100	-1.332300
H	4.330600	-0.147000	-2.449700
H	5.925700	3.070400	-0.061300
C	3.924900	-2.072900	1.774900
C	3.897200	-0.557600	2.017300
C	3.082300	-2.806200	2.832800
C	5.376800	-2.536900	1.935200
H	4.523700	-0.035700	1.277300
H	2.877800	-0.160400	1.936300
H	4.287600	-0.333300	3.023000
H	3.186400	-3.896000	2.720000
H	3.425800	-2.533700	3.843300
H	2.017000	-2.556000	2.740900
H	5.712600	-2.310400	2.957500
H	5.480400	-3.620800	1.781300
H	6.051100	-2.016200	1.239200
C	-4.131300	1.643200	2.032100
C	-4.478000	0.358800	1.258000
C	-3.359600	1.315600	3.323300
C	-5.450600	2.300700	2.452600
H	-5.206200	0.582200	0.463300
H	-3.594600	-0.094300	0.785900
H	-4.936000	-0.379300	1.936900
H	-3.125200	2.238500	3.876000
H	-3.977100	0.677600	3.974700
H	-2.420000	0.792400	3.110000
H	-6.018100	1.597200	3.079000
H	-5.281400	3.213800	3.042300
H	-6.077600	2.553700	1.585600
C	-1.432400	-1.742200	1.905300

H	-2.318100	-1.356000	2.432900
H	-1.723800	-1.754300	0.809700
S	-0.475100	-0.673800	-1.438000
S	1.233400	2.002500	0.756600
H	-0.241700	-2.838000	-2.451700
H	0.680200	3.554000	-0.972700
C	-1.009500	-3.126500	2.356700
H	-0.776900	-3.098100	3.433100
H	-0.082400	-3.422700	1.840400
C	-2.106000	-4.165600	2.110200
H	-1.793400	-5.157000	2.466100
H	-3.035100	-3.891500	2.631000
H	-2.335800	-4.250400	1.036200
O	6.422100	1.178400	-1.973200
O	-6.319900	-0.295800	-2.273000
C	-7.197900	-1.406000	-2.090200
H	-7.053900	-1.809100	-1.071100
H	-6.965100	-2.200000	-2.819800
C	-8.598700	-0.914800	-2.270500
H	-8.881800	-0.051900	-1.661000
C	-9.473700	-1.486000	-3.093400
H	-9.197000	-2.344200	-3.711300
H	-10.498100	-1.120300	-3.174100
C	7.547600	2.010500	-1.694100
H	7.834300	1.921000	-0.632400
H	7.274000	3.061300	-1.897500
C	8.667700	1.576500	-2.584700
H	8.438800	1.543400	-3.653700
C	9.882700	1.272900	-2.136400
H	10.117300	1.298800	-1.068900
H	10.686700	0.995400	-2.819100
C	0.047700	-0.470400	3.856000
H	-0.987200	-0.592400	4.179700
H	0.710800	-1.335200	3.939900
C	0.527700	0.727700	3.474800
H	1.592800	0.863800	3.278300
H	-0.108600	1.617200	3.442400

Ti-3(O,S)_TS_2

C	0.173600	2.719600	-0.322000
C	-1.197900	3.062700	0.196100
C	-2.003200	2.124600	0.872300
H	-1.074300	5.073200	-0.562000
H	0.144800	2.060200	-1.202900
C	-1.700000	4.343600	-0.044800
C	-3.303000	2.455900	1.324000
C	-3.761000	3.745500	1.040200
C	-2.982600	4.682000	0.362600
H	-4.756400	4.041000	1.365700
H	-3.376500	5.679400	0.168500
O	-1.492600	0.890700	1.102400
C	0.056700	-2.306200	-1.614800
C	1.520800	-2.492600	-1.333000
C	2.029800	-2.174600	-0.058000
H	1.964700	-3.255600	-3.297300
H	-0.546600	-2.849300	-0.870300
C	2.363700	-3.025100	-2.307800
C	3.368300	-2.467700	0.289600
C	4.170700	-3.012300	-0.719900
C	3.695900	-3.273900	-2.003500
H	5.211700	-3.243200	-0.502900
H	4.364900	-3.691200	-2.755700
O	1.182100	-1.565800	0.809300
Ti	-0.185200	-0.385500	1.174600
C	-2.159000	-0.503100	-1.787000
C	-2.964300	-1.637200	-1.765000
C	-2.734800	0.755600	-2.017200
C	-4.345600	-1.526200	-1.951600
H	-2.539900	-2.630700	-1.620400
C	-4.100500	0.869800	-2.193200
H	-2.113000	1.651800	-2.051100
C	-4.921900	-0.269000	-2.152300
H	-4.951300	-2.430100	-1.937900
H	-4.567900	1.840500	-2.358700
C	2.785000	1.762200	0.047600
C	2.968700	0.839500	-0.989800
C	3.846300	2.570000	0.450600
C	4.199400	0.727700	-1.611000
H	2.150500	0.196000	-1.306800
C	5.090300	2.466900	-0.173000
H	3.709000	3.285600	1.262200
C	5.272600	1.542200	-1.209700
H	4.363300	0.007700	-2.412700
H	5.903500	3.109300	0.159200
C	3.926200	-2.209900	1.694900
C	3.969300	-0.699600	1.964700
C	3.050400	-2.918100	2.741800
C	5.352900	-2.749200	1.849300
H	4.652100	-0.195600	1.262300
H	2.979200	-0.245500	1.837400
H	4.321300	-0.507900	2.991100
H	3.025900	-4.002800	2.555900
H	3.463600	-2.753500	3.748900
H	2.020200	-2.541500	2.717700
H	5.692300	-2.569600	2.879600
H	5.404300	-3.831900	1.662200
H	6.058200	-2.241900	1.175400
C	-4.160300	1.457300	2.111500
C	-4.481900	0.232100	1.236900
C	-3.415300	1.046200	3.393700
C	-5.496800	2.068000	2.548900
H	-5.212000	0.507400	0.460900
H	-3.593200	-0.169300	0.728900
H	-4.934200	-0.563200	1.853000
H	-3.239900	1.924200	4.033900
H	-4.019400	0.323600	3.965700
H	-2.443800	0.594700	3.163900
H	-6.071900	1.309600	3.100200
H	-5.354400	2.930900	3.215900
H	-6.103600	2.384400	1.688400
C	-1.491700	-1.880900	1.889400
H	-2.460900	-1.516600	2.256000
H	-1.544700	-1.729700	0.760200
S	-0.390300	-0.529900	-1.522300
S	1.241200	1.892600	0.934900
H	-0.203800	-2.662200	-2.619300
H	0.707800	3.635500	-0.603500
C	-1.261700	-3.356400	2.145000
H	-1.356900	-3.554900	3.223300
H	-0.234300	-3.627000	1.849900
C	-2.277400	-4.216000	1.390300
H	-2.129000	-5.279700	1.619800
H	-3.307900	-3.945500	1.664000
H	-2.175200	-4.093300	0.300800
O	6.425700	1.357100	-1.876000
O	-6.241300	-0.042100	-2.301300
C	-7.125700	-1.158800	-2.230900
H	-6.992800	-1.655800	-1.252200
H	-6.890400	-1.883700	-3.028600
C	-8.522500	-0.645500	-2.378000
H	-8.806600	0.162600	-1.697800
C	-9.393300	-1.137100	-3.254900
H	-9.115200	-1.939000	-3.943900
H	-10.415100	-0.760000	-3.312400
C	7.529300	2.206900	-1.564100
H	7.839300	2.060900	-0.515300
H	7.217800	3.258700	-1.696400
C	8.645100	1.867700	-2.499800
H	8.391600	1.878700	-3.563800
C	9.883300	1.597400	-2.095600
H	10.143700	1.580200	-1.034000
H	10.681000	1.393400	-2.810900
C	-0.323900	-1.063200	3.546100
H	-1.296200	-0.979200	4.033300
H	0.192400	-2.017900	3.658400
C	0.423400	0.075700	3.280100
H	1.510900	-0.006400	3.218100
H	-0.001100	1.065600	3.466800

