

Electronic Supplementary Information

Metal π -Lewis Base Activation in Palladium(0)-Catalyzed trans-Alkylative Cyclization of Alkynals

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1. Comparison of the metal π -Lewis acid activation and π -Lewis base activation

In Chatt-Dewar-Duncanson coordination mode, the metal can act as π -Lewis acids by accepting π -electrons of alkynes to enhance their electrophilic reactivity toward diverse nucleophiles. Meanwhile, the empty antibonding molecular orbital of the alkyne (π^*) is able to accept electrons from the d -orbitals of metal via π -back-donation. To distinguish the role of Lewis acid or base in the metal-alkyne complex, the electron density of typical Lewis acid metal-alkyne complexes was considered. As shown in Figure S1, in the Au(I)-alkyne complex **int-Au(I)** and Pd(II)-alkyne complex **int-Pd(II)**, there are significant charge transfers from alkyne to metal, indicating the canonical Lewis acid role of Au(I) and Pd(II). However, in the Pd(0)-alkyne complex **int-Pd(0)**, a considerable amount of charge transfer from PdL_2 to alkyne suggests the intrinsic Lewis base role of Pd(0), which is consistent with the Lewis base mode in the $(Ph_3)_2P_2Pd(0)$ -alkynal complex.

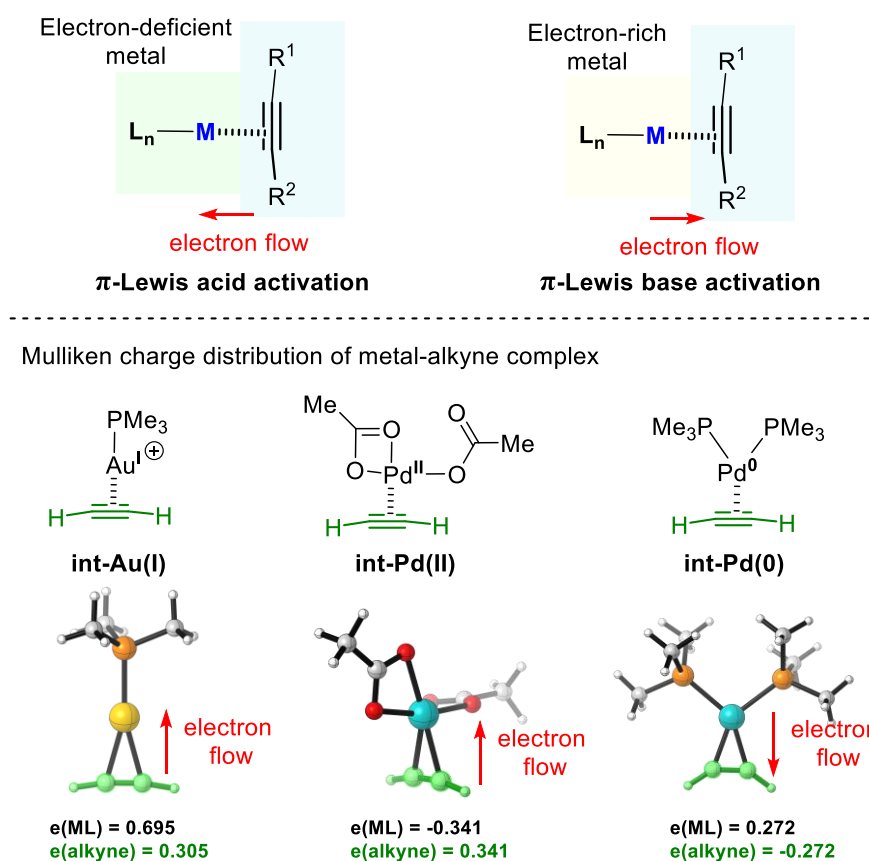


Figure S1. Comparison of the metal π -Lewis acid activation and π -Lewis base activation.

2. MeOH acting as an H-bond donor in the π -Lewis base activation

As depicted in Figure S2, we also considered the MeOH acting as an H-bond donor in the π -

Lewis base activation. The relative free energy of **TS-endo-MeOH** is 4.9 kcal/mol higher than that of **TS-endo**, which indicates that MeOH didn't play a crucial role in the π -Lewis base activation. While MeOH was considered as a proton source, and the generated counter ion MeO^- could be considered as an activator of phenylboronic acid to realize the subsequent Suzuki reaction (see Figure 3 in the text). Moreover, we also have considered the stabilizing effects of arylboronic acid in the π -Lewis base activation. The activation free energy of this process (via **TS-endo-PhB(OH)₂**) is 11.7 kcal/mol higher than that of **TS-endo**, which indicates the weak Lewis acid ability of arylboronic acid.

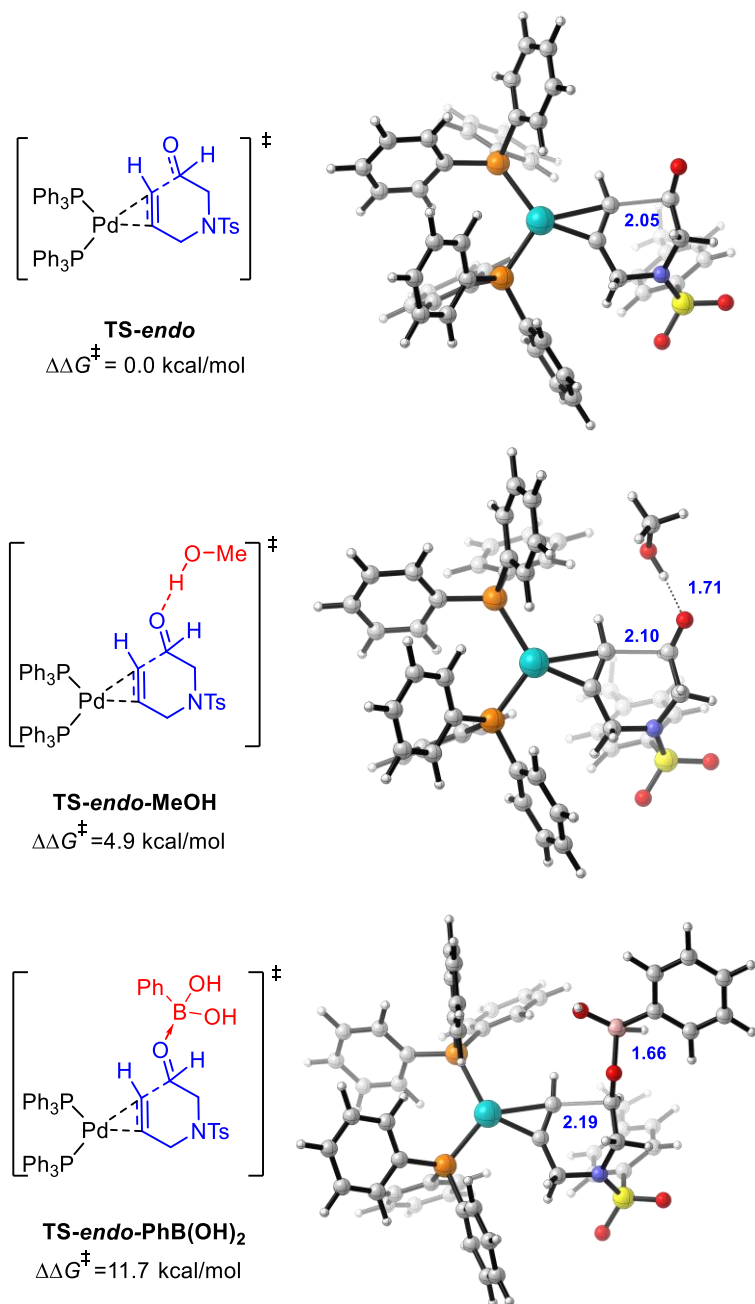


Figure S2. Consideration for the MeOH and arylboronic acid to stabilize the alkoxide in the π -Lewis base activation..

3. Competitive β -H elimination and protonation starting from **int-3**

The competitive β -H elimination and protonation starting from **int-3** were also taken into consideration. As shown in Figure S3, the free energy barrier of the β -H elimination (via **TS- β -H**) is 13.6 kcal/mol higher than that of the transmetalation (via **TS-TM**). Meanwhile, the free energy barrier of the protonation (via **TS-proton**) is extremely high about 50.0 kcal/mol. These results suggest that the transmetalation would preferentially proceed starting from **int-3**, which corroborates that no corresponding hydroalkylative byproduct was detected in the reaction system.

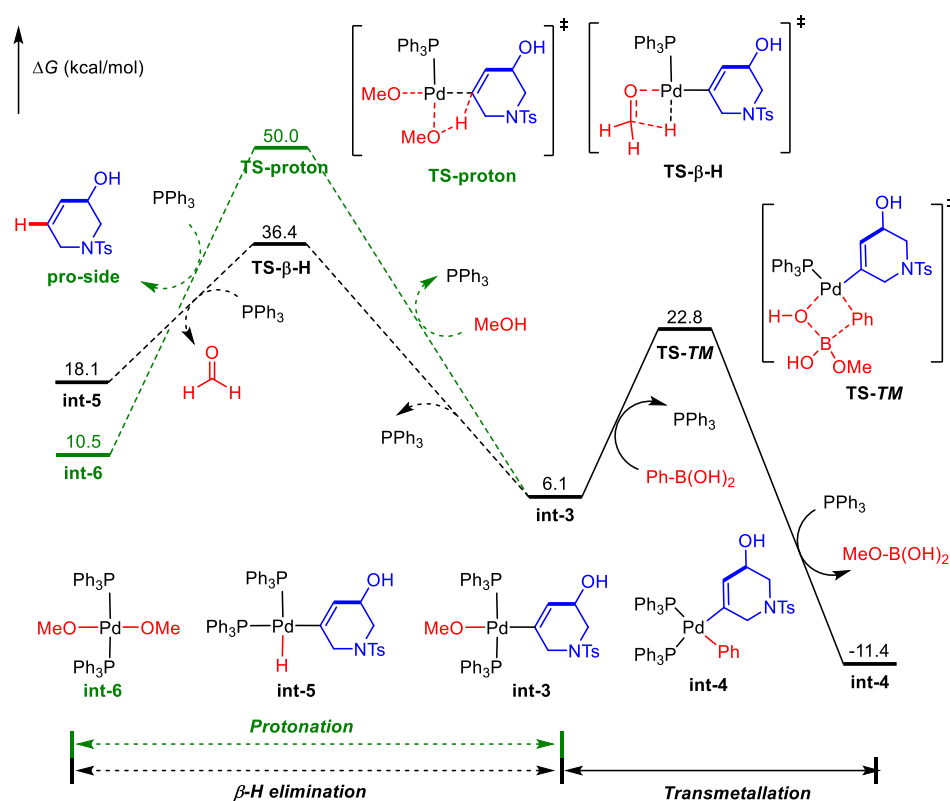


Figure S3. Free energy profile for the competitive β -H elimination and protonation starting from **int-3**.

4. Exclusion the possibility of Pd(II)-catalyzed mechanism

To distinguish the rationality of Pd(0)-catalyzed or Pd(II)-catalyzed mechanism in this Pd(0)-catalyzed trans-alkylative cyclization of alkynals, further calculations and control experiments were conducted in the revision, and corresponding results were summarized in below:

Initially, we conducted the calculation for the probable reaction pathway starting from the Pd(II) catalyst. As shown in Figure S4, the $\text{Pd}(\text{OMe})_2(\text{PPh}_3)_2$ **int-6** was chosen as the initial catalyst complex. The transmetalation between **int-6** and phenylboronic acid proceeds via **TS-1** with an energy barrier of 17.5 kcal/mol to generate aryl-Pd(II) intermediate **int-7** irreversibly. Starting from **int-7**, the

migration insertion (via **TS-2**) of **1a** affords the *cis*-vinyl-Pd(II) intermediate **int-8**, in which following *Z/E*-isomerization (via **TS-3**) generates *trans*-vinyl-Pd(II) intermediate **int-10** reversibly. Then the intramolecular aldehyde 1,2-addition proceeds via **TS-4** to form alkoxy-Pd(II) intermediate **int-11**, from which the subsequent protonation could release the final product. Overall the rate-determining step of the Pd(II)-mediated reaction pathway (black line in Fig S4) is the *Z/E*-isomerization with an energy barrier of 28.6 kcal/mol (referring to **int-8** → **TS-3**), which is close to the activation energy of the Pd(0)-mediated reaction pathway in Fig 3 (28.0 kcal/mol, via **TS-endo**).

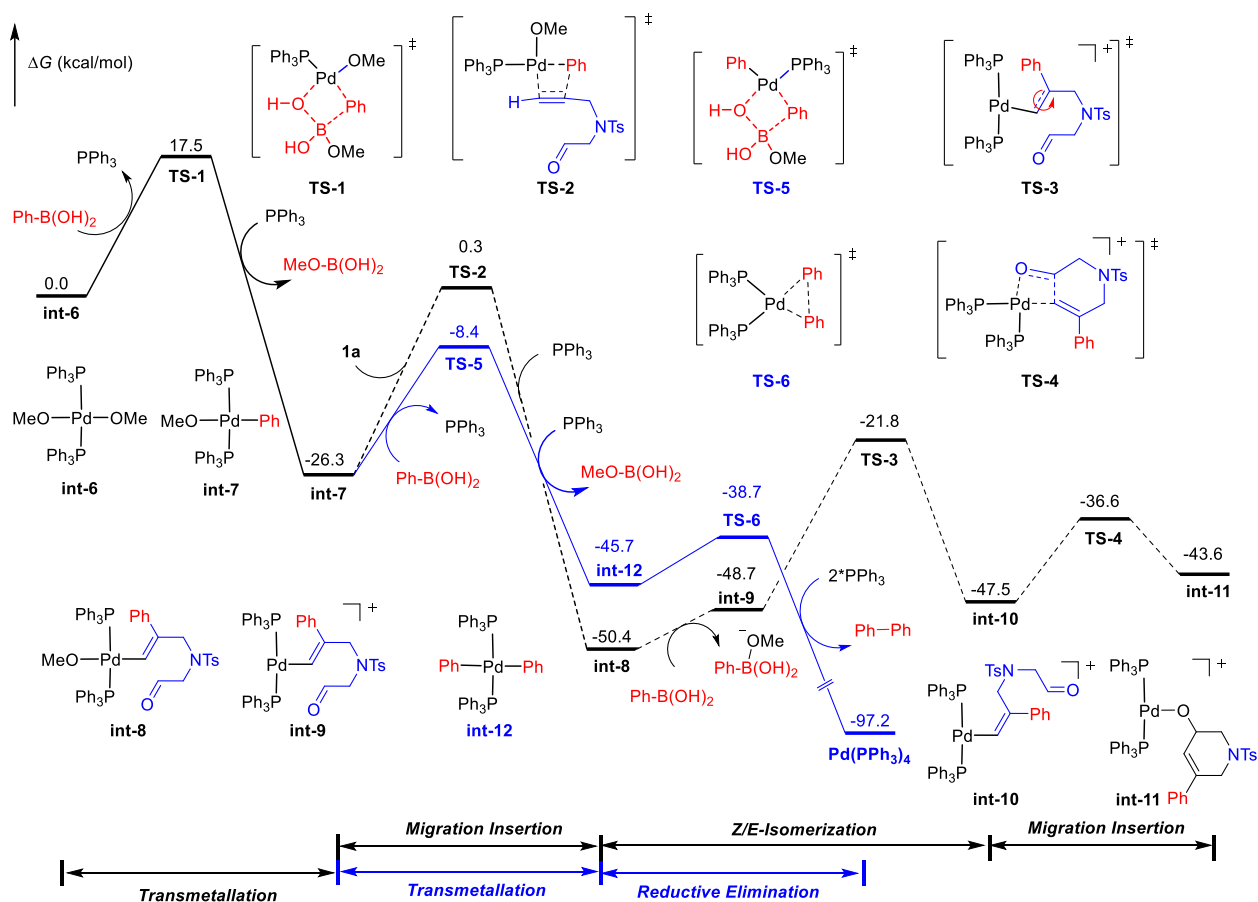


Figure S4. Free energy profile for the probable reaction pathway starting from Pd(II) catalyst.

Meanwhile, starting from **int-7**, an alternative pathway undergoing the second transmetalation via **TS-5** (blue line in Figure S4) generates the diaryl-Pd(II) intermediate **int-7**, in which the following reductive elimination could proceed rapidly to afford Pd(0) species Pd(PPh₃)₄. The energy barrier of the second transmetalation is only 17.9 kcal/mol, which is 8.7 kcal/mol lower than that of the corresponding migration insertion (via **TS-2**). It suggests that even if a Pd(II) catalyst is generated, the reduction of Pd(II) with the assistance of phenylboronic acid would preferentially occur rather than a Pd(II)-mediated reaction pathway to generate the final product in this catalytic system. Therefore, the π -Lewis base activation mode starting from the Pd(0) catalyst is proven to be more

theoretically favorable in this reaction.

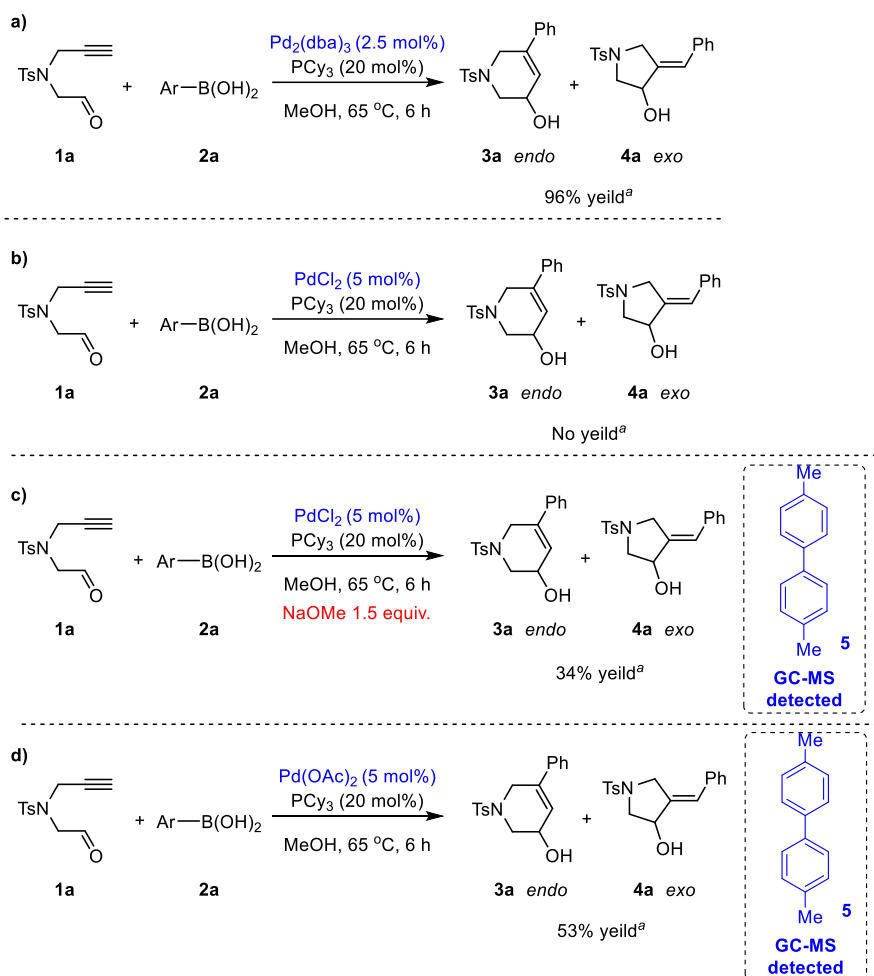


Figure S5. Comparison of Pd(0) and Pd(II) catalysts for the *trans*-alkylative cyclization of alkyne **1a**.

^aThe yield was determined by ¹H NMR analysis. The Ar of Ar-B(OH)₂ represents p-methyl phenyl.

Furthermore, to validate our theoretical results, the control experiments were then conducted. As shown in Figure S5a, the *trans*-alkylative cyclization of alkyne **1a** and **2a** proceeds smoothly mediated by Pd(0) catalyst (Pd₂(dba)₃) and PCy₃, which obtained a 96% yield (mixture of **3a** and **4a**) after 6 hours. While using PdCl₂ as the catalyst (Figure S5b), the corresponding reaction didn't work. It indicates that the Pd(II)-catalyzed mechanism may be not relevant. When adding NaOMe as an additive (Figure S5c), the reaction obtained a 34% yield. Meanwhile, the 4,4'-dimethylbiphenyl **5** was detected by GC-MS as a by-product, which suggests that adding NaOMe promotes two-step transmetalation guiding the generation of **5** and Pd(0) catalyst in situ, thus the reaction can proceed via a Pd(0)-catalyzed pathway. The Pd(OAc)₂ with enhanced transmetalation reactivity could also catalyze this reaction, in which the by-product **5** was also detected (Figure S5d). It is consistent with the aforementioned calculated results in Figure S3, that the reduction of Pd(II) with the assistance of phenylboronic acid might preferentially occur in this Pd(II) system.

Further kinetic studies for the comparison of Pd(0) and Pd(II) catalysts show a low reaction rate as well as an obvious induction period in the Pd(II)-catalyzed system (Figure S6). This result validates our mechanistic speculation of the reduction of Pd(II) with the assistance of phenylboronic acid to generate the active Pd(0) catalyst *in situ*. Therefore, these theoretical and experimental results suggest that the Pd(0)-catalyzed mechanism is more favorable in this Pd-catalyzed *trans*-alkylative cyclization of alkynal.

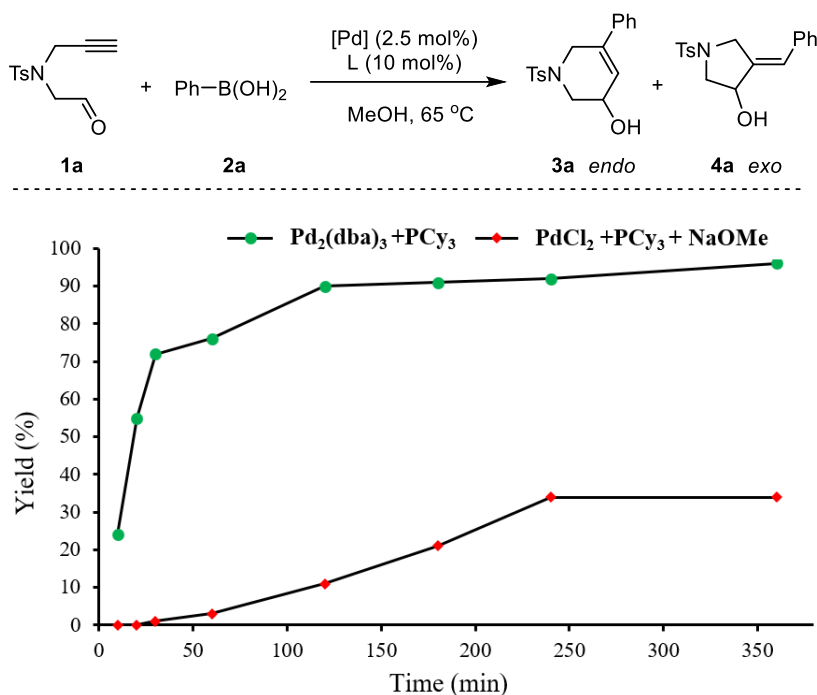


Figure S6. Kinetic studies for the comparison of Pd(0) and Pd(II) catalysts. The yield indicates the total yield of **3a** and **4a**.

5. FMO analysis for TS-endo(Y-Shape) and TS-endo(T-Shape)

To get more insights into the different conformation of transition states in π -Lewis base activation, frontier molecular orbital (FMO) analysis was then conducted. As shown in Figure S7, there is a significant orbital overlap between Pd and reactant in **TS-endo(Y-Shape)**. It accordingly reduces owing to the reacting alkyne being perpendicular to the P-Pd-P plane in **TS-endo(T-Shape)**. Thus it results in the high activation free energy of **TS-endo(T-Shape)**.

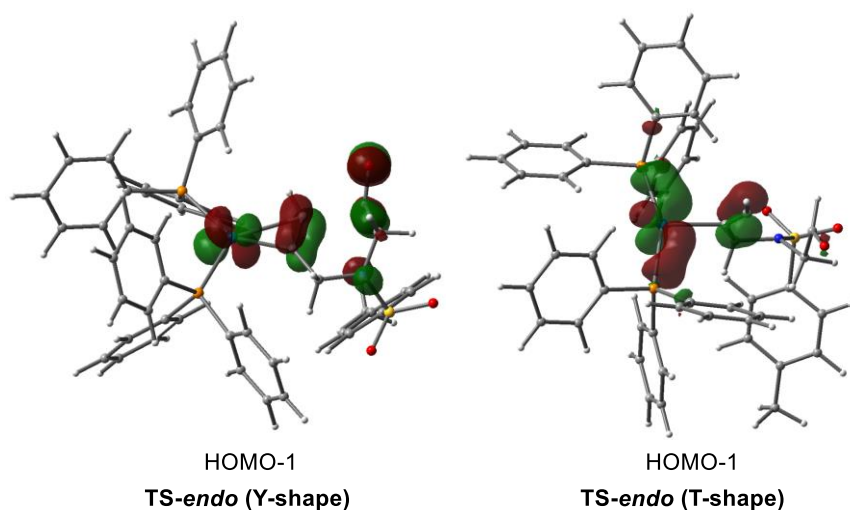


Figure S7. Frontier molecular orbital diagram for **TS-endo(Y-Shape)** and **TS-endo(T-Shape)**.

6. Reactivities for π -Lewis base activation with PPh_3 (**L1**) and PCy_3 (**L4**)

The energy barriers for π -Lewis base activation with PPh_3 (**L1**) and PCy_3 (**L4**) were calculated to evaluate the electron effect of the ligand. As shown in Figure S8, The relative free energy of Pd(0)-alkyne complex **int-1** and **int-1-L4** were set to zero for an intuitionistic comparison. Calculated results showed that the free energy barrier of the **L4**-involved case is 8.7 kcal/mol lower than that of **L1**, correlating with the electron-donating effects. It indicates ligands with greater electron-donating abilities would accelerate this Pd(0)-catalyzed π -Lewis base activation reaction (see Figure 6 and Figure 7 in the text).

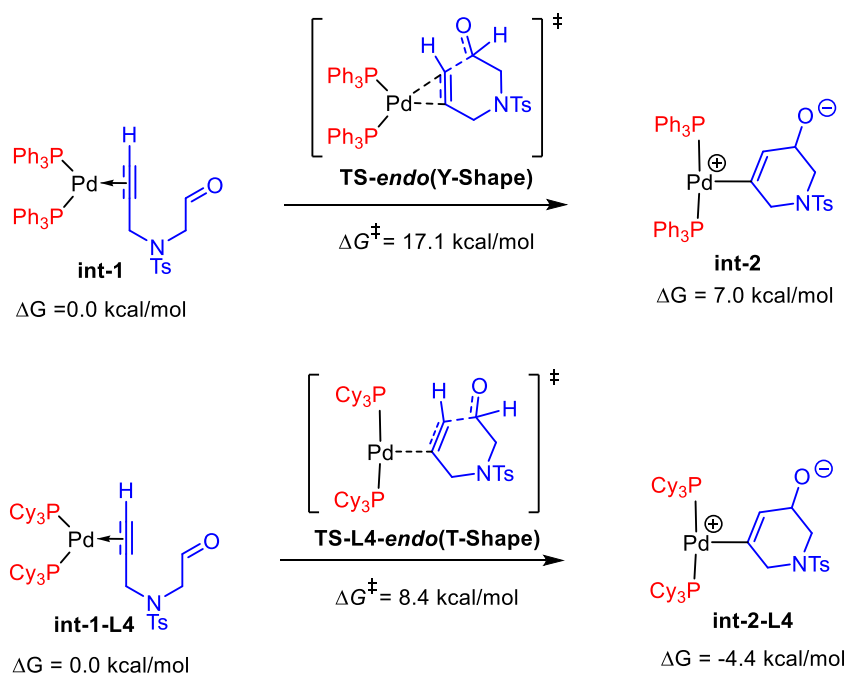


Figure S8. Comparison of the reactivities for π -Lewis base activation with PPh_3 (**L1**) and PCy_3 (**L4**).

7. Regioselectivities for the Pd(PCy₃)₂-catalyzed π -Lewis base activation of **1a**, **1e**, **1f**, and **1g**

Previous experimental results showed that *endo*-regioselectivity could be regulated by both steric and electronic effects of the substituent group in the PCy₃ (**L4**) involved case. As shown in Figure S9, the relative free energy of **TS-L4-*exo*** is 0.8 kcal/mol lower than that of **TS-L4-*endo*** due to the weak electron-donating effects of alkyl moiety at **1a**, which is consistent with the observation of the mixture (*endo/exo* = 32 : 68) in the experiment. Meanwhile, large substituents at the terminal position of NTs-tether reactants **1e** and **1f** lead to *endo*-selectivity in the presence of **L4**. Furthermore, the electron-withdrawing as well as steric aryl substituent **1g** performs more *endo*-selective. These results indicate that the regioselectivity depends on both steric and electronic effects in the PCy₃ (**L4**) involved case.