Ti-3(O,S)_P_2

C	0.584600	2.820300	0.136100
C	-0.795800	3.205600	0.582900
C	-1.688500	2.253000	1.108800
H	-0.510000	5.268500	0.034300
H	0.581900	2.269600	-0.817100
C	-1.208100	4.530500	0.433000
C	-2.999000	2.608800	1.502300
C	-3.369300	3.943800	1.309700
C	-2.499800	4.897100	0.782600
H	-4.370700	4.262200	1.592300
H	-2.831500	5.927800	0.660700
O	-1.225400	0.986500	1.255800
C	0.016300	-1.899700	-2.053100
C	1.498300	-2.097600	-1.879000
C	2.080200	-2.005700	-0.598700
H	1.837500	-2.548300	-3.958600
H	-0.536900	-2.645600	-1.463000
C	2.282000	-2.491100	-2.963400
C	3.394400	-2.455500	-0.350800
C	4.138500	-2.845500	-1.471300
C	3.613300	-2.835400	-2.762600
H	5.166600	-3.176300	-1.337300
H	4.235000	-3.136500	-3.605400
O	1.326700	-1.461500	0.387100
Ti	0.045300	-0.309600	1.022300
C	-2.277900	-0.191300	-1.847500
C	-3.101400	-1.310500	-1.756600
C	-2.812700	1.046500	-2.228200
C	-4.460100	-1.208500	-2.053700
H	-2.702200	-2.282000	-1.459500
C	-4.163400	1.154400	-2.509000
H	-2.168500	1.924400	-2.304500
C	-5.000100	0.029100	-2.427600
H	-5.082400	-2.099100	-1.990900
H	-4.605600	2.105200	-2.806300
C	3.072000	1.641500	0.491200
C	3.184300	1.001400	-0.749600
C	4.194000	2.204400	1.093000
C	4.417400	0.913600	-1.369300
H	2.309300	0.561700	-1.231500
C	5.439900	2.122200	0.471900
H	4.104100	2.704200	2.058500
C	5.557800	1.471700	-0.763800
H	4.533100	0.408800	-2.328700
H	6.304500	2.566300	0.961100
C	3.943900	-2.600500	1.075100
C	4.034000	-1.248800	1.797600
C	3.021300	-3.554500	1.854900
C	5.351400	-3.208000	1.070400
H	4.671200	-0.549400	1.235600
H	3.046600	-0.787900	1.933300
H	4.479900	-1.396000	2.793300
H	3.009100	-4.550300	1.386700
H	3.383800	-3.665800	2.888400
H	1.989800	-3.176300	1.884700
H	5.692400	-3.333700	2.108000
H	5.370500	-4.197100	0.590100
H	6.073400	-2.554400	0.557700