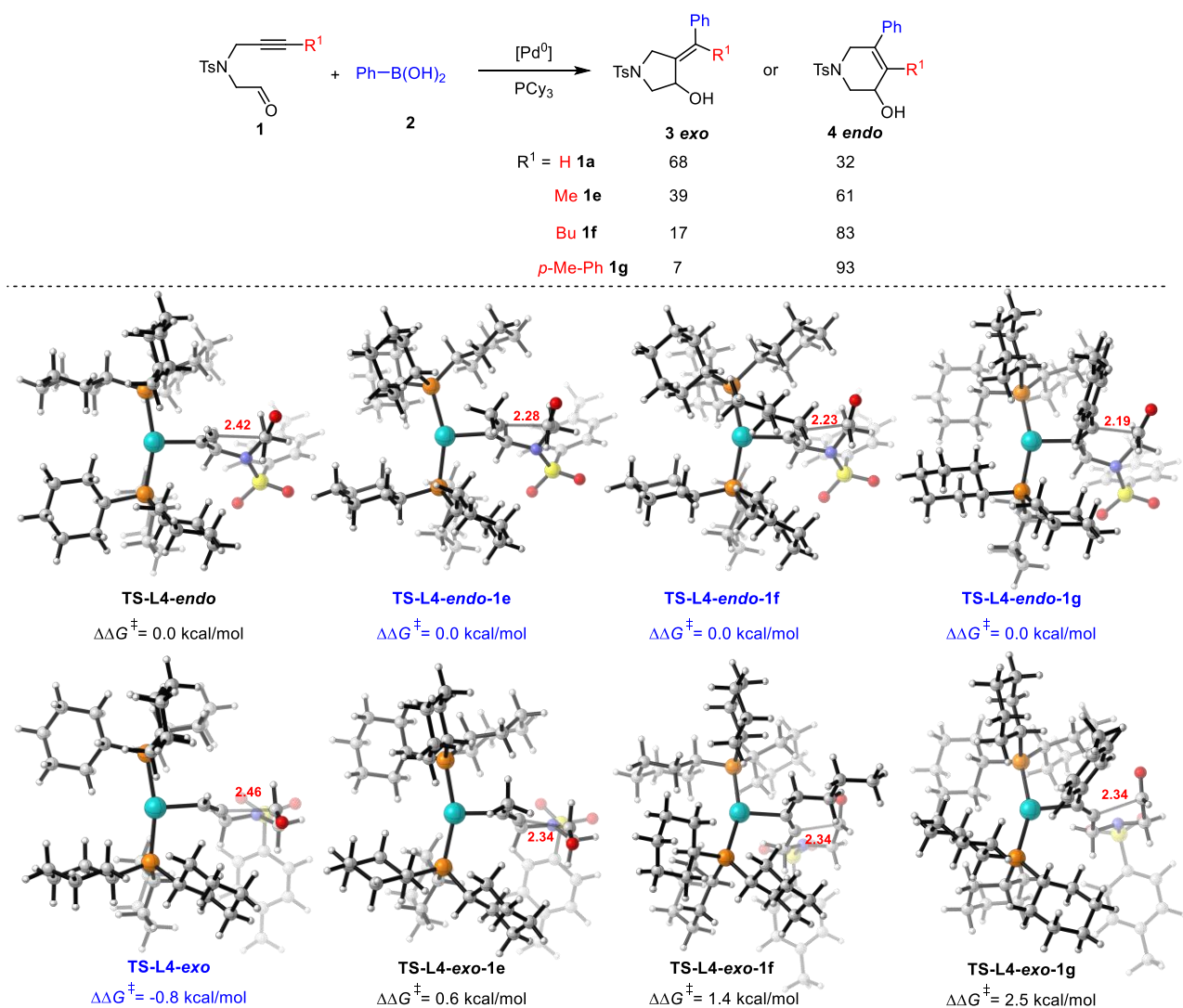
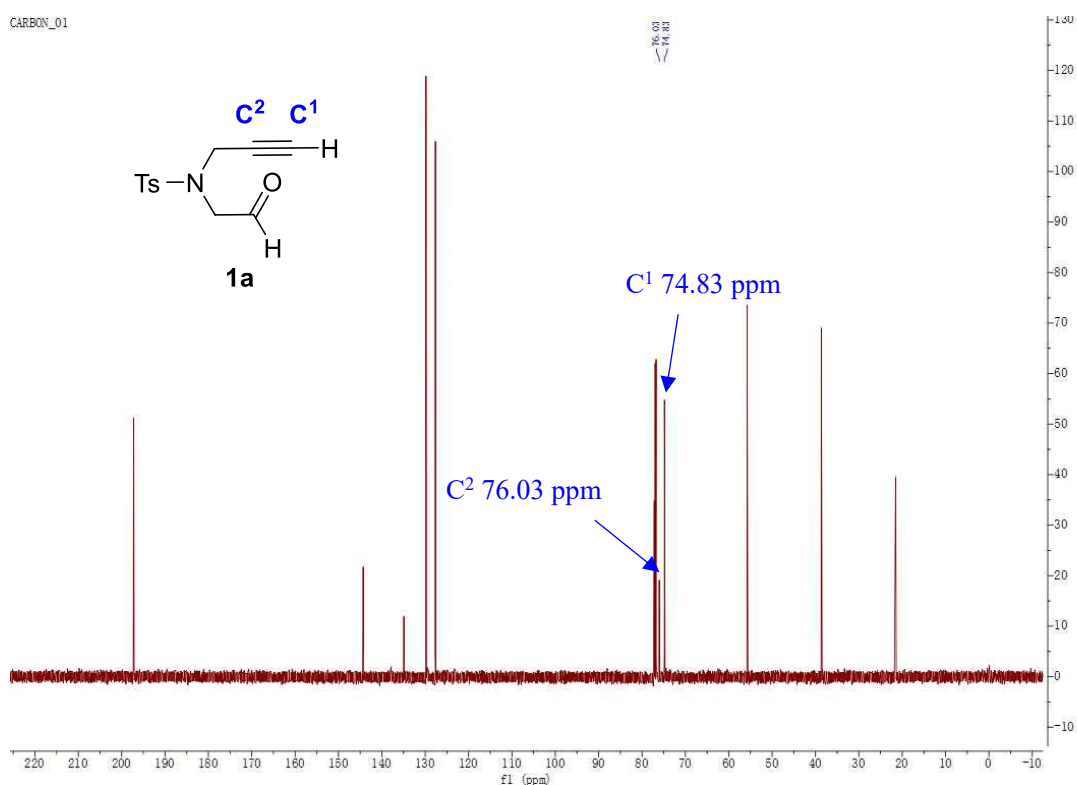
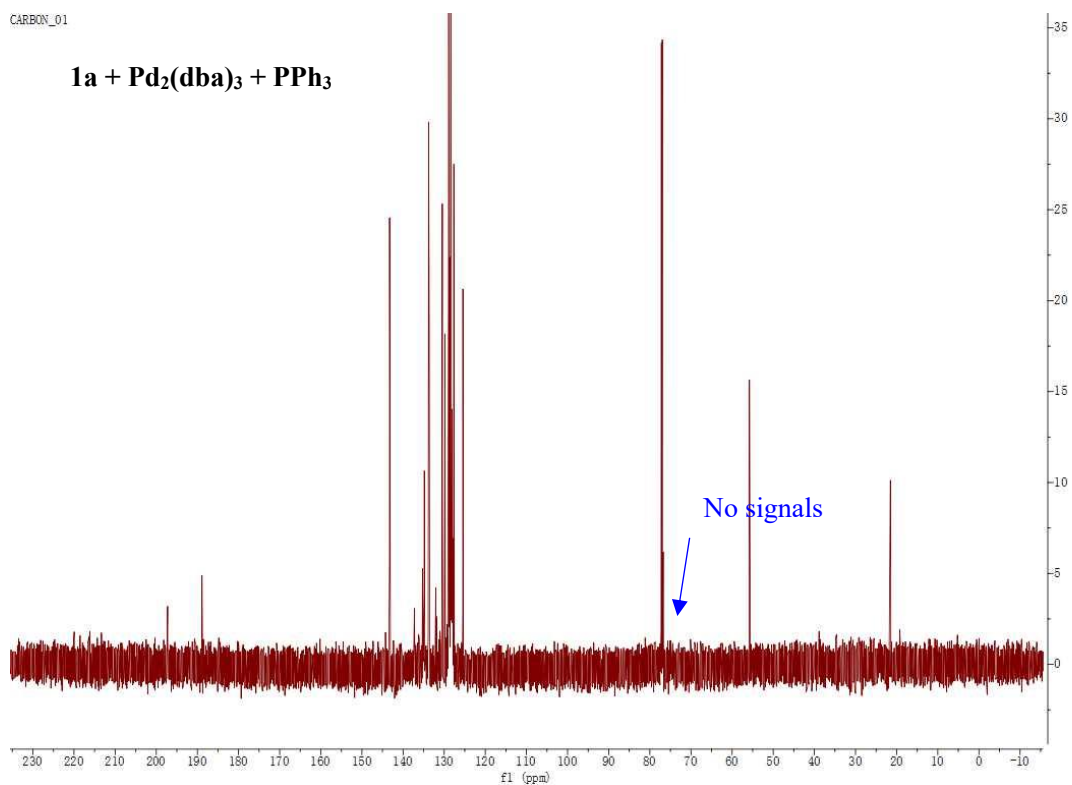
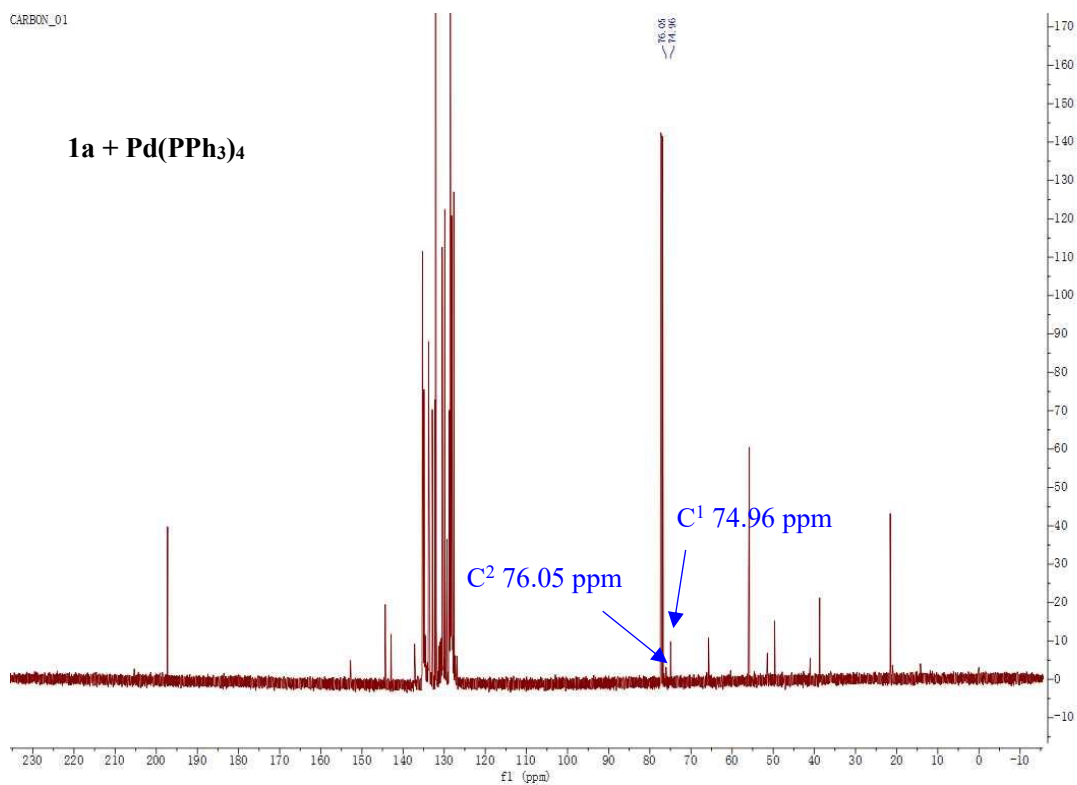


Figure S9. Regioselectivities for the Pd(PCy₃)₂-catalyzed π -Lewis base activation of **1a**, **1e**, **1f**, and **1g**.

8. Detected the coordination of **1a** and Pd(0) by ^{13}C NMR

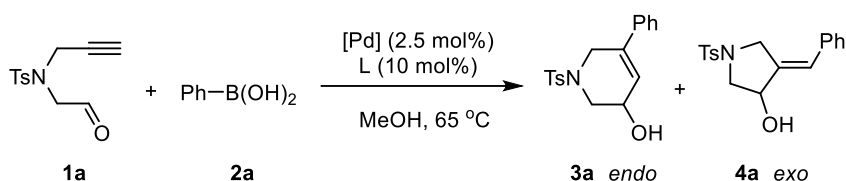
To validate the coordination of **1a** and Pd(0) by ^{13}C NMR, we have carried out NMR studies on the *in situ* generated complexes between alkyne of **1a** and Pd(0). As shown below, when we mix and heat **1a** and Pd(PPh₃)₄, the ^{13}C NMR signals of the triple bond of **1a** are still clear without apparent field shift. However, when we add Pd₂(dba)₃/PPh₃ and reduce the ratio of ligand and metal (P/Pd = 3/1), the ^{13}C NMR signals of the triple bond of **1a** disappeared around 70-80 ppm. These results show that the coordination of **1a** and Pd(0) is only present in the system with a low P/Pd ratio, indicating a weak coordination capacity of alkyne compared with PPh₃. It corroborates the endotherm of ligand exchange between **1a** and PPh₃ in the theoretical calculation.





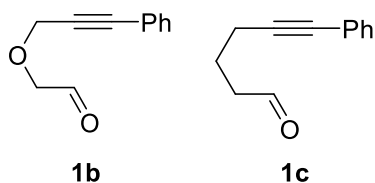
9. Experimental procedures

9.1 General Procedure

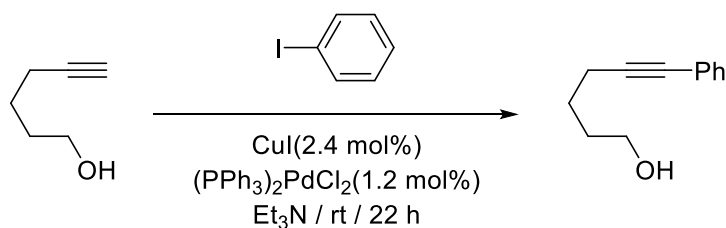


In an N_2 -filled glovebox, an oven-dried Schlenk tube equipped with a stirrer bar was charged with **1a** (0.2 mmol), *p*-tolylboronic acid **2a** (0.3 mmol, 1.5 equiv), PCy_3 (30 mol%), $\text{Pd}_2(\text{dba})_3$ (5 mol%), and MeOH (2 mL). Under a nitrogen atmosphere, The Schlenk tube was sealed with a Teflon screwcap, and the reaction mixture was stirred at 65°C for 24 h. Upon cooling to room temperature, the reaction mixture was diluted with 10 mL of ethyl acetate, and filtered through a pad of silica gel, followed by washing the pad of the silica gel with ethyl acetate (20 mL). Subsequently, the filtrate was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel to afford the desired products.

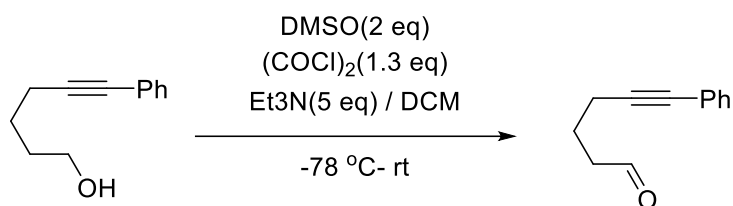
9.2 Preparation of reactants



The **1b** and **1c** were prepared according to literature procedures, The structure of the product was identified by comparison with the NMR spectra of the previous report.

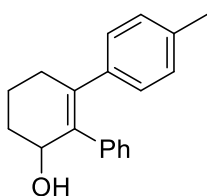


Under nitrogen atmosphere, Iodobenzene (5.4 ml, 48 mmol) was added to a mixture of CuI (183 mg, 0.96 mmol), $(\text{PPh}_3)_2\text{PdCl}_2$ (337 mg, 0.48 mmol), and Et_3N (80 ml). The solution was stirred at 25°C for 30 min. Hex-5-yn-1-ol (3.7 ml, 40 mmol) is then added and the mixture is stirred for an additional 22 h at 25°C . The resulting solution is diluted with EtOAc, filtered over celite and concentrated under reduced pressure. The residue is purified by flash chromatography on silica gel (10% EtOAc/hexane) to afford 6-Phenylhex-5-yn-1-ol (5.1g, 73%) as a yellow oil (*J. Am. Chem. Soc.* **2003**, *125*, 8076-8077).



To a solution of oxalyl chloride (3.5 mL, 40 mmol) in anhydrous CH₂Cl₂ (100 mL) was added DMSO (4.5 mL, 62 mmol) at -78 °C. The mixture was stirred at -78 °C for 10 min, and then a solution of 6-Phenylhex-5-yn-1-ol (5.0 g, 30mmol) in anhydrous CH₂Cl₂ (10 mL) was added. The mixture was stirred at -78 °C for 2 h, and then triethylamine (22mL, 160 mmol) was added. The reaction was allowed to warm up to 25 °C over 2 h and then partitioned between EtOAc and saturated aqueous NH₄Cl. The aqueous layer was extracted with EtOAc twice. The combined organic layers were washed with brine, dried over MgSO₄, and concentrated in vacuo. The residue is purified by flash chromatography on silica gel (20% EtOAc/hexane) to afford 6-phenylhex-5-ynal (1.1g, 21%) as a yellow oil (*Chem. Eur. J.* **2004**, *10*, 5681–5688).

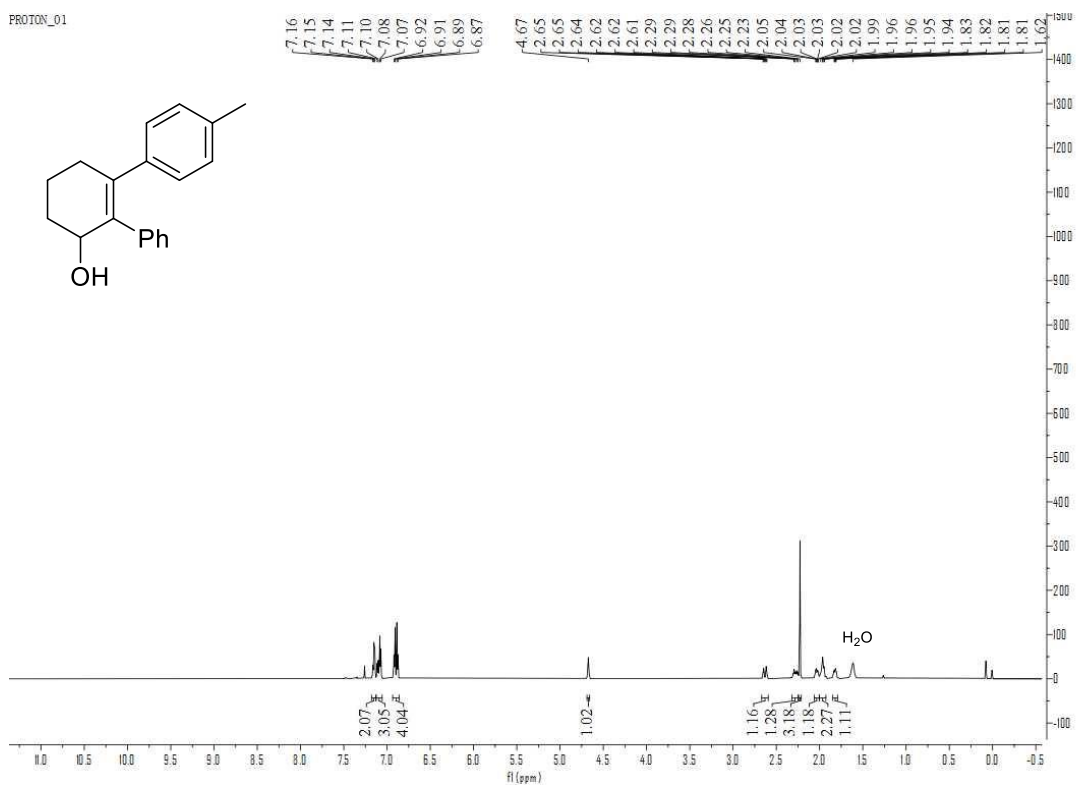
10. Spectrum for compounds



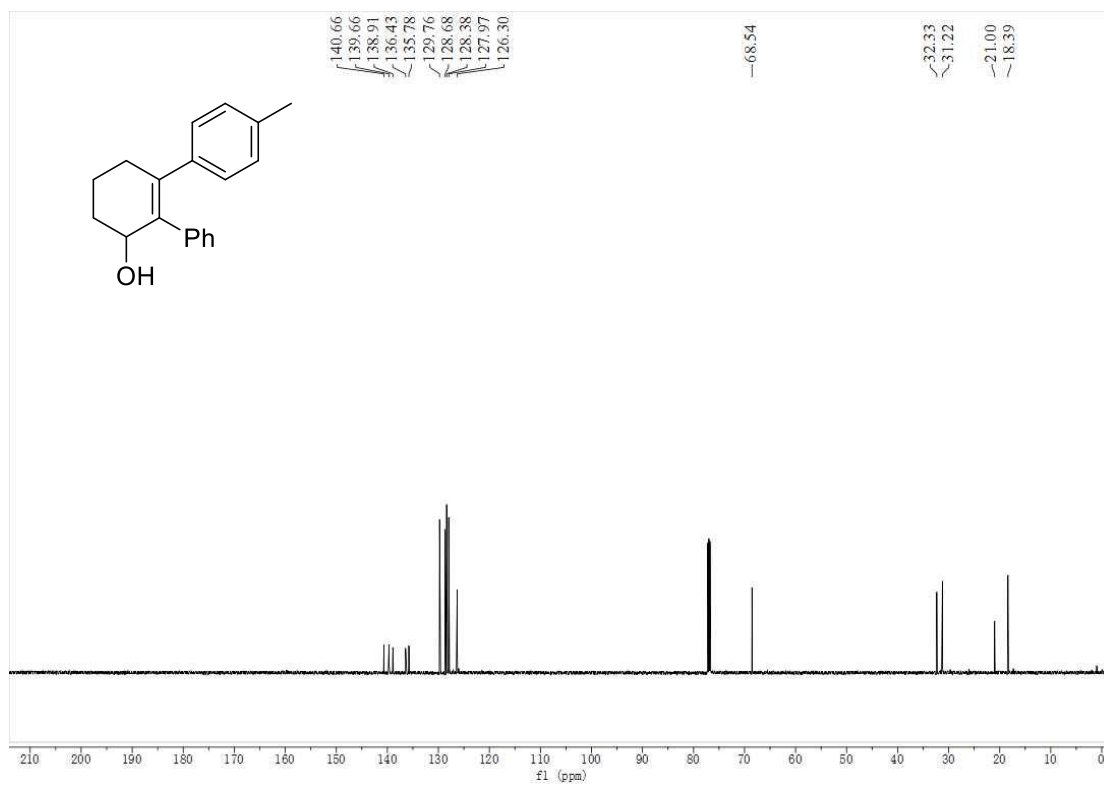
4-methyl-3',4',5',6'-tetrahydro-[1,1':2',1''-terphenyl]-3'-ol (3b): Colorless oil; ¹H NMR (600 MHz, CDCl₃): δ 7.15 (t, J = 7.4 Hz, 2H), 7.012-7.06 (m, 3H), 6.93 – 6.86 (m, 4H), 4.67 (br-s, 1H), 2.63 (dt, J = 18.3, 4.6 Hz, 1H), 2.31-2.25 (m, 1H), 2.23 (s, 3H), 2.06-2.01 (m, 1H), 1.99 – 1.94 (m, 2H), 1.85-1.79 (m, 1H). ¹³C NMR (150 MHz, CDCl₃): δ 140.66, 139.66, 138.91, 136.43, 135.78, 129.76, 128.68, 128.38, 127.97, 126.30, 68.54, 32.33, 31.22, 21.00, 18.39. HRMS(ESI): Calcd for C₁₉H₂₀O [M + Na]⁺ 287.1406, found 287.1406.

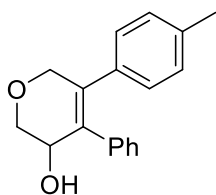
¹H NMR Spectrum of **3b**

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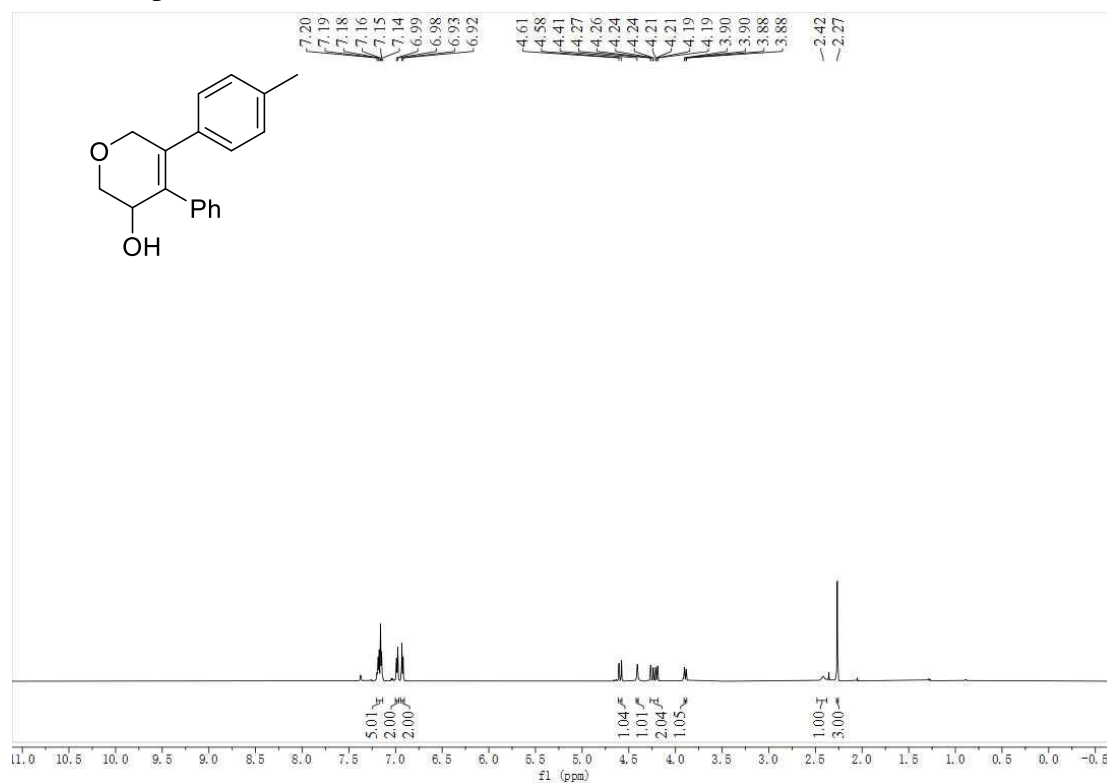
¹³C NMR Spectrum of 3b



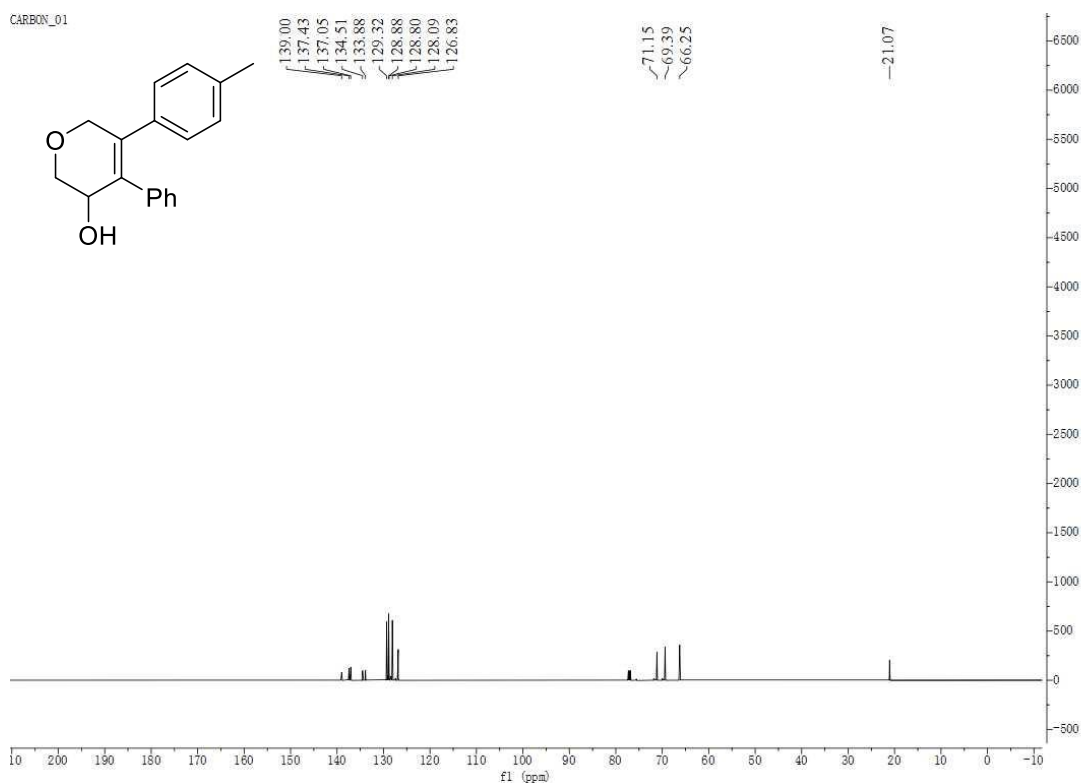


4-phenyl-5-(p-tolyl)-3,6-dihydro-2H-pyran-3-ol (3c): Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.20-7.10 (m, 5H), 6.98 (d, $J = 7.8$ Hz, 2H), 6.93 (d, $J = 7.9$ Hz, 2H), 4.62-4.56 (m, 1H), 4.41 (s, 1H), 4.27 – 4.19 (m, 2H), 3.92-3.86 (m, 1H), 2.42 (br-s, 1H), 2.27 (s, 3H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 139.00, 137.43, 137.05, 134.51, 133.88, 129.32, 128.88, 128.80, 128.09, 126.83, 71.15, 69.39, 66.25, 21.07. **HRMS(ESI):** Calcd for $\text{C}_{18}\text{H}_{18}\text{O}_2$ $[\text{M} + \text{Na}]^+$ 289.1199, found 289.1197.

$^1\text{H NMR}$ Spectrum of **3c**



$^{13}\text{C NMR}$ Spectrum of **3c**



11. Complete Reference for Gaussian 09

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2013**.

12. Absolute Calculation Energies, Enthalpies, and Free Energies

Geometry	$E_{(\text{elec-B3LYP})}^1$	$G_{(\text{corr-B3LYP})}^2$	$H_{(\text{corr-B3LYP})}^3$	$E_{(\text{solv, M06})}^4$	IF ⁵
1a	-1142.9141	0.180957	0.247223	-1143.414418	-
3a	-1375.088152	0.284825	0.359497	-1375.638188	-
Ph-B(OH)₂	-407.99627	0.092014	0.133953	-408.175033	-

PPh₃	-1035.72921	0.227006	0.290261	-1035.991688	-
MeOH	-115.639087	0.028236	0.055241	-115.706896	-
MeO-B(OH)₂	-291.586525	0.046122	0.083147	-291.777246	-
Pd(PPh₃)₄	-4270.906622	0.97875	1.170719	-4272.065515	-
int-1	-3342.3854	0.677882	0.834772	-3343.455577	-
int-2	-3342.381059	0.685322	0.836814	-3343.447631	-
int-3	-3458.066639	0.738986	0.894719	-3459.198729	-
int-4	-3574.484924	0.782803	0.945088	-3575.622444	-
int-5	-3343.606962	0.705455	0.857484	-3344.668357	-
int-6	-2429.520786	0.552739	0.676046	-2430.208896	-
int-7	-2545.955571	0.597894	0.726653	-2546.64792	-
int-8	-3688.938573	0.809254	0.978493	-3690.135625	-
int-9	-3573.758974	0.769987	0.934392	-3574.878304	-
int-10	-3573.758224	0.771035	0.934341	-3574.877494	-
int-11	-3573.771622	0.778047	0.937011	-3574.874187	-
int-12	-2662.380432	0.644081	0.777392	-2663.076845	-
pro-side	-1144.19183	0.210156	0.273639	-1144.685458	-
int-Au(I)	-673.905873	0.104599	0.154635	-674.028555	-
int-Pd(II)	-661.886634	0.086476	0.145772	-662.190248	-
int-Pd(0)	-1127.151396	0.207797	0.276167	-1127.422363	-
int-oxcyc	-3342.41541	0.690176	0.836273	-3343.471945	-
int-LA	-3342.338765	0.684006	0.833400	-3343.398324	-
int-1-L2	-3349.632157	0.816568	0.975380	-3350.709912	-
int-1-L3	-3356.875789	0.954073	1.115926	-3357.960138	-
int-1-L4	-3364.107858	1.090786	1.256611	-3365.198869	-
int-2-L4	-3364.121741	1.100912	1.259315	-3365.211843	-
TS-endo	-3342.354265	0.678735	0.83292	-3343.429094	411.08i
TS-exo	-3342.353066	0.679442	0.833235	-3343.423411	384.61i
TS-endo-side	-3342.353611	0.680683	0.833111	-3343.424134	446.50i
TS-endo-MeOH	-3458.007592	0.726319	0.890552	-3459.143344	471.00i
TS-endo-PhB(OH)₂	-3750.356307	0.79499	0.968591	-3751.605676	537.68i