C	-3.962200	1.594900	2.130700
C	-4.234700	0.452200	1.141000
C	-3.353500	1.054400	3.435300
C	-5.311300	2.232900	2.479800
H	-4.698100	0.846600	0.224300
H	-3.312800	-0.072200	0.856800
H	-4.928000	-0.277900	1.589000
H	-3.201100	1.869100	4.158800
H	-4.035200	0.318100	3.890800
H	-2.385400	0.571700	3.253600
H	-5.962900	1.467900	2.926400
H	-5.203200	3.046800	3.211400
H	-5.821400	2.626700	1.588400
C	-1.318000	-2.274200	1.713900
C	-0.409300	-1.463500	2.607600
H	0.488100	-1.976800	2.974000
H	-0.929800	-0.900700	3.393700
S	-0.531800	-0.242600	-1.486600
S	1.510400	1.754900	1.343800
H	-0.274100	-1.984900	-3.107700
H	1.214800	3.710300	0.016600
O	6.706600	1.329000	-1.445500
O	-6.293800	0.242200	-2.721000
C	-7.200300	-0.856700	-2.626300
H	-7.155100	-1.268300	-1.601600
H	-6.913500	-1.649000	-3.338400
C	-8.571200	-0.340400	-2.925500
H	-8.890600	0.522200	-2.333800
C	-9.381400	-0.887900	-3.827000
H	-9.069100	-1.745400	-4.428800
H	-10.387900	-0.501100	-3.991000
C	7.887300	1.929700	-0.911700
H	8.130900	1.484000	0.067800
H	7.704800	3.010200	-0.772400
C	8.995400	1.704200	-1.889800
H	8.791300	2.015900	-2.918200
C	10.174400	1.187800	-1.553700
H	10.384900	0.869600	-0.529100
H	10.972200	1.072600	-2.288200
C	-2.698700	-2.571900	2.305100
H	-3.147100	-1.625600	2.645200
H	-3.360200	-2.973500	1.519500
C	-2.621000	-3.554900	3.469900
H	-2.178000	-4.501900	3.118000
H	-1.933500	-3.155500	4.234200
C	-3.989100	-3.816600	4.088800
H	-4.428300	-2.885100	4.477900
H	-4.686500	-4.231200	3.345500
H	-3.921300	-4.530100	4.920700
H	-0.813200	-3.190700	1.372400
H	-1.520800	-1.706100	0.744400

Ti-3(half)_R_2

C	0.900300	-2.044800	-0.962500
C	2.297200	-1.892000	-0.770700
C	2.837700	-0.716600	-0.162000
H	2.743100	-3.862400	-1.569200
H	0.498600	-3.036900	-1.208800
C	3.158100	-2.959900	-1.117500
C	4.209300	-0.576100	0.093900
C	5.010400	-1.657400	-0.305700
C	4.510900	-2.828400	-0.896800
H	6.084900	-1.596200	-0.137400
H	5.197000	-3.628900	-1.170700
O	1.959400	0.249700	0.198900
N	0.045000	-1.049300	-0.843500
C	4.790700	0.661900	0.788100
C	4.453100	1.932300	-0.014200
C	4.217500	0.755900	2.213300
C	6.317500	0.570400	0.896000
H	4.795500	1.845000	-1.056100
H	3.376000	2.150700	-0.010600
H	4.967900	2.792700	0.437000
H	4.507900	-0.119900	2.811500
H	4.615400	1.652300	2.711100
H	3.119700	0.821400	2.210300
H	6.693000	1.471100	1.399900
H	6.637600	-0.295900	1.492700
H	6.797300	0.519400	-0.092700
C	0.561000	1.968500	-1.698800
H	1.600200	2.317600	-1.767500
H	0.245900	1.492300	-2.642200
C	-6.207500	0.067900	0.189200
H	-5.821700	1.080500	0.398000
H	-6.291300	-0.078800	-0.899300
C	-7.513600	-0.174000	0.869000
H	-7.522200	-0.068000	1.956800
C	-8.622900	-0.472200	0.197700
H	-8.622300	-0.578600	-0.890400
H	-9.574500	-0.611700	0.711900
O	-5.249200	-0.884600	0.716800
C	-4.009600	-0.876000	0.276500
C	-3.490800	0.021700	-0.674400
C	-3.160600	-1.875000	0.832600
C	-2.161800	-0.104700	-1.079900
H	-4.123200	0.775900	-1.139400
C	-1.843800	-1.975700	0.458800
H	-3.595100	-2.553600	1.567700
C	-1.326100	-1.095300	-0.524600
H	-1.800400	0.500600	-1.918800
H	-1.194500	-2.728400	0.911500
C	-0.441100	2.935600	-1.101900
H	-1.056200	2.435800	-0.329300
H	0.066900	3.740800	-0.552000
C	-1.450900	3.506300	-2.105500
H	-2.185800	4.147400	-1.603100
H	-0.916800	4.107500	-2.852500
H	-1.982900	2.703100	-2.636100
Ti	0.283100	0.750000	-0.144400
C	-0.639500	0.733600	2.231800
H	-1.720100	0.599400	2.107200
H	-0.047200	-0.148200	2.503400
C	-0.068100	1.952300	2.147600
H	1.004200	2.092400	2.334000
H	-0.668700	2.849800	1.975700