TS-proton	-2537.926979	0.53005	0.653493	-2538.833817	<i>1115.25i</i>
TS-β-H	-2422.287381	0.478684	0.596128	-2423.129739	<i>253.99i</i>
TS-1	-1801.764575	0.413924	0.517138	-1802.360604	<i>320.65i</i>
TS-2	-2653.110321	0.550501	0.681661	-2654.026849	<i>264.73i</i>
TS-3	-3573.706853	0.766398	0.930753	-3574.831857	<i>66.76i</i>
TS-4	-3573.740959	0.776537	0.934371	-3574.865701	<i>315.88i</i>
TS-5	-1918.198117	0.461674	0.567945	-1918.801407	<i>332.96i</i>
TS-6	-2662.362477	0.642611	0.775393	-2663.064227	<i>322.15i</i>
TS-oxcyc	-3342.352029	0.681661	0.833318	-3343.417913	<i>341.52i</i>
TS-LA	-3342.324444	0.678404	0.832751	-3343.387116	<i>511.41i</i>
TS-TM	-2830.312661	0.601009	0.735866	-2831.352568	<i>318.85i</i>
TS-RE	-3574.466167	0.782259	0.943482	-3575.607074	<i>337.60i</i>
TS-endo(T-shape)	-3342.351905	0.677137	0.832871	-3343.420804	<i>241.29i</i>
TS-L2-endo(Y-shape)	-3349.603442	0.819029	0.973827	-3350.681596	<i>465.26i</i>
TS-L2-endo(T-shape)	-3349.601791	0.817154	0.973595	-3350.67703	<i>243.23i</i>
TS-L3-endo(Y-shape)	-3356.846994	0.954242	1.11422	-3357.934349	<i>424.27i</i>
TS-L3-endo(T-shape)	-3356.85098	0.95136	1.113644	-3357.932479	<i>229.24i</i>
TS-L4-endo(Y-shape)	-3364.081614	1.093638	1.255105	-3365.173929	<i>387.13i</i>
TS-L4-endo(T-shape)	-3364.086047	1.088337	1.254243	-3365.178951	<i>151.29i</i>
TS-endo-1d	-2660.13499	0.610189	0.74291	-2660.876059	<i>350.51i</i>
TS-exo-1d	-2660.135956	0.607099	0.742955	-2660.870399	<i>356.46i</i>
TS-L4-exo	-3364.095235	1.087379	1.254021	-3365.179243	<i>74.95i</i>
TS-L4-endo-1d	-2681.864626	1.017822	1.16398	-2682.624236	<i>213.45i</i>
TS-L4-exo-1d	-2681.87829	1.018774	1.164284	-2682.628802	<i>222.49i</i>
TS-L4-endo-1e	-3403.379811	1.115763	1.284225	-3404.483817	<i>240.35i</i>
TS-L4-exo-1e	-3403.382598	1.11711	1.284235	-3404.484219	<i>180.54i</i>
TS-L4-endo-1f	-3521.234543	1.197803	1.373719	-3522.370871	<i>246.60i</i>
TS-L4-exo-1f	-3521.235433	1.196462	1.373489	-3522.367295	<i>143.24i</i>
TS-L4-endo-1g	-3634.277734	1.189808	1.370278	-3635.443638	<i>221.86i</i>
TS-L4-exo-1g	-3634.273232	1.189842	1.369951	-3635.439654	<i>136.17i</i>

¹The electronic energy calculated by B3LYP in methanol solvent. ²The thermal correction to Gibbs free energy

calculated by B3LYP in methanol solvent. ³The thermal correction to enthalpy calculated by B3LYP in methanol solvent. ⁴The electronic energy calculated by M06 in methanol solvent. ⁵The B3LYP calculated imaginary frequencies for the transition states.

13. Geometries for All the Optimized Compounds and Transition State

1a				H	1.21262800	1.94357700	-0.77651100
C	1.69584800	1.30906000	1.89800900	C	-0.87439900	2.42214700	-0.32661300
C	1.21200300	2.35748700	2.26815200	O	-1.04976400	3.57722000	-1.13868300
H	0.77786100	3.28730500	2.59759500	H	-0.57630300	2.72573500	0.69632500
C	2.30374000	0.04678800	1.45146200	S	1.08693200	-0.08080600	1.07065300
H	3.40214200	0.15252500	1.46105200	O	0.63068000	-1.35070200	1.66278100
H	2.06630500	-0.75814400	2.16158700	O	1.10838500	1.12503900	1.92339900
N	1.91357200	-0.38597400	0.10682600	C	2.74151400	-0.31218100	0.43531800
C	2.43745100	0.33985000	-1.03988300	C	3.03710000	-1.48419500	-0.27456200
H	3.53053800	0.45131400	-0.94302300	C	3.72154100	0.65032400	0.68177200
H	2.26079900	-0.25422200	-1.95260500	C	4.33176500	-1.67683000	-0.74726200
C	1.82545100	1.70645500	-1.28346800	H	2.26682700	-2.23789400	-0.45226100
O	2.43107700	2.60520800	-1.82374800	C	5.01593300	0.43845100	0.19696900
H	0.75961300	1.82689000	-0.97341700	H	3.47929000	1.55110100	1.24788200
S	0.73622600	-1.56391800	-0.08845800	C	5.34304200	-0.72066800	-0.52272900
O	0.95152800	-2.13978200	-1.42473800	H	4.56779800	-2.58989500	-1.30110600
O	0.81176900	-2.42381700	1.10258500	H	5.78534000	1.19166900	0.38629700
C	-0.87207200	-0.78210500	-0.08854700	H	-3.06444000	2.35264100	-0.15840000
C	-1.44318800	-0.38296900	-1.30236200	H	-0.27979500	4.15198900	-1.01137100
C	-1.53397800	-0.57051100	1.12610200	C	-3.65658400	-0.30920300	-0.21000300
C	-2.68968000	0.24320400	-1.28933000	C	-4.75876300	0.31915800	0.40856900
H	-0.92693500	-0.56722100	-2.24617100	C	-3.85364000	-1.60142100	-0.74047200
C	-2.77928900	0.05816300	1.11656700	C	-6.00396100	-0.30686600	0.47524400
H	-1.08965900	-0.89915700	2.06723500	H	-4.63585800	1.30437500	0.86344100
C	-3.37858700	0.47515800	-0.08529100	C	-5.10218800	-2.22744400	-0.67404800
H	-3.13911100	0.55407900	-2.23642600	H	-3.03198900	-2.12813900	-1.22944300
H	-3.29870800	0.22420700	2.06428200	C	-6.18477700	-1.58434800	-0.06823200
C	-4.73813700	1.12139900	-0.08730900	H	-6.83777300	0.20319200	0.96571300
H	-4.84504500	1.83435000	-0.91911700	H	-5.22622700	-3.22651400	-1.10107200
H	-5.52811300	0.35864300	-0.20859000	H	-7.15972700	-2.07593600	-0.01222300
H	-4.93667300	1.64918700	0.85774300	C	6.73611800	-0.95352900	-1.04343100
3a				H	7.17247600	-1.86657500	-0.60382900
C	-2.33106800	0.36068800	-0.29343100	H	6.72927600	-1.09977200	-2.13668700
C	-2.19035900	1.70079000	-0.25088000	H	7.40274300	-0.10994900	-0.81274400
C	-1.11401100	-0.53398400	-0.46459600	Ph-B(OH)₂			
H	-1.12377000	-0.98356700	-1.47384000	C	-0.17402100	0.00017000	0.00035300
H	-1.14703900	-1.36867200	0.24757100	C	0.55499500	-1.20603000	0.01361200
N	0.15888300	0.17450900	-0.30223600	C	0.55524500	1.20615600	-0.01306500
C	0.21162900	1.50648500	-0.90556300	C	1.95300800	-1.21067700	0.01428800
H	0.03569800	1.39728600	-1.98882000	H	0.01767400	-2.15873300	0.02449600

C	1.95328100	1.21058800	-0.01440300
H	0.01809400	2.15899000	-0.02358700
C	2.65559300	-0.00010400	-0.00027700
H	2.49776600	-2.15912800	0.02585600
H	2.49821000	2.15893900	-0.02631700
H	3.74946000	-0.00020900	-0.00058300
B	-1.74933200	0.00003200	0.00006700
O	-2.39360200	-1.20599800	-0.02870500
H	-3.36149400	-1.15224800	-0.02947000
O	-2.39388300	1.20589900	0.02837200
H	-3.36178300	1.15240200	0.02888500

PPh₃

P	0.00006200	0.00076700	-1.19199000
C	-1.46340800	0.81551400	-0.39684700
C	-2.71553100	0.60599000	-1.00587900
C	-1.39533300	1.64736700	0.73366500
C	-3.87142300	1.19521300	-0.48653900
H	-2.78676600	-0.02499100	-1.89745500
C	-2.55156900	2.24700200	1.24636200
H	-0.43611700	1.83102600	1.22308600
C	-3.79171700	2.02062000	0.64102300
H	-4.83618200	1.01735900	-0.96991100
H	-2.48074200	2.89289600	2.12615400
H	-4.69375200	2.49000800	1.04314600
C	1.43764900	0.85928700	-0.39534700
C	1.89221100	2.04086800	-1.01127900
C	2.11252000	0.39150000	0.74526800
C	2.98009500	2.74675200	-0.48999300
H	1.39015700	2.41200500	-1.91036600
C	3.20935700	1.09215900	1.25985700
H	1.78291900	-0.52476800	1.24049300
C	3.64413200	2.27158900	0.64662000
H	3.31683200	3.66500200	-0.97930900
H	3.72472600	0.71394900	2.14732000
H	4.50151400	2.81710000	1.05037100
C	0.02608000	-1.67407000	-0.39675700
C	-0.74488000	-2.03794600	0.72034900
C	0.85135200	-2.64697200	-0.99288200
C	-0.68590300	-3.33961600	1.23181000
H	-1.39652000	-1.30427300	1.20038300
C	0.91913600	-3.94286800	-0.47431300
H	1.44651600	-2.38786300	-1.87424100
C	0.14709900	-4.29374300	0.63922100
H	-1.29354300	-3.60694400	2.10103600
H	1.56936300	-4.68399000	-0.94758200
H	0.19147300	-5.30989300	1.04069800

MeOH

C	0.65933200	-0.01908400	0.00000000
H	1.10161500	0.99026400	-0.00000100
H	1.03511400	-0.55150700	-0.89554200
H	1.03511500	-0.55150600	0.89554200
O	-0.74882800	0.12384100	0.00000000
H	-1.13721100	-0.76348000	0.00000000

MeO-B(OH)₂

B	0.51523000	-0.03383700	-0.00011900
O	1.63821100	-0.81875300	0.00005900
H	2.46568100	-0.31709100	0.00255700
O	0.51336100	1.33446600	0.00028900
H	1.39814700	1.72675700	-0.00307700
O	-0.67396900	-0.71054800	-0.00065200
C	-1.91401500	-0.02261300	0.00027700
H	-2.72015600	-0.77171600	-0.02631400
H	-2.03853300	0.59163600	0.90876300
H	-2.01801900	0.63395100	-0.88055700

Pd(PPh₃)₄

Pd	0.00244700	0.00401000	0.00609900
P	0.13873900	2.44658000	0.77164900
P	2.03376100	-1.30829900	0.88308400
P	-2.18446100	-1.06508900	0.85691700
P	0.01384800	-0.07387300	-2.50016400
C	3.74198400	-0.64991000	0.50639100
C	4.82213600	-1.45818300	0.11007600
C	3.96475600	0.72987700	0.65714000
C	6.08400500	-0.90124100	-0.12895200
H	4.69161200	-2.53454900	-0.01089000
C	5.22748000	1.28580200	0.43209500
H	3.14202500	1.38131400	0.95487100
C	6.29307400	0.47150600	0.03283500
H	6.90873600	-1.54934500	-0.43888500
H	5.37475900	2.36127000	0.56190500
H	7.27992100	0.90506400	-0.15120000
C	2.23501000	-3.07377900	0.30457800
C	2.39103900	-4.16777000	1.17325000
C	2.22847500	-3.32030700	-1.08117400
C	2.53435000	-5.46742400	0.67061000
H	2.40576800	-4.01729800	2.25373400
C	2.38388500	-4.61506100	-1.58319400
H	2.11321600	-2.48960100	-1.77960400
C	2.53399800	-5.69690100	-0.70807800
H	2.65343600	-6.30298400	1.36627900
H	2.38307000	-4.77806900	-2.66452400
H	2.65009300	-6.71140600	-1.09908700

C	2.17788400	-1.54477300	2.73190500	C	-1.36885200	-3.75950900	0.76884900
C	3.39253800	-1.45986900	3.43553100	C	-3.81514500	-4.82438600	-0.03882900
C	1.00787800	-1.83284300	3.45622500	H	-4.54387900	-2.80209700	-0.02815600
C	3.43287500	-1.65976500	4.82057500	C	-1.50769900	-5.14026900	0.60009200
H	4.32227800	-1.24063900	2.90784300	H	-0.40359400	-3.35507400	1.07608200
C	1.04890100	-2.04764400	4.83705900	C	-2.73250300	-5.67871800	0.19037700
H	0.05064100	-1.88924400	2.93618200	H	-4.77846300	-5.23244300	-0.35786700
C	2.26302700	-1.95800400	5.52623400	H	-0.65143000	-5.79519200	0.78182500
H	4.38825100	-1.58624000	5.34798700	H	-2.84163100	-6.75764500	0.04992100
H	0.12548100	-2.27638400	5.37573100	C	-2.52777000	-0.99078300	2.69302800
H	2.29668100	-2.11695700	6.60758200	C	-3.06349500	-2.06316700	3.42825000
C	1.65158200	-0.37349900	-3.34566000	C	-2.24144600	0.20554100	3.37424300
C	1.82048200	-1.24300700	-4.43796700	C	-3.30660200	-1.93949000	4.80142000
C	2.77798900	0.31530600	-2.86091500	H	-3.30120500	-3.00673400	2.93449300
C	3.07895900	-1.41662800	-5.02633900	C	-2.49744900	0.33534300	4.74245900
H	0.96845100	-1.79169500	-4.84309000	H	-1.81219900	1.04855500	2.83094400
C	4.03149300	0.15551100	-3.45885300	C	-3.02841200	-0.73967600	5.46334300
H	2.67548400	0.98363300	-2.00392300	H	-3.72166100	-2.78764200	5.35338100
C	4.18773800	-0.71590600	-4.54237600	H	-2.27176200	1.27857500	5.24701100
H	3.18873000	-2.10106400	-5.87241700	H	-3.22170500	-0.64353000	6.53530400
H	4.89034500	0.70789700	-3.06855300	C	-3.79232600	-0.38874500	0.18719600
H	5.16947600	-0.85026200	-5.00488100	C	-4.85008400	0.05880900	0.99741200
C	-1.03594900	-1.37688000	-3.32857900	C	-3.95144800	-0.32620900	-1.20987700
C	-1.02136500	-2.67493400	-2.78730800	C	-6.02926100	0.55508400	0.42690400
C	-1.83398600	-1.13515600	-4.46102300	H	-4.76673700	0.02209000	2.08465100
C	-1.76643600	-3.70518700	-3.36858600	C	-5.13238700	0.15739400	-1.77916800
H	-0.42222900	-2.88363300	-1.89900600	H	-3.14884800	-0.67207700	-1.86352200
C	-2.59397800	-2.16233200	-5.03317200	C	-6.17691200	0.60472500	-0.96208400
H	-1.86756600	-0.14099800	-4.91007800	H	-6.83855400	0.89832300	1.07770400
C	-2.56038500	-3.45116000	-4.49238600	H	-5.23350000	0.18771300	-2.86761700
H	-1.73244800	-4.70783900	-2.93425300	H	-7.09954800	0.98852200	-1.40597200
H	-3.21106500	-1.95145000	-5.91128600	C	1.55431800	3.47327800	0.11323300
H	-3.15208400	-4.25318000	-4.94227700	C	2.44359700	4.19488100	0.92814900
C	-0.56192300	1.45083900	-3.41124700	C	1.73814700	3.52516700	-1.28117700
C	0.08689400	1.97996100	-4.54115200	C	3.48566700	4.94255300	0.36473900
C	-1.71477200	2.10254900	-2.93744800	H	2.33100400	4.18447400	2.01331900
C	-0.40437800	3.12683700	-5.17638200	C	2.76988800	4.28087200	-1.84408400
H	0.98208200	1.49889000	-4.93909700	H	1.05902000	2.97923500	-1.93831100
C	-2.21559600	3.23767200	-3.58152000	C	3.65249900	4.99093800	-1.02208100
H	-2.22669100	1.71957000	-2.05254100	H	4.16584600	5.49519100	1.01916200
C	-1.55846000	3.75754400	-4.70216000	H	2.88585600	4.31035500	-2.93107400
H	0.11791600	3.52414900	-6.05143300	H	4.46397400	5.57817100	-1.46056600
H	-3.11769700	3.72219700	-3.19865700	C	-1.29298100	3.57731200	0.36345100
H	-1.94264300	4.65146400	-5.20120100	C	-1.13995700	4.90196100	-0.08290200
C	-2.45129800	-2.88952200	0.55060800	C	-2.59670300	3.08285600	0.54189100
C	-3.67815600	-3.44333300	0.14408400	C	-2.25718400	5.70398300	-0.34366500