Ti-3(half)_TS_2

C	-0.951400	-2.179500	1.104300
C	-2.346600	-1.971500	0.868100
C	-2.823800	-0.834700	0.150300
H	-2.894400	-3.831200	1.837000
H	-0.602400	-3.179100	1.397900
C	-3.260100	-2.952800	1.302500
C	-4.185800	-0.641300	-0.116600
C	-5.046600	-1.640800	0.371000
C	-4.608800	-2.774400	1.063100
H	-6.115300	-1.539300	0.188600
H	-5.332700	-3.513200	1.404800
O	-1.901000	0.060500	-0.316700
N	-0.073200	-1.221300	0.966800
C	-4.709800	0.570800	-0.898600
C	-4.346800	1.865200	-0.149400
C	-4.109900	0.579300	-2.315900
C	-6.236600	0.524400	-1.035400
H	-4.771500	1.866000	0.865400
H	-3.258600	2.003600	-0.074600
H	-4.761000	2.728700	-0.689900
H	-4.361700	-0.345700	-2.854800
H	-4.529600	1.423000	-2.883000
H	-3.016800	0.689200	-2.302800
H	-6.570000	1.409900	-1.593200
H	-6.572300	-0.361400	-1.593900
H	-6.739600	0.541600	-0.057500
C	-0.209000	2.412000	0.638100
H	-1.184200	2.853200	0.361600
H	-0.447600	1.686100	1.429400
C	6.121200	0.029600	-0.207800
H	5.697400	1.001400	-0.514900
H	6.207300	-0.007600	0.889700
C	7.437500	-0.226000	-0.862500
H	7.446300	-0.217500	-1.955300
C	8.553800	-0.426500	-0.166500
H	8.553100	-0.435900	0.926700
H	9.511000	-0.579600	-0.666100
O	5.202500	-1.006300	-0.639500
C	3.967600	-1.015300	-0.186800
C	3.409200	-0.049100	0.672400
C	3.164200	-2.103000	-0.628000
C	2.088200	-0.197200	1.100400
H	4.006100	0.779600	1.049700
C	1.855300	-2.233000	-0.228100
H	3.623900	-2.828200	-1.301000
C	1.300400	-1.286400	0.668500
H	1.699500	0.475400	1.877400
H	1.243200	-3.058700	-0.597400
C	0.750700	3.436400	1.213800
H	1.736300	2.977700	1.395600
H	0.895400	4.228500	0.463600
C	0.198600	4.047700	2.505200
H	0.898100	4.802500	2.886800
H	-0.768600	4.538300	2.328700
H	0.064800	3.285400	3.286600
Ti	-0.205200	0.486200	-0.030600
C	0.607400	0.969300	-1.992600
H	1.455400	0.267700	-1.995700
H	-0.214600	0.771700	-2.690500
C	0.777100	2.235000	-1.455200
H	0.097000	3.047900	-1.721400
H	1.733600	2.521600	-1.010400

Ti-3(half)_P_2

C	1.456400	-2.200300	0.456100
C	2.832300	-1.870300	0.350200
C	3.264300	-0.560700	-0.032100
H	3.458700	-3.884800	0.866800
H	1.167100	-3.227100	0.715300
C	3.789100	-2.886800	0.574300
C	4.616800	-0.250600	-0.216800
C	5.515000	-1.307200	0.022300
C	5.127100	-2.596200	0.411400
H	6.580300	-1.114700	-0.098000
H	5.884500	-3.361000	0.576900
O	2.303400	0.385300	-0.200100
N	0.505900	-1.325000	0.213100
C	5.095100	1.142700	-0.644500
C	4.499800	1.491400	-2.020200
C	4.677700	2.182400	0.411100
C	6.622800	1.190300	-0.769900
H	4.811000	0.759000	-2.779500
H	3.401900	1.530700	-2.002700
H	4.865500	2.479000	-2.335900
H	5.100400	1.934000	1.395800
H	5.063300	3.169900	0.118700
H	3.586300	2.262500	0.508100
H	6.920200	2.199100	-1.086000
H	7.122600	0.986200	0.188500
H	6.997600	0.485200	-1.526200

C	0.259900	1.610100	1.518400
H	-0.144100	1.008700	2.348500
H	1.171200	2.152500	1.807600
C	-0.782100	2.395100	0.740600
H	-0.523100	3.462400	0.682800
C	-5.723900	-0.464100	-1.053000
H	-5.328300	0.542700	-1.274200
H	-5.539300	-1.132300	-1.909200
C	-7.172700	-0.417000	-0.700800
H	-7.444600	0.206500	0.155300
C	-8.099900	-1.068000	-1.398700
H	-7.836700	-1.692500	-2.256300
H	-9.157300	-0.991700	-1.142300
O	-5.003700	-0.973900	0.099200
C	-3.690000	-1.063100	0.055800
C	-2.889500	-0.662300	-1.030000
C	-3.075100	-1.608600	1.216700
C	-1.506800	-0.832400	-0.947600
H	-3.329500	-0.277600	-1.948000
C	-1.708100	-1.741900	1.311800
H	-3.728800	-1.912300	2.035600
C	-0.905300	-1.377300	0.208800
H	-0.903500	-0.691300	-1.861100
H	-1.248400	-2.141200	2.217700
Ti	0.534500	0.568100	-0.139200
C	-2.225000	2.159800	1.182700
H	-2.394600	1.073100	1.285700
H	-2.332500	2.588700	2.192000
C	-3.262400	2.759400	0.240600
H	-3.072700	3.838000	0.118900
H	-3.141500	2.308100	-0.762400
C	-4.681300	2.536300	0.754100
H	-4.880000	1.465600	0.923300
H	-4.836600	3.054600	1.711100
H	-5.425700	2.920800	0.044200
H	-0.766000	2.119100	-0.379900

Ni-3(Octahedral)_R_2

C	0.545200	-2.530100	0.411600
C	1.950100	-2.422600	0.725800
C	2.541100	-1.196400	1.177200
H	2.246000	-4.486600	0.175500
H	0.202200	-3.552000	0.171300
C	2.739400	-3.573700	0.522500
C	3.970300	-1.195400	1.434900
C	4.688400	-2.354900	1.199900
C	4.098700	-3.551900	0.738300
H	5.764600	-2.357800	1.379700
H	4.711000	-4.438400	0.572300
O	1.866200	-0.124800	1.362300
N	-0.311600	-1.568300	0.320700
C	4.636600	0.081100	1.960500
C	4.473200	1.230800	0.949500
C	4.006100	0.471400	3.309700
C	6.138800	-0.114400	2.195300
H	5.064400	1.029900	0.041300
H	3.421900	1.368500	0.662700
H	4.845600	2.170300	1.391800
H	4.155700	-0.333300	4.047600
H	4.485100	1.386500	3.695900
H	2.931000	0.655300	3.197500
H	6.569100	0.828000	2.568000
H	6.338600	-0.897200	2.944000
H	6.670600	-0.379800	1.267100
C	-6.324100	-1.949300	-1.797300
H	-6.159500	-0.889000	-1.526200
H	-5.964700	-2.094000	-2.832100
C	-7.778800	-2.286900	-1.694200
H	-8.179700	-2.312500	-0.676000
C	-8.567300	-2.520000	-2.740600
H	-8.171600	-2.507300	-3.759700
H	-9.632000	-2.724800	-2.617500
O	-5.624800	-2.782600	-0.893900
C	-4.302100	-2.494800	-0.688000
C	-3.578700	-1.560900	-1.435400
C	-3.680800	-3.174400	0.361700
C	-2.256200	-1.286900	-1.100000
H	-4.034000	-1.009100	-2.257000
C	-2.358600	-2.894000	0.690800
H	-4.269800	-3.889500	0.936700
C	-1.638700	-1.934300	-0.030500
H	-1.685900	-0.541200	-1.651900
H	-1.889500	-3.377000	1.549400
C	-0.604700	1.887300	-2.042400
C	-1.965100	2.114000	-1.576100
C	-2.454500	1.672500	-0.291700
H	-2.377900	3.161900	-3.408300
H	-0.303300	2.500500	-2.916000
C	-2.800100	2.832000	-2.454000
C	-3.828100	2.014500	0.037500
C	-4.601400	2.692900	-0.891200
C	-4.113600	3.108600	-2.143400
H	-5.635100	2.937400	-0.643500
H	-4.756500	3.653800	-2.834700
O	-1.758700	1.005500	0.557400
N	0.206700	1.032400	-1.540800
C	-4.386600	1.643600	1.417700
C	-4.408800	0.115700	1.599100
C	-3.531700	2.308500	2.512600
C	-5.825100	2.139000	1.610200
H	-5.155900	-0.336800	0.926200
H	-3.432900	-0.333200	1.374800
H	-4.691700	-0.135800	2.636000
H	-3.609300	3.405300	2.436100
H	-3.892100	2.005000	3.509900
H	-2.476100	2.030900	2.415000
H	-6.168200	1.855300	2.617500
H	-5.895700	3.234400	1.524300
H	-6.517000	1.688000	0.881500
C	6.286100	-0.616600	-2.138000
H	5.887200	-0.905800	-1.146200
H	6.092300	-1.449800	-2.837700
C	7.754300	-0.343800	-2.037100
H	8.023800	0.549700	-1.464800
C	8.696000	-1.125300	-2.560600
H	8.432300	-2.013500	-3.141000
H	9.757100	-0.910500	-2.424000
O	5.652300	0.572100	-2.573700
C	4.289300	0.618900	-2.440500
C	3.500300	-0.492500	-2.135600
C	3.696400	1.879000	-2.562700
C	2.141400	-0.316700	-1.899600
H	3.928900	-1.487700	-2.016100
C	2.336800	2.043200	-2.324100
H	4.339500	2.731700	-2.783900
C	1.539300	0.942600	-1.969000
H	1.521900	-1.164000	-1.608600
H	1.900400	3.043700	-2.343700
C	0.458700	2.147600	1.741700
H	-0.296300	2.265000	2.544500
H	1.448500	2.067200	2.225100
C	0.426600	3.369700	0.833500
H	1.170900	3.246900	0.024900
H	-0.557400	3.447700	0.339300
C	0.713900	4.679700	1.572200
H	0.695300	5.553900	0.899700
H	-0.034200	4.846300	2.364400
H	1.703600	4.643700	2.056700
Ni	0.089900	0.443000	0.874600
C	-1.229700	-0.773800	3.425100
H	-0.164600	-0.604500	3.611700
H	-1.706400	-0.114600	2.692500
C	-1.910200	-1.743100	4.035200
H	-2.969800	-1.906900	3.819500
H	-1.438000	-2.411200	4.760600

Ni-3(Octahedral)_TS_2

C	-0.786700	2.549500	0.533600
C	-2.203500	2.468300	0.783300
C	-2.880800	1.264300	1.234900
H	-2.390800	4.530500	0.168800
H	-0.442800	3.568400	0.279700
C	-2.940400	3.643500	0.500400
C	-4.339800	1.342900	1.375600
C	-4.985500	2.519000	1.057600
C	-4.309000	3.683400	0.614100
H	-6.071500	2.575200	1.157400
H	-4.869200	4.589400	0.383500
O	-2.257500	0.203200	1.491600
N	0.116600	1.616800	0.486400
C	-5.089300	0.116900	1.910100
C	-4.895100	-1.095000	0.982100
C	-4.562600	-0.226900	3.316000
C	-6.595800	0.371700	2.027400
H	-5.408200	-0.936500	0.020000
H	-3.829900	-1.275200	0.787600
H	-5.331600	-1.994800	1.448500
H	-4.716600	0.622700	4.000600
H	-5.106600	-1.098200	3.718400
H	-3.491600	-0.459000	3.272000
H	-7.087600	-0.536200	2.410800
H	-6.819200	1.197400	2.721000
H	-7.046900	0.609500	1.050100
C	6.164100	2.050300	-1.465200
H	5.911600	0.988100	-1.279300
H	5.885400	2.289200	-2.507300
C	7.627400	2.275400	-1.245400
H	7.956700	2.208200	-0.203300
C	8.502400	2.509600	-2.220400
H	8.179000	2.586500	-3.262100
H	9.567900	2.625200	-2.015100
O	5.459800	2.869600	-0.548800
C	4.124000	2.607000	-0.398700
C	3.399600	1.758200	-1.237300
C	3.492900	3.206500	0.694400
C	2.068000	1.482300	-0.944100
H	3.859300	1.265700	-2.094000
C	2.162800	2.915700	0.982700
H	4.084000	3.858400	1.338300
C	1.441600	2.030300	0.172500
H	1.503400	0.799600	-1.574300
H	1.686000	3.337500	1.869800
C	0.798600	-1.597600	-1.733700
C	2.218000	-1.736400	-1.522800
C	2.879500	-1.453700	-0.260600
H	2.433200	-2.315500	-3.592800
H	0.468500	-1.933800	-2.733700
C	2.970800	-2.113900	-2.660700
C	4.338200	-1.610800	-0.232800
C	5.000400	-1.963200	-1.389900
C	4.340700	-2.211800	-2.619600
H	6.087000	-2.070600	-1.371100
H	4.914200	-2.493200	-3.502800
O	2.240200	-1.095500	0.761900
N	-0.118100	-1.086400	-0.968800
C	5.070700	-1.403900	1.097000
C	4.880900	0.036500	1.604400
C	4.519600	-2.394700	2.139600