H	-0.14465500	5.32534800	-0.22567800	C	-0.83805700	5.61842100	-1.39712300
C	-3.71356400	3.88672400	0.29518600	H	-2.17947000	4.00881600	-1.89782100
H	-2.74422000	2.05571200	0.87778300	C	0.47198800	5.33733300	0.61377800
C	-3.54793900	5.20156400	-0.15371000	H	0.18741200	3.49366200	1.68902500
H	-2.11353800	6.73058200	-0.69256200	C	0.11272100	6.10865100	-0.49872100
H	-4.71643900	3.47879600	0.44680300	H	-1.12716600	6.21177700	-2.26910000
H	-4.41995200	5.82992400	-0.35488100	H	1.21528700	5.71071500	1.32371000
C	0.30447300	2.78347700	2.60347200	H	0.57334200	7.08669000	-0.66220300
C	-0.38488000	3.81191300	3.27044300	C	-0.58731800	-3.21081100	-1.36427600
C	1.17111500	1.96888900	3.35352000	C	-0.36561500	-4.56917900	-1.08356300
C	-0.20919200	4.01843700	4.64396100	C	-0.18797900	-2.70556500	-2.61536700
H	-1.06451400	4.46660400	2.72259300	C	0.24020400	-5.40130600	-2.03231800
C	1.35880300	2.18326100	4.72217200	H	-0.66315000	-4.98956300	-0.12076900
H	1.70723300	1.15458600	2.86429400	C	0.40644000	-3.53955800	-3.56636600
C	0.66536100	3.20823400	5.37462800	H	-0.33673600	-1.64701500	-2.84568800
H	-0.75768900	4.82297400	5.14213300	C	0.62536500	-4.89082000	-3.27554800
H	2.04349300	1.53937800	5.28056400	H	0.41070600	-6.45514700	-1.79515400
H	0.80384700	3.37269100	6.44677100	H	0.71001500	-3.12806600	-4.53285900
int-1				H	1.09938100	-5.54246500	-4.01467400
P	-1.37289300	-2.03376400	-0.16234800	C	-3.17730400	-2.19294300	-0.57207000
P	-1.75928100	1.88033000	0.21789700	C	-3.65326500	-2.93681200	-1.66445100
C	-3.27062700	1.86037600	-0.85685400	C	-4.10669000	-1.50040000	0.22731300
C	-3.12754100	1.33502100	-2.15395500	C	-5.02386300	-2.99120800	-1.94655400
C	-4.53093800	2.33413600	-0.45556700	H	-2.95871500	-3.48375100	-2.30448700
C	-4.21289000	1.29969700	-3.03471100	C	-5.47429400	-1.56545500	-0.04832000
H	-2.15735500	0.94539400	-2.47547500	H	-3.76249300	-0.90783500	1.07836500
C	-5.61932100	2.28692300	-1.33330500	C	-5.93833200	-2.31005700	-1.13943000
H	-4.67714300	2.73862500	0.54743900	H	-5.37458700	-3.57542000	-2.80191400
C	-5.46335900	1.77388000	-2.62499700	H	-6.18054200	-1.02642600	0.58893800
H	-4.08197500	0.89161600	-4.04059400	H	-7.00845800	-2.35624400	-1.35891200
H	-6.59490700	2.65434800	-1.00306600	C	-1.24773100	-2.92751000	1.45877200
H	-6.31571600	1.73895800	-3.30900000	C	-2.19573700	-3.87146700	1.89209000
C	-2.39791200	2.03239600	1.95213700	C	-0.14526800	-2.64810400	2.28662800
C	-2.96020500	3.21976400	2.45776300	C	-2.04202400	-4.51971700	3.12218300
C	-2.29449300	0.91908700	2.80328000	H	-3.06140800	-4.10810100	1.26981200
C	-3.42318400	3.28142800	3.77526500	C	0.01069800	-3.30204600	3.51279000
H	-3.03264400	4.10764200	1.82564900	H	0.59455700	-1.90797600	1.96950400
C	-2.75900100	0.98139400	4.12203100	C	-0.93904200	-4.23811300	3.93499400
H	-1.83523200	-0.00083700	2.43364100	H	-2.78923300	-5.24985700	3.44524400
C	-3.32628200	2.16190700	4.60985800	H	0.87419700	-3.07225300	4.14300200
H	-3.85854700	4.21074800	4.15280000	H	-0.82191200	-4.74472000	4.89688100
H	-2.66807900	0.10538800	4.76988900	Pd	-0.21269300	0.08608500	-0.17094300
H	-3.68566900	2.21404800	5.64122900	C	1.76013500	0.78091200	-0.45369300
C	-1.07911000	3.58692900	-0.07441400	C	1.74750600	-0.49437100	-0.52941400
C	-1.43368400	4.36806500	-1.18587000	H	2.28737800	-1.42448400	-0.68516100
C	-0.11204300	4.08573500	0.81953500	C	2.51263200	2.05954100	-0.52857600

H	1.98145300	2.77206300	-1.18099000	H	3.59987300	1.46668700	-1.01408700
H	2.55157700	2.53896700	0.45948500	C	4.15400000	4.02234200	-3.20351500
N	3.88891400	1.95654300	-1.04557500	H	2.84315100	5.72093800	-3.49500900
C	4.07421500	1.72650300	-2.47046500	H	5.25407200	2.22641400	-2.69735300
H	3.45672800	2.43847700	-3.04316500	H	4.88233600	4.35633000	-3.94734400
H	5.12697100	1.92411500	-2.73409000	C	-0.53314700	3.26376400	-0.54472400
C	3.76562500	0.32051400	-2.94686700	C	-1.09582100	4.39528400	0.06697500
O	3.23224200	0.08738300	-4.01024300	C	-1.20362300	2.66235000	-1.62577900
H	4.11267800	-0.50265200	-2.27878200	C	-2.31202300	4.91215500	-0.39399800
S	5.18647700	1.94602800	0.00416800	H	-0.59048100	4.88283400	0.90251800
O	6.37229800	2.29854800	-0.79492400	C	-2.41182300	3.18791800	-2.08930400
O	4.80827400	2.78321200	1.15431800	H	-0.77618200	1.78055500	-2.11095900
C	5.43046300	0.28151300	0.61768600	C	-2.97079300	4.31228800	-1.47084500
C	6.25782200	-0.59857900	-0.09171200	H	-2.74236800	5.79166500	0.09223000
C	4.78811300	-0.12178200	1.79158500	H	-2.92203500	2.71267000	-2.93113800
C	6.42711600	-1.89818900	0.38227500	H	-3.92051600	4.71900000	-1.82837300
H	6.77337800	-0.26898400	-0.99565000	C	1.47676700	-3.28263800	1.21612800
C	4.97176400	-1.42844200	2.25042600	C	0.15732700	-3.61135700	1.58189700
H	4.16074900	0.57585100	2.34912600	C	2.54067800	-3.74218000	2.00984100
C	5.78673100	-2.33789700	1.55643700	C	-0.08611200	-4.39054600	2.71542100
H	7.07609300	-2.58589400	-0.16730700	H	-0.69042100	-3.27360100	0.98283300
H	4.47364800	-1.74433100	3.17092600	C	2.28961200	-4.51869800	3.14658800
C	5.98354900	-3.74706900	2.04826900	H	3.57250700	-3.50101200	1.74772400
H	5.63135200	-4.47730300	1.30003000	C	0.97818700	-4.84454500	3.50256100
H	7.05205500	-3.95930700	2.22110100	H	-1.11636500	-4.63893000	2.98400600
H	5.44028100	-3.92944400	2.98679000	H	3.12810000	-4.87132600	3.75314400
int-2				H	0.78412500	-5.45133300	4.39104300
P	1.75205000	-2.18775400	-0.23796500	C	3.55288200	-2.28945700	-0.61197800
P	1.08245700	2.54423200	-0.03925000	C	4.08922500	-3.17996100	-1.55709300
C	1.56037100	3.37698100	1.53224300	C	4.41554300	-1.41473400	0.07564200
C	0.74919800	3.22752300	2.67416000	C	5.46564800	-3.19765000	-1.80335700
C	2.76426500	4.09609700	1.64210900	H	3.43763400	-3.86335100	-2.10532000
C	1.13805500	3.78716900	3.89385400	C	5.79170300	-1.44140400	-0.16890800
H	-0.18577700	2.66632300	2.64241100	H	4.00843800	-0.71164600	0.80847000
C	3.14437800	4.65724000	2.86570600	C	6.31832300	-2.33164700	-1.11072300
H	3.41372000	4.22421000	0.77420400	H	5.87255000	-3.89400400	-2.54143400
C	2.33433900	4.50440800	3.99511700	H	6.45210700	-0.76060800	0.37458100
H	0.49827500	3.63933600	4.76791700	H	7.39365600	-2.34846100	-1.30730500
H	4.08131800	5.21680000	2.93248600	C	0.89692800	-3.00902400	-1.64251700
H	2.63614000	4.94043700	4.95127900	C	0.71503000	-4.40148100	-1.70985900
C	2.27572700	3.16523000	-1.29801900	C	0.43365200	-2.20342200	-2.69763400
C	2.07324300	4.36358700	-2.00363400	C	0.08192200	-4.97416800	-2.81704400
C	3.42724000	2.40121900	-1.55743200	H	1.06554400	-5.04463700	-0.89971900
C	3.00962700	4.78730700	-2.95100300	C	-0.19394800	-2.78059600	-3.80538900
H	1.18493600	4.97103700	-1.81658200	H	0.56074600	-1.11773900	-2.64674200
C	4.36288100	2.82933600	-2.50445600	C	-0.37216500	-4.16668100	-3.86531300

H	-0.05721700	-6.05768500	-2.85918200	H	0.17219900	4.38431200	4.68552900
H	-0.55027000	-2.14440300	-4.61981500	H	-2.28880000	3.99647200	4.87709900
H	-0.86916400	-4.61837600	-4.72802300	C	1.89278700	3.82096100	-0.07850900
Pd	1.29379900	0.15307400	-0.06097400	C	1.85794900	5.01856000	-0.81178500
C	-0.31640400	-0.12084000	1.09243400	C	3.06304100	3.49102200	0.63012600
C	-0.26750400	0.03921500	2.41354100	C	2.96622900	5.87205400	-0.82580100
C	-1.57029100	-0.50535000	0.34431600	H	0.97154300	5.29380000	-1.38501800
H	-1.95037900	0.35461400	-0.24077600	C	4.16557300	4.35029000	0.62079800
H	-1.36521000	-1.31974700	-0.36330200	H	3.11472800	2.55636500	1.19336400
N	-2.57580100	-0.96430700	1.31563000	C	4.12034800	5.54261600	-0.10857000
C	-2.78530100	-0.05200200	2.44407600	H	2.92471300	6.79872100	-1.40455200
H	-3.00298100	0.97121000	2.08042100	H	5.06556300	4.08084500	1.17988500
H	-3.63556900	-0.39573200	3.04616200	H	4.98538900	6.21118000	-0.12238400
C	-1.51718300	0.02511300	3.33967800	C	-0.69160600	3.10480700	-1.34135000
O	-1.54590600	1.08772800	4.16673300	C	-1.42856600	4.30417700	-1.32420300
H	-1.46548600	-0.97415300	3.86974200	C	-0.84998800	2.22237500	-2.42337100
S	-3.81306200	-1.93623100	0.77492400	C	-2.29330300	4.61539700	-2.37674500
O	-3.20756100	-2.91421200	-0.15081900	H	-1.33603100	4.99767700	-0.48550000
O	-4.52114400	-2.42389100	1.97041800	C	-1.71678300	2.53674400	-3.47556500
C	-4.96740100	-0.95067200	-0.17627400	H	-0.29535000	1.28065700	-2.43624800
C	-4.77460400	-0.79768200	-1.55586300	C	-2.43750800	3.73410300	-3.45462900
C	-6.03401900	-0.32066600	0.47327200	H	-2.85966900	5.55021900	-2.35282400
C	-5.65822900	0.00139400	-2.27988200	H	-1.83032900	1.84027900	-4.31042600
H	-3.95397500	-1.31058300	-2.06062400	H	-3.11671100	3.97993400	-4.27539400
C	-6.90785500	0.47599200	-0.27014600	C	1.62947200	-3.11245000	1.00539100
H	-6.19319000	-0.46214900	1.54375100	C	0.37025600	-3.71385000	0.82399600
C	-6.73616700	0.65426400	-1.65286300	C	2.38733200	-3.45765100	2.13641700
H	-5.51306000	0.11460200	-3.35806000	C	-0.11726100	-4.63774700	1.75101900
H	-7.74532600	0.96323300	0.23638200	H	-0.24433800	-3.46673100	-0.04325800
H	0.66032900	0.28427700	2.94104900	C	1.89749100	-4.38691200	3.06202900
C	-7.67267800	1.52028200	-2.45312800	H	3.36782500	-3.00887100	2.30489400
H	-8.53074400	1.85457000	-1.85184500	C	0.64544900	-4.97857800	2.87399000
H	-7.15112200	2.41768600	-2.82864600	H	-1.10641000	-5.07768500	1.59827800
H	-8.05555300	0.98198100	-3.33577800	H	2.50345200	-4.64798700	3.93395800
int-3				H	0.26372000	-5.70210200	3.59941200
P	2.19020900	-1.83466300	-0.20962600	C	4.00654700	-1.70434600	0.09358200
P	0.47392900	2.63760300	0.00644400	C	4.96305900	-2.44449000	-0.61885000
C	-0.41127600	3.13961900	1.55318100	C	4.43798200	-0.81536900	1.09475800
C	-1.79636000	2.92228300	1.67179700	C	6.32454400	-2.30318300	-0.32806100
C	0.28578700	3.66573600	2.65383600	H	4.65701100	-3.13223000	-1.40908800
C	-2.46550900	3.23080300	2.85880300	C	5.79749900	-0.68359400	1.38958500
H	-2.36390800	2.51094000	0.83460700	H	3.70462700	-0.21883600	1.64440100
C	-0.38738300	3.97142300	3.84180400	C	6.74474100	-1.42682900	0.67678000
H	1.36006500	3.84792200	2.59556000	H	7.05918000	-2.88235500	-0.89408000
C	-1.76383000	3.75588100	3.94875000	H	6.11755000	0.00846000	2.17308900
H	-3.54230800	3.05623800	2.93097500	H	7.80938600	-1.31860900	0.90108800

C 1.99124700 -2.69145500 -1.82995200
C 2.22903000 -4.07034000 -1.98210700
C 1.58681300 -1.94187700 -2.94668800
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H 2.53388500 -4.67613500 -1.12594200
C 1.42876200 -2.55500500 -4.19389100
H 1.39199700 -0.87410900 -2.83653100
C 1.67150800 -3.92398200 -4.33785000
H 2.25900200 -5.75165200 -3.33540200
H 1.11036500 -1.95917000 -5.05341000
H 1.54473500 -4.40470000 -5.31168100
Pd 1.24050300 0.38065100 -0.17647800
C -0.30650300 -0.26341700 0.95824400
C -0.32857700 -0.32820800 2.30010200
C -1.49318900 -0.75095300 0.15189100
H -2.05309000 0.11954500 -0.24797500
H -1.15432500 -1.33579000 -0.71272500
N -2.37553200 -1.60485700 0.96878600
C -2.74625100 -1.03783700 2.26356300
H -3.22544600 -0.04822100 2.13921000
H -3.45418800 -1.70304000 2.77356200
C -1.48629300 -0.86523700 3.11429500
O -1.85328800 0.01760000 4.17676700
H -1.20726000 -1.85068200 3.53944200
S -3.45032700 -2.62221600 0.20392000
O -2.75828000 -3.13472400 -0.99319400
O -3.92955000 -3.57649300 1.21929600
C -4.85826800 -1.66738500 -0.35279300
C -4.80112000 -1.01337700 -1.59149500
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H -3.92719600 -1.12094500 -2.23655700
C -7.06231800 -0.77539800 0.03951100
H -6.03201700 -2.08589700 1.42001400
C -7.03168300 -0.10203300 -1.19259400
H -5.84376900 0.26993700 -2.96606700
H -7.94661500 -0.69387800 0.67720700
H 0.53553300 0.00037800 2.89303200
C -8.18993500 0.74215700 -1.65396500
H -9.01972400 0.72400000 -0.93245400
H -7.88015500 1.79175400 -1.79428600
H -8.57162600 0.39088000 -2.62734400
H -1.09311800 0.10231200 4.77175300
O 2.90478000 0.88094300 -1.38806600
C 2.76803900 1.57340500 -2.58256900
H 3.76350400 1.77304800 -3.04182800

H 2.18761500 1.02901600 -3.36526700
H 2.27959500 2.56963200 -2.48588700
int-4
P -1.16801900 2.14321700 0.00099400
P -2.60624100 -1.49582400 -0.39241100
C -4.06311800 -0.77727400 -1.29945000
C -3.78341100 0.00489700 -2.43511200
C -5.40251400 -1.03771500 -0.97077900
C -4.81734400 0.50599900 -3.22839000
H -2.74677700 0.21526200 -2.71231000
C -6.43860000 -0.52623500 -1.76246200
H -5.65277300 -1.64918200 -0.10235200
C -6.15091200 0.24299100 -2.89268500
H -4.58077900 1.10695000 -4.11049700
H -7.47672200 -0.74036400 -1.49354100
H -6.96164700 0.63651200 -3.51173500
C -3.35665200 -2.44394500 1.00111100
C -3.18998400 -3.82672700 1.17909400
C -4.02285200 -1.70872700 2.00111000
C -3.69884600 -4.46216700 2.31794000
H -2.65057700 -4.41973300 0.43915200
C -4.53745900 -2.34694800 3.13221700
H -4.14134700 -0.62630800 1.89984600
C -4.37839400 -3.72806900 3.29341500
H -3.55763900 -5.53948000 2.44020200
H -5.05880200 -1.76062600 3.89368600
H -4.77676400 -4.22753400 4.18064400
C -2.09891000 -2.72340400 -1.68466800
C -2.95981100 -3.74882100 -2.11834700
C -0.87134400 -2.54487100 -2.34196700
C -2.58252500 -4.59414700 -3.16461000
H -3.93624900 -3.88581000 -1.64775900
C -0.50032600 -3.38416500 -3.39905600
H -0.20528500 -1.73731300 -2.02731600
C -1.35121100 -4.41461800 -3.80679000
H -3.25798300 -5.39146400 -3.48651300
H 0.45819700 -3.23018000 -3.90192500
H -1.06078000 -5.07397600 -4.62926600
C 0.08864100 2.95960200 -1.07519800
C 1.11629700 3.78065000 -0.58288000
C 0.07892200 2.63735700 -2.44680400
C 2.09152300 4.29129300 -1.44866100
H 1.18009200 4.01389300 0.48088200
C 1.04853200 3.15495700 -3.30917100
H -0.69202300 1.97463900 -2.84947700
C 2.05754100 3.98793500 -2.81231800

H 2.88355800 4.92973700 -1.04798500
H 1.01815200 2.90089800 -4.37211400
H 2.81844600 4.39189000 -3.48549300
C -2.79614200 2.81584000 -0.60343900
C -2.93114600 3.75759800 -1.63522200
C -3.94913300 2.40119900 0.08878600
C -4.19144900 4.27126700 -1.96673600
H -2.05717500 4.11105400 -2.18417500
C -5.20303700 2.92270800 -0.23534800
H -3.86734900 1.67201900 0.89944500
C -5.32887700 3.85956400 -1.26815100
H -4.27735000 5.00575000 -2.77239100
H -6.08616100 2.59325900 0.31845400
H -6.31050100 4.26686000 -1.52486900
C -1.13878700 3.01974200 1.63355600
C -1.15043800 4.42386000 1.72377800
C -1.23724500 2.26288900 2.81167900
C -1.22765700 5.05187700 2.96938700
H -1.11010300 5.03588400 0.81961400
C -1.32746000 2.89341400 4.05801700
H -1.24815500 1.17154800 2.74941700
C -1.31554300 4.28827100 4.13966300
H -1.22878300 6.14388600 3.02553900
H -1.40499700 2.28952500 4.96611600
H -1.38139000 4.78235600 5.11286200
Pd -0.63610900 -0.23357600 0.37042000
C 1.30578000 0.35461000 0.77128300
C 1.79559600 0.88531100 1.90567100
C 2.22563300 0.11157300 -0.40679000
H 2.01308400 0.84050900 -1.20854200
H 2.05525700 -0.87883200 -0.84628700
N 3.67324700 0.22620400 -0.09582600
C 3.99742200 1.35308100 0.78472800
H 3.71296600 2.27204200 0.24712000
H 5.08422300 1.40047400 0.95425900
C 3.22654200 1.31983900 2.11179200
O 3.20964700 2.62621000 2.69625700
H 3.72665500 0.62172600 2.81084000
S 4.52927600 -1.19276000 0.16205100
O 3.95960500 -2.20364800 -0.75047400
O 4.62564400 -1.54593300 1.59621200
C 6.17656100 -0.78481800 -0.40280700
C 6.38114200 -0.51972200 -1.76102700
C 7.24277200 -0.79466600 0.50139100
C 7.67411300 -0.25020500 -2.20929100
H 5.54402300 -0.52318000 -2.46240000

C 8.52871400 -0.52238300 0.03340700
H 7.06679300 -1.01427100 1.55564000
C 8.76756400 -0.24551200 -1.32433000
H 7.83850100 -0.04154000 -3.26979400
H 9.36495200 -0.52699500 0.73829000
H 1.16083000 1.03337600 2.78604000
H 4.10690700 2.82947300 3.00238700
C 0.03395900 -1.98635000 1.24757400
C 0.76322000 -3.01770500 0.62747500
C -0.24971600 -2.14586200 2.62125500
C 1.17700200 -4.15743800 1.33476400
H 1.02995900 -2.94899900 -0.42928900
C 0.15776400 -3.28095700 3.33402000
H -0.80187400 -1.36988200 3.16145300
C 0.87474100 -4.29774400 2.69207500
H 1.74482900 -4.93662300 0.81595800
H -0.08422300 -3.36817000 4.39820500
H 1.19697100 -5.18494700 3.24501400
C 10.16340100 0.04530800 -1.80823100
H 10.58530000 0.92290900 -1.28988200
H 10.83752200 -0.80221100 -1.59809400
H 10.18636800 0.24184400 -2.88994000

int-5

P -1.13633900 1.92887900 -0.28768500
P -2.54850300 -1.77488000 0.05713700
C -3.99086600 -1.31279600 -1.01269600
C -3.69817200 -0.87447200 -2.31732900
C -5.33377000 -1.42875800 -0.62045200
C -4.72560100 -0.57103200 -3.21332200
H -2.65744000 -0.77632500 -2.63977600
C -6.36207400 -1.11364800 -1.51716100
H -5.59041500 -1.77089400 0.38394000
C -6.06230700 -0.68762400 -2.81409100
H -4.48142400 -0.23652200 -4.22514300
H -7.40351700 -1.20905500 -1.19762100
H -6.86754100 -0.44565600 -3.51294900
C -3.27322900 -2.14073700 1.71709000
C -3.13073700 -3.38722900 2.34831100
C -3.88862200 -1.08990300 2.42456400
C -3.60703800 -3.58222400 3.65020500
H -2.64221800 -4.21562200 1.83216100
C -4.37200100 -1.29059200 3.71975700
H -3.99439000 -0.10511100 1.96267700
C -4.23226600 -2.53869600 4.33757900
H -3.48637700 -4.55913500 4.12631900
H -4.85457400 -0.46524900 4.25012400

H -4.60570800 -2.69417800 5.35330200
C -2.14455300 -3.43138700 -0.67390900
C -3.15277400 -4.39303700 -0.87860500
C -0.83526000 -3.72605100 -1.08424500
C -2.85032500 -5.62475400 -1.46294900
H -4.18292200 -4.18305300 -0.58060900
C -0.53506500 -4.95796600 -1.67827200
H -0.04492200 -2.98701600 -0.93869500
C -1.53964300 -5.91025500 -1.86537900
H -3.64278200 -6.36392800 -1.60867700
H 0.48997800 -5.16957300 -1.99435500
H -1.30546100 -6.87321600 -2.32750100
C 0.22805700 2.57404600 -1.35080800
C 1.19213100 3.48979800 -0.89897900
C 0.37063600 2.02297800 -2.63982600
C 2.25386100 3.86937000 -1.72979600
H 1.13771000 3.90060300 0.11023900
C 1.42509300 2.41147200 -3.46995300
H -0.34647100 1.28143800 -3.00250700
C 2.36938400 3.34042800 -3.01805800
H 2.99486300 4.58379700 -1.36102300
H 1.51261700 1.98045000 -4.47092900
H 3.19702800 3.64275600 -3.66531500
C -2.69177200 2.47269100 -1.15446000
C -2.72050500 3.17031400 -2.37222500
C -3.90967400 2.20174500 -0.50301900
C -3.93902800 3.58502700 -2.92472500
H -1.79546700 3.40951800 -2.89849100
C -5.12249400 2.62555700 -1.04956500
H -3.91217100 1.66557700 0.44926900
C -5.14159300 3.31707900 -2.26668000
H -3.94096500 4.12951300 -3.87306100
H -6.05682600 2.41157700 -0.52394100
H -6.09082000 3.64687300 -2.69743100
C -1.23286700 3.03979100 1.18863300
C -1.30958200 4.43923300 1.06126900
C -1.33643100 2.46579300 2.46542500
C -1.46078000 5.24445500 2.19252300
H -1.25936400 4.90595100 0.07445100
C -1.49774300 3.27370100 3.59728600
H -1.29679500 1.37834400 2.57158700
C -1.55415900 4.66331300 3.46331000
H -1.51371700 6.33088400 2.08089000
H -1.57918700 2.81224100 4.58506300
H -1.67697800 5.29561300 4.34690000
Pd -0.61581900 -0.38203800 0.39404600

C 1.32657500 0.18847500 0.84065700
C 1.74616800 0.86441600 1.92749500
C 2.33367700 -0.24318900 -0.20613000
H 2.18954400 0.34515300 -1.13025400
H 2.18306800 -1.29190600 -0.48973000
N 3.75314900 -0.08019600 0.19425200
C 4.02776300 1.16170100 0.92210700
H 3.78137300 1.99694400 0.24623100
H 5.10143000 1.23664900 1.15398600
C 3.16893000 1.30104900 2.18622900
O 3.13691400 2.66819300 2.60808100
H 3.60735800 0.68604400 2.99588600
S 4.61351800 -1.43266200 0.67603100
O 4.01470700 -2.59157100 -0.01381700
O 4.75689100 -1.50692500 2.14658800
C 6.24606500 -1.15362700 -0.00148800
C 6.41165700 -1.14031000 -1.39089100
C 7.33801500 -1.00368500 0.85787100
C 7.69078200 -0.96423500 -1.91723400
H 5.55454400 -1.26390300 -2.05647600
C 8.61048900 -0.82783500 0.31171900
H 7.19228100 -1.02486200 1.93901000
C 8.81026000 -0.80595700 -1.07943500
H 7.82431500 -0.95033900 -3.00227000
H 9.46582100 -0.70633200 0.98228100
H 1.04880400 1.16368100 2.71754600
H 4.01153500 2.89294900 2.96106900
C 10.19261300 -0.63706000 -1.65195100
H 10.74152000 0.17026100 -1.14107500
H 10.78398200 -1.56007300 -1.51903200
H 10.16157800 -0.41199000 -2.72813400
H -0.05435400 -1.72497700 1.00067600

int-6

P -2.39520700 -0.00895000 0.00309500
P 2.40800600 -0.02142500 0.01119800
C 3.24607600 -1.07784000 1.27686300
C 3.26245700 -2.47220300 1.08213100
C 3.81569700 -0.55348800 2.44919000
C 3.83905000 -3.31659700 2.03345700
H 2.83352500 -2.90729700 0.17749500
C 4.38984900 -1.40318400 3.40160100
H 3.82652800 0.52217400 2.62950300
C 4.40319600 -2.78536900 3.19853400
H 3.84667900 -4.39639000 1.86182200
H 4.83299500 -0.97545700 4.30498000
H 4.85356000 -3.44723500 3.94314000

C	3.02348000	1.68566100	0.32826800	C	-2.09734200	1.63359800	2.25777000
C	3.96960500	2.32855500	-0.48620200	C	-4.81529500	1.68871600	2.91061300
C	2.49036100	2.37825100	1.43193400	H	-5.11220500	0.41840600	1.19576700
C	4.38624000	3.63128500	-0.19097800	C	-2.53346800	2.34992800	3.37766000
H	4.38640400	1.82178500	-1.35818700	H	-1.03299000	1.59664300	2.01277600
C	2.92053500	3.67344600	1.73231200	C	-3.89231500	2.38222300	3.70258900
H	1.73588100	1.90184900	2.06357700	H	-5.87817200	1.70328900	3.16630000
C	3.86948100	4.30381900	0.92018600	H	-1.80625100	2.87892700	3.99925200
H	5.12117200	4.12019600	-0.83614700	H	-4.23369900	2.94088400	4.57830100
H	2.50414600	4.19467300	2.59841700	Pd	0.01255400	-0.07919600	-0.05466500
H	4.20009500	5.32034100	1.14981300	O	0.13260600	1.62939600	-1.16373600
C	3.16114800	-0.56814900	-1.57685800	O	-0.01133000	-1.86284100	0.91687000
C	4.53846500	-0.83423000	-1.69210200	C	-0.34254800	2.83867700	-0.66229500
C	2.33438800	-0.73663500	-2.70008500	H	-0.14877300	3.65018300	-1.39748500
C	5.07515500	-1.25094200	-2.91278500	H	-1.43857000	2.85118400	-0.47286600
H	5.19658100	-0.71984300	-0.82743900	H	0.14713600	3.15966600	0.28243100
C	2.87578200	-1.15359900	-3.92096000	C	-0.07716300	-2.94444100	0.03559600
H	1.26096800	-0.55086500	-2.61498600	H	-0.08491200	-3.89826500	0.60593200
C	4.24547500	-1.40991000	-4.02913300	H	-0.99238000	-2.95063000	-0.59543800
H	6.14638500	-1.45488200	-2.99171100	H	0.78529800	-3.00483000	-0.66463500
H	2.22161500	-1.28332300	-4.78712200	int-7			
H	4.66815400	-1.73905200	-4.98228500	P	-2.39639400	0.22097900	-0.01032200
C	-3.08915400	0.75824200	-1.52166700	P	2.40878200	0.23957600	-0.04339700
C	-4.09602100	1.73702400	-1.52095100	C	3.20318400	1.67874300	-0.90603100
C	-2.54190500	0.34148400	-2.75005800	C	3.20622200	2.92961400	-0.25904000
C	-4.55598500	2.27658300	-2.72716200	C	3.75731600	1.58678000	-2.19357900
H	-4.52504700	2.09218700	-0.58266200	C	3.75497900	4.05261500	-0.88253500
C	-3.01127500	0.87523100	-3.95317900	H	2.79139300	3.03141600	0.74526800
H	-1.74708400	-0.40895800	-2.76621800	C	4.30321600	2.71490100	-2.81655800
C	-4.01903000	1.84556200	-3.94392300	H	3.78133100	0.63440200	-2.72374600
H	-5.33853200	3.04001000	-2.71177000	C	4.30385200	3.95076500	-2.16530200
H	-2.58158400	0.53723900	-4.89988000	H	3.75327700	5.01304100	-0.35998600
H	-4.38105000	2.26951700	-4.88444700	H	4.73463100	2.61908700	-3.81666700
C	-3.28513100	-1.61845700	0.17518600	H	4.73310600	4.83055200	-2.65217100
C	-3.94702000	-2.23393300	-0.89984300	C	3.18326300	-1.24437000	-0.82300000
C	-3.25000100	-2.27544000	1.42024800	C	4.11151600	-2.06777700	-0.16555500
C	-4.56318200	-3.47939200	-0.73284600	C	2.78424500	-1.58256800	-2.13044600
H	-3.99356600	-1.74630000	-1.87508600	C	4.64750900	-3.18804000	-0.81147300
C	-3.86533000	-3.51872300	1.58159900	H	4.42234500	-1.84842300	0.85672300
H	-2.74499300	-1.81551000	2.27235200	C	3.33243400	-2.69225300	-2.77792900
C	-4.52269600	-4.12587200	0.50542500	H	2.03518600	-0.97807300	-2.64749700
H	-5.07935100	-3.94208300	-1.57837500	C	4.26762500	-3.49848700	-2.11968400
H	-3.83168800	-4.01517700	2.55518300	H	5.36778500	-3.81912600	-0.28379800
H	-5.00492700	-5.09861300	0.63431100	H	3.01805000	-2.93399600	-3.79672000
C	-3.01751800	0.94494400	1.45062200	H	4.69163500	-4.37156500	-2.62304300
C	-4.38256600	0.96880100	1.79433200	C	3.11488700	0.36008900	1.65537600