C	6.577000	-1.654200	0.969100
H	5.433800	0.748300	0.970500
H	3.820100	0.318800	1.601800
H	5.275700	0.128000	2.630700
H	4.659700	-3.431200	1.792500
H	5.056400	-2.273000	3.095400
H	3.449400	-2.217300	2.300900
H	7.054800	-1.495700	1.948700
H	6.795500	-2.684900	0.648000
H	7.047300	-0.962000	0.251900
C	-6.172400	0.275300	-2.438000
H	-5.945100	0.698300	-1.440200
H	-5.885400	1.024500	-3.198000
C	-7.630600	-0.047800	-2.534400
H	-7.958800	-0.892700	-1.920600
C	-8.502300	0.636800	-3.270900
H	-8.180600	1.476800	-3.892300
H	-9.565000	0.388300	-3.273300
O	-5.452600	-0.931200	-2.615900
C	-4.120300	-0.903600	-2.301200
C	-3.414900	0.264400	-2.004600
C	-3.472100	-2.139400	-2.242700
C	-2.086500	0.175100	-1.602900
H	-3.887100	1.246300	-2.033500
C	-2.141700	-2.216100	-1.840000
H	-4.047700	-3.036500	-2.472700
C	-1.439300	-1.054200	-1.497000
H	-1.539100	1.075100	-1.333200
H	-1.648500	-3.185800	-1.743700
C	-0.606400	-2.341700	1.646400
H	-1.214000	-2.678500	2.495800
H	-1.351000	-2.144100	0.855700
C	0.361400	-3.444100	1.251500
H	0.896100	-3.181800	0.328100
H	1.145100	-3.554600	2.021800
C	-0.346400	-4.789400	1.070800
H	0.358400	-5.584600	0.779500
H	-0.847700	-5.103100	2.001100
H	-1.122600	-4.722200	0.291200
C	0.205800	-1.094100	3.169600
H	-0.688700	-1.261100	3.769000
H	0.997000	-1.838400	3.282600
C	0.539900	0.228900	2.870700
H	1.580000	0.489000	2.658500
H	-0.147200	1.026800	3.155600
Ni	-0.012600	-0.375300	1.020000

Ni-3(Octahedral)_P_2

C	0.788900	0.158100	2.770000
C	2.068900	0.809900	2.535400
C	2.551100	1.190500	1.229700
H	2.415400	0.802200	4.658200
H	0.460900	0.157600	3.829400
C	2.829500	1.091600	3.687300
C	3.839900	1.855800	1.171700
C	4.546000	2.072500	2.344400
C	4.063100	1.700200	3.612300
H	5.515800	2.569100	2.296300
H	4.648700	1.905300	4.508800
O	1.918200	0.965300	0.135100
N	0.072200	-0.402500	1.866900
C	4.379700	2.329800	-0.184800
C	4.597700	1.133500	-1.127100
C	3.387700	3.320300	-0.821500
C	5.724800	3.052200	-0.044300
H	5.350100	0.445200	-0.707700
H	3.664000	0.578700	-1.279200
H	4.968100	1.488100	-2.104200
H	3.250600	4.196600	-0.167200
H	3.778300	3.672200	-1.791200
H	2.412300	2.844800	-0.977300
H	6.062500	3.378900	-1.040100
H	5.646200	3.944400	0.596200
H	6.501500	2.392500	0.374000
C	-5.781900	-2.743400	1.281600
H	-5.462600	-2.254900	0.340500
H	-5.441400	-3.794300	1.251600
C	-7.271000	-2.677200	1.415900
H	-7.680500	-1.675600	1.583100
C	-8.076900	-3.731600	1.314700
H	-7.673400	-4.735700	1.158200
H	-9.161500	-3.629500	1.378500
O	-5.216900	-2.056000	2.382900
C	-3.880200	-1.767300	2.297900
C	-3.025800	-2.308200	1.336000
C	-3.394800	-0.818700	3.203900
C	-1.709100	-1.863400	1.271200
H	-3.376200	-3.027300	0.595100
C	-2.083400	-0.369700	3.118400
H	-4.094100	-0.392400	3.924300
C	-1.216300	-0.885400	2.139500
H	-1.038900	-2.239800	0.498900
H	-1.747600	0.437400	3.771600
C	-0.307200	-1.802200	-2.001900
C	-1.729200	-1.590300	-2.118400
C	-2.382100	-0.420200	-1.600900
H	-1.928400	-3.499200	-3.101900
H	0.062200	-2.720100	-2.492600
C	-2.470700	-2.627200	-2.724000
C	-3.829200	-0.352200	-1.731300
C	-4.493400	-1.409200	-2.328000
C	-3.840300	-2.556900	-2.827800
H	-5.579500	-1.365900	-2.423100
H	-4.414200	-3.358600	-3.292800
O	-1.745600	0.538200	-1.040700
N	0.544200	-1.089300	-1.340900
C	-4.581500	0.868100	-1.187900
C	-4.381200	0.963200	0.334600
C	-4.072300	2.152000	-1.865900
C	-6.088800	0.776600	-1.451200
H	-4.925400	0.150600	0.842300
H	-3.317500	0.894800	0.601500
H	-4.778800	1.922100	0.708500
H	-4.177000	2.077600	-2.960500
H	-4.664800	3.016200	-1.521200
H	-3.018500	2.324900	-1.622200
H	-6.578500	1.670400	-1.034500
H	-6.315800	0.736200	-2.528400
H	-6.540000	-0.105100	-0.968200
C	6.569500	-2.854600	-0.078200
H	6.472900	-1.884100	0.444000
H	6.165400	-3.639300	0.586800
C	8.007600	-3.123300	-0.395800
H	8.446700	-2.468600	-1.155000
C	8.740000	-4.062600	0.197300
H	8.304900	-4.728200	0.947700
H	9.796300	-4.197400	-0.041000
O	5.862300	-2.807800	-1.300700
C	4.550800	-2.419300	-1.244700
C	3.845300	-2.197400	-0.057400
C	3.916200	-2.227500	-2.472900
C	2.525600	-1.758800	-0.108700
H	4.313100	-2.331500	0.916700
C	2.593200	-1.799400	-2.516300
H	4.490100	-2.395200	-3.384700
C	1.887100	-1.557400	-1.333600
H	1.968900	-1.546600	0.804200
H	2.109000	-1.613100	-3.476900
C	-1.505600	4.659900	-0.264400
H	-2.489600	4.284200	0.073000
H	-1.045100	5.147300	0.614700
C	-0.646800	3.466600	-0.690900
H	-1.110500	3.014200	-1.587100
H	0.340000	3.839700	-1.020300
C	-0.470200	2.400500	0.386100
H	-1.442100	2.201600	0.878500
H	0.245900	2.735000	1.159100
C	-1.716600	5.690600	-1.369700
H	-0.735600	6.059500	-1.716400
H	-2.180700	5.190800	-2.238100
C	-2.583700	6.867300	-0.931800
H	-2.729100	7.600200	-1.740100
H	-3.577800	6.519200	-0.608500
H	-2.126500	7.392800	-0.078100
Ni	0.066300	0.697300	-0.371100

Ni-3(half)_R_2

C	0.044600	-1.643500	-0.180000
C	1.422200	-2.009900	-0.293400
C	2.486000	-1.083100	-0.060400
H	0.852900	-4.038100	-0.789500
H	-0.665000	-2.467500	-0.359600
C	1.694100	-3.364400	-0.606800
C	3.842600	-1.586500	-0.081700
C	4.037600	-2.918700	-0.395600
C	2.984800	-3.819500	-0.673300
H	5.054400	-3.309200	-0.428300
H	3.205200	-4.858100	-0.917100
O	2.276200	0.167400	0.170700
N	-0.464200	-0.486200	0.131600
C	5.012800	-0.655500	0.258400
C	5.085800	0.510200	-0.742400
C	4.836300	-0.105000	1.685000
C	6.355000	-1.393800	0.208300
H	5.194500	0.130900	-1.770600
H	4.183800	1.129600	-0.688100
H	5.961900	1.138900	-0.514900
H	4.843100	-0.927800	2.417000
H	5.668700	0.575300	1.927100
H	3.891800	0.444800	1.780300
H	7.160000	-0.693400	0.476100
H	6.389100	-2.232500	0.920200
H	6.570900	-1.782000	-0.799000
C	1.876200	2.727000	0.227100
H	1.458000	3.646400	0.677700
H	2.778000	2.442900	0.793200
C	-6.854800	-0.188300	-0.629500
H	-6.548300	0.737500	-1.151300
H	-6.735000	-1.034300	-1.329100
C	-8.275000	-0.076000	-0.172200
H	-8.456900	0.658500	0.617900
C	-9.275600	-0.785500	-0.686800
H	-9.101100	-1.529200	-1.468700
H	-10.303000	-0.646900	-0.347200
O	-6.043200	-0.369300	0.519800
C	-4.698300	-0.402000	0.341000
C	-4.058100	-0.320300	-0.898200
C	-3.930200	-0.535600	1.505400
C	-2.662100	-0.355800	-0.960000
H	-4.626100	-0.234200	-1.823000
C	-2.545600	-0.571200	1.432900
H	-4.451500	-0.616700	2.459400
C	-1.893700	-0.471100	0.196400
H	-2.158400	-0.286200	-1.926200
H	-1.948800	-0.687900	2.339800
C	2.218600	2.966000	-1.240400
H	2.532900	2.013700	-1.700100
H	1.319300	3.289400	-1.796900

C	3.323200	4.007400	-1.432800
H	3.541700	4.179900	-2.497600
H	3.036300	4.971100	-0.983000
H	4.252100	3.674800	-0.943900
Ni	0.691400	1.201000	0.314400
C	-0.838100	2.388600	1.393000
H	-1.418400	1.622600	1.910600
H	-0.188400	3.024400	1.996300
C	-1.020000	2.614800	0.072000
H	-0.522500	3.444500	-0.432500
H	-1.756000	2.040200	-0.495000

Ni-3(half)_TS_2

C	-0.043400	-1.830500	-0.178900
C	-1.423500	-2.191100	-0.099000
C	-2.452000	-1.209200	0.050100
H	-0.910800	-4.291200	-0.210300
H	0.657600	-2.680300	-0.180500
C	-1.728700	-3.573900	-0.105500
C	-3.816700	-1.671900	0.184300
C	-4.047400	-3.035000	0.160300
C	-3.025300	-4.000500	0.018300
H	-5.070500	-3.398300	0.255000
H	-3.273200	-5.061100	0.011600
O	-2.193400	0.052500	0.074100
N	0.484900	-0.641200	-0.219100
C	-4.961100	-0.661100	0.318600
C	-4.755400	0.220000	1.563300
C	-5.022900	0.212300	-0.946900
C	-6.319400	-1.355300	0.468500
H	-4.729000	-0.402400	2.471300
H	-3.820000	0.786600	1.496200
H	-5.593800	0.928800	1.659100
H	-5.269100	-0.405200	-1.824600
H	-5.805300	0.980500	-0.836700
H	-4.062200	0.708600	-1.126600
H	-7.104600	-0.590300	0.561800
H	-6.562000	-1.978300	-0.405700
H	-6.357300	-1.987200	1.369000
C	1.031700	2.012500	-1.173200
H	1.862000	1.967700	-0.468100
H	1.121500	1.404500	-2.076900
C	0.105300	3.025500	-1.089200
H	-0.541000	3.270100	-1.933600
H	0.232100	3.807700	-0.343600
C	6.807500	0.050100	0.752800
H	6.451900	1.078000	0.954000
H	6.660200	-0.550700	1.667600
C	8.251300	0.070900	0.360200
H	8.465900	0.526200	-0.611400
C	9.233000	-0.398500	1.125100
H	9.026200	-0.864600	2.092200
H	10.276700	-0.331400	0.814700
O	6.073100	-0.495700	-0.330700
C	4.719300	-0.517700	-0.225800
C	4.002200	-0.105000	0.902200
C	4.027500	-0.995200	-1.345100
C	2.607600	-0.160700	0.893200
H	4.511900	0.256300	1.793800
C	2.640400	-1.049600	-1.342600
H	4.607400	-1.310900	-2.212400
C	1.917000	-0.627000	-0.222200
H	2.041300	0.165500	1.767500
H	2.101600	-1.406500	-2.222500
Ni	-0.587600	1.047600	-0.293100
C	-1.897800	2.624300	0.046900
H	-2.679600	2.249000	-0.629200
H	-2.059100	2.157500	1.033300
C	-2.030900	4.131100	0.207500
H	-1.282100	4.515800	0.921300
H	-1.851200	4.657200	-0.745400
C	-3.427900	4.494600	0.713700
H	-3.542100	5.582400	0.834000
H	-4.199400	4.144400	0.010900
H	-3.627700	4.019600	1.686200

Ni-3(half)_P_2

C	-0.061900	-1.858800	-0.371200
C	-1.448300	-2.220500	-0.365400
C	-2.489000	-1.317400	0.027500
H	-0.936900	-4.210400	-1.044600
H	0.623600	-2.665600	-0.672900
C	-1.755800	-3.547900	-0.753200
C	-3.850400	-1.798900	0.022700
C	-4.079700	-3.104600	-0.370600
C	-3.052900	-3.992000	-0.761900
H	-5.102500	-3.480700	-0.382400
H	-3.296800	-5.011000	-1.059500
O	-2.234900	-0.103000	0.380200
N	0.489100	-0.722800	-0.050300
C	-4.989500	-0.863800	0.443700
C	-4.778000	-0.398600	1.895400
C	-5.043700	0.353800	-0.496000
C	-6.351100	-1.563700	0.375300
H	-4.774200	-1.263300	2.577100
H	-3.827700	0.137300	2.002300
H	-5.600900	0.269700	2.196000
H	-5.229800	0.030000	-1.532000
H	-5.866900	1.021100	-0.193500
H	-4.101600	0.914100	-0.466600
H	-7.134100	-0.858900	0.692800
H	-6.591400	-1.893200	-0.647100
H	-6.395400	-2.437800	1.042700
C	0.684400	2.232200	0.534900
H	1.343400	2.217000	1.410300
H	1.236900	2.425800	-0.394300
C	-0.587200	3.002200	0.697800
C	6.863700	-0.066000	0.508800
H	6.551400	0.945600	0.829300
H	6.756200	-0.749100	1.369800
C	8.280900	-0.045000	0.028900
H	8.453400	0.494000	-0.907500
C	9.289600	-0.614900	0.682700
H	9.123100	-1.165000	1.612700
H	10.314700	-0.548700	0.315600
O	6.048600	-0.488500	-0.572000
C	4.705200	-0.519200	-0.373500
C	4.073400	-0.217100	0.837400
C	3.931400	-0.882700	-1.481500
C	2.683500	-0.278500	0.927100
H	4.647100	0.063400	1.718900
C	2.548800	-0.947200	-1.380600
H	4.443500	-1.102400	-2.418200
C	1.910700	-0.648900	-0.170800
H	2.183300	-0.046000	1.867900
H	1.948800	-1.211400	-2.252900
Ni	-0.575300	0.811400	0.422600
C	-1.012800	3.896200	-0.463700
H	-0.304100	4.739300	-0.523200
H	-0.906100	3.330900	-1.405800
C	-2.438100	4.424600	-0.339000
H	-3.135800	3.571500	-0.279900
H	-2.538500	4.973700	0.612800
C	-2.829500	5.330200	-1.501300
H	-3.859000	5.699700	-1.396100
H	-2.161700	6.203200	-1.561500
H	-2.760800	4.791100	-2.458500
H	-0.672800	3.523500	1.663400
H	-1.473900	2.244900	0.816400