C	4.49084000	0.56395400	1.87267300	H	-0.14461400	4.09114400	1.15217300
C	2.25405900	0.27955600	2.76162100	H	-0.95752400	2.67208600	1.84317600
C	4.99180000	0.66564400	3.17246500	H	0.81322500	2.80805300	1.91911900
H	5.17621400	0.64853600	1.02594200	C	-0.02731700	-1.77314900	0.02178400
C	2.75852000	0.38255200	4.06321800	C	-0.27483600	-2.54288900	-1.13267400
H	1.18060400	0.15155900	2.60055200	C	0.18518300	-2.48341600	1.22178000
C	4.12724800	0.57216200	4.27005700	C	-0.31458400	-3.94419600	-1.09309800
H	6.06239800	0.82245800	3.32927500	H	-0.44210700	-2.05303200	-2.09471300
H	2.07632400	0.32045800	4.91516200	C	0.15156000	-3.88415000	1.26875400
H	4.52228500	0.65482700	5.28620600	H	0.38001300	-1.94439400	2.15295900
C	-3.10130800	-1.09444900	1.07051500	C	-0.10102500	-4.62511200	0.10937900
C	-3.84533600	-2.18287200	0.58877300	H	-0.51317500	-4.50467700	-2.01246900
C	-2.78844600	-1.03928900	2.44257300	H	0.32322200	-4.39717800	2.22061400
C	-4.29167700	-3.17814800	1.46629900	H	-0.13063400	-5.71810500	0.14314600
H	-4.07560100	-2.27228900	-0.47360700	int-8			
C	-3.24794700	-2.02619500	3.31747800	P	1.31162800	2.55381700	-0.20209600
H	-2.17184100	-0.22446400	2.83175900	C	0.43688300	3.27236000	1.25125800
C	-4.00410300	-3.09874400	2.83117400	C	-0.83910300	3.85373400	1.17192300
H	-4.86811900	-4.02050000	1.07436400	C	1.05813000	3.16545900	2.51050400
H	-3.00398800	-1.96223700	4.38124800	C	-1.46512100	4.34574900	2.32306300
H	-4.35863800	-3.87553600	3.51399100	H	-1.35846400	3.92528800	0.21537200
C	-3.30141200	1.77199400	0.46265700	C	0.43635200	3.67100400	3.65474700
C	-4.07682400	1.89890400	1.62643600	H	2.03526200	2.68433100	2.60147400
C	-3.19239500	2.87912600	-0.40165000	C	-0.82692300	4.26595100	3.56349000
C	-4.72372900	3.10504600	1.92150400	H	-2.45856800	4.79534800	2.24381300
H	-4.19650100	1.05885200	2.31130700	H	0.93778200	3.58948000	4.62251200
C	-3.83771300	4.08078200	-0.10294800	H	-1.31587200	4.65713200	4.45965400
H	-2.60649900	2.80593200	-1.32027000	C	2.83648700	3.58550600	-0.42279100
C	-4.60434400	4.19959200	1.06194700	C	3.23202100	4.60514000	0.45700000
H	-5.32786800	3.18152300	2.82966000	C	3.62387600	3.32566300	-1.56106000
H	-3.74263200	4.92824800	-0.78729600	C	4.39420500	5.34505700	0.20653100
H	-5.11051600	5.14045600	1.29424600	H	2.63675600	4.84044700	1.34022900
C	-3.05013800	-0.03293900	-1.71683500	C	4.78188700	4.06585500	-1.80743700
C	-4.43103100	-0.14360000	-1.96793600	H	3.32504100	2.54947900	-2.26936800
C	-2.15895700	-0.01217200	-2.80138200	C	5.17337300	5.07631400	-0.92145400
C	-4.90188800	-0.26519200	-3.27720100	H	4.68565800	6.13867000	0.89989500
H	-5.14537100	-0.12496300	-1.14133200	H	5.38070900	3.85187500	-2.69683200
C	-2.63436500	-0.12549800	-4.11312200	H	6.08103400	5.65464400	-1.11412300
H	-1.08858900	0.11120100	-2.61702900	C	0.36122100	3.06235500	-1.70348600
C	-4.00429600	-0.25990100	-4.35206200	C	0.07945600	4.42115400	-1.94462100
H	-5.97597900	-0.35618000	-3.46003300	C	-0.00772700	2.11064300	-2.66673800
H	-1.92931000	-0.10472500	-4.94830500	C	-0.58491200	4.80964500	-3.10964800
H	-4.37642400	-0.35099100	-5.37615700	H	0.38562500	5.18382100	-1.22454200
Pd	0.00293900	0.26988600	0.01602300	C	-0.66852100	2.50363100	-3.83694500
O	0.03408600	2.37305300	0.01009300	H	0.23558500	1.05849100	-2.51333300
C	-0.06425400	2.98410800	1.25290000	C	-0.96430200	3.85083400	-4.05711600

H -0.80154000 5.86740500 -3.28160300
H -0.94744600 1.75006000 -4.57812500
H -1.48199500 4.15756600 -4.97002200
Pd 1.67812500 0.19119300 -0.05833700
O 3.77520800 0.35378500 -0.21049700
C 4.38232300 0.70241700 0.99046000
H 4.10603400 1.71944800 1.35535300
H 4.15852900 0.00225300 1.82775200
H 5.49160500 0.70871400 0.89126000
C -0.89777900 0.01403100 2.51171900
C -1.82408900 0.42528100 3.49774300
C 0.37780900 -0.38280600 2.97331900
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H -3.91464000 -3.15431700 1.40440200
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O -3.19752200 -1.28363600 -2.01176200
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C 0.90813000 -3.48228300 -0.22476100
C 1.11443400 -4.68439000 0.47346200
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H 2.26675200 -2.72100800 2.51827400
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H 6.42540400 -3.57970300 3.24880900
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H -9.36279100 1.95225200 -2.47867200
H -10.00495500 1.25719900 -0.96529400
int-9
P -2.71299000 -1.86542700 -0.50033100
C -3.19254000 -2.88009800 0.95492300
C -3.34634700 -4.27619900 0.89407400
C -3.46444000 -2.20995600 2.16039100
C -3.76599200 -4.98554400 2.02364000
H -3.14166000 -4.81664300 -0.03233700
C -3.89014200 -2.92244400 3.28472800

H	-3.33851000	-1.12540700	2.22131600	C	3.25734100	0.95561900	-0.93333200
C	-4.03955700	-4.31157800	3.21834100	H	2.23699600	1.36961400	-0.97602500
H	-3.88104200	-6.07121200	1.96702700	H	3.89229400	1.77501800	-0.55687200
H	-4.09816400	-2.39063500	4.21675500	C	3.71536000	0.64114300	-2.34484700
H	-4.36618700	-4.87011100	4.09960000	O	3.40420100	1.31548700	-3.30127000
C	-4.29574000	-1.47944200	-1.36390000	H	4.38198800	-0.24978700	-2.45446900
C	-5.40883000	-2.33624800	-1.30802000	S	4.55334700	-0.25021400	1.09378000
C	-4.38152500	-0.28914900	-2.10834600	O	4.73651800	1.10775600	1.63874300
C	-6.58268600	-2.00750900	-1.99127300	O	4.23380900	-1.36289500	2.00065100
H	-5.36673500	-3.26305100	-0.73215600	C	6.05495100	-0.66776900	0.21450200
C	-5.55787200	0.03457800	-2.79220200	C	6.92208600	0.34644400	-0.20109000
H	-3.52430800	0.38941500	-2.15233500	C	6.33410300	-2.01402400	-0.05849800
C	-6.65972500	-0.82382800	-2.73401400	C	8.07474900	0.00376400	-0.91282400
H	-7.44252700	-2.68084600	-1.94172000	H	6.70960800	1.39025400	0.03593400
H	-5.61188100	0.96220600	-3.36791800	C	7.48880800	-2.33389200	-0.76868200
H	-7.58100800	-0.56985800	-3.26511800	H	5.66492400	-2.80328900	0.28951800
C	-1.79747100	-2.98751400	-1.63391000	C	8.37685900	-1.33437000	-1.21166500
C	-2.10561400	-3.04616800	-3.00334800	H	8.75486800	0.79593100	-1.23700900
C	-0.71840800	-3.74508900	-1.14058000	H	7.71133700	-3.38370700	-0.97964800
C	-1.35073600	-3.85227200	-3.86241500	P	-1.06000900	2.55882300	0.15027100
H	-2.93720500	-2.46680000	-3.40931900	C	-0.13840100	3.17770200	1.61664600
C	0.02710100	-4.55355500	-2.00217100	C	-0.66623800	4.15378500	2.47776300
H	-0.46278200	-3.71513300	-0.07924900	C	1.13518600	2.64209700	1.88456300
C	-0.28530900	-4.60781700	-3.36530800	C	0.07153600	4.58628600	3.58565700
H	-1.60363000	-3.89093600	-4.92527400	H	-1.65108500	4.58543300	2.28937900
H	0.85668900	-5.14433300	-1.60474700	C	1.87034400	3.08265300	2.98664000
H	0.30050800	-5.24021500	-4.03768400	H	1.56011600	1.87690600	1.23342100
Pd	-1.74738400	0.26511900	0.00612000	C	1.33876400	4.05476800	3.84178200
C	0.73687800	-1.41568800	1.83662500	H	-0.34927500	5.34706300	4.24851000
C	1.22394300	-2.65290200	2.30905400	H	2.85930700	2.65651400	3.17275900
C	-0.00931600	-0.62554300	2.73350200	H	1.91235200	4.39648800	4.70751200
C	0.96926500	-3.08179300	3.61427500	C	-0.13613300	3.18430400	-1.30794100
H	1.80049800	-3.30380200	1.64863500	C	0.74148700	4.27870300	-1.22377000
C	-0.25582900	-1.04850800	4.04265800	C	-0.33256100	2.55212800	-2.54883000
H	-0.39273300	0.34038700	2.40294800	C	1.41582200	4.72625700	-2.36416500
C	0.23130500	-2.28017800	4.49109300	H	0.90445900	4.78508500	-0.27011800
H	1.35264200	-4.05031100	3.94721000	C	0.34083800	3.00559200	-3.68568300
H	-0.82875000	-0.40639300	4.71761900	H	-1.01146900	1.69849600	-2.62424200
H	0.03981100	-2.61178300	5.51519700	C	1.22033500	4.08961800	-3.59369700
C	0.97820500	-0.98848700	0.42663800	H	2.09920700	5.57618300	-2.28843600
C	0.08281300	-0.35796600	-0.35870200	H	0.18524600	2.50343500	-4.64400100
H	0.34039000	-0.12092000	-1.39958700	H	1.75588500	4.43681900	-4.48123100
C	2.34851300	-1.27915000	-0.19835900	C	-2.67309300	3.43871900	0.15501300
H	2.78782500	-2.19096600	0.22084700	C	-2.92949700	4.57461100	-0.63041200
H	2.23637400	-1.44979900	-1.27943100	C	-3.69733700	2.91384600	0.96586900
N	3.31553100	-0.17559600	-0.02326200	C	-4.19034100	5.17856500	-0.59641100

H	-2.14856800	4.99327400	-1.26869300	Pd	1.38995700	0.24003800	-0.11965100
C	-4.95435400	3.52339800	0.99871700	C	-1.87970600	-0.64853900	2.62682100
H	-3.50871400	2.02703200	1.57942800	C	-2.94473700	0.09455700	3.17549200
C	-5.20225300	4.65647300	0.21628100	C	-1.44912400	-1.79553500	3.32260600
H	-4.38143800	6.06370600	-1.20888400	C	-3.54816200	-0.29129700	4.37601500
H	-5.74175600	3.11003100	1.63430000	H	-3.29718300	0.99862100	2.67295200
H	-6.18641400	5.13195300	0.23814300	C	-2.05280300	-2.18112700	4.52279500
C	9.61990700	-1.70594000	-1.97516600	H	-0.64216000	-2.40329000	2.90676400
H	10.27741400	-2.34973100	-1.36647000	C	-3.10593700	-1.43128400	5.05612500
H	9.36849100	-2.27784300	-2.88416600	H	-4.36678500	0.30772800	4.78483300
H	10.19346600	-0.81691100	-2.27506400	H	-1.70331300	-3.08020200	5.03818100
int-10				H	-3.58151300	-1.73432000	5.99283800
P	2.15362500	-2.03586200	-0.25004500	C	-1.20438000	-0.21630300	1.35875600
C	1.16166600	-3.31619400	-1.11925500	C	0.14314400	-0.19071600	1.34275400
C	-0.11055100	-3.64482900	-0.61571200	H	0.70872800	-0.47746100	2.23852700
C	1.63845400	-3.97433300	-2.26517300	C	-2.07877700	0.22931700	0.19019300
C	-0.88160900	-4.62882400	-1.23826100	H	-3.06208300	0.55223700	0.56103300
H	-0.50562400	-3.13559800	0.26588200	H	-1.62981400	1.11246800	-0.28107400
C	0.85723400	-4.95253300	-2.88990200	N	-2.28379700	-0.74779100	-0.90058300
H	2.62151700	-3.73329900	-2.67375600	C	-1.52152500	-0.59445200	-2.12909500
C	-0.39959900	-5.28478100	-2.37662400	H	-0.43996900	-0.60664500	-1.90738200
H	-1.86878400	-4.86991700	-0.83842200	H	-1.72384400	-1.44816400	-2.79592100
H	1.23896900	-5.45898900	-3.78040400	C	-1.86051300	0.66067900	-2.90431900
H	-1.00628100	-6.05203100	-2.86500600	O	-1.05460200	1.25717700	-3.58554500
C	3.71742900	-1.88043600	-1.20509400	H	-2.92110100	1.00480000	-2.83038200
C	4.86674400	-2.63341700	-0.91118700	S	-3.54275300	-1.83924400	-0.80024000
C	3.75290400	-0.95240000	-2.26163500	O	-3.46810200	-2.67970200	-2.00911300
C	6.02955500	-2.46050800	-1.66793900	O	-3.47813700	-2.47787700	0.52541900
H	4.85938200	-3.35755500	-0.09378200	C	-5.07426100	-0.91671600	-0.87042400
C	4.91744200	-0.78373500	-3.01606900	C	-5.55096000	-0.48694700	-2.11723800
H	2.86508400	-0.35786800	-2.50034200	C	-5.78001500	-0.64517600	0.30400800
C	6.05756800	-1.53753700	-2.71917600	C	-6.74273000	0.23087000	-2.17327600
H	6.91901000	-3.05120900	-1.43321900	H	-5.00536200	-0.72238700	-3.03330600
H	4.93342500	-0.05839100	-3.83363300	C	-6.97364400	0.07832200	0.22564200
H	6.97037000	-1.40378200	-3.30577800	H	-5.41074900	-1.00233900	1.26638700
C	2.63652800	-2.79745800	1.35258600	C	-7.47332500	0.52929000	-1.00585600
C	2.50277100	-4.17262900	1.60681000	H	-7.12044900	0.56308000	-3.14433900
C	3.19044900	-1.96616900	2.34280400	H	-7.52823900	0.29042900	1.14360800
C	2.91741800	-4.70392200	2.83286600	P	1.20111900	2.61056600	0.13162300
H	2.07869200	-4.83732000	0.85193700	C	-0.42772100	3.46452500	0.12987900
C	3.60909300	-2.50224500	3.56281700	C	-0.95875500	4.03732600	-1.03819000
H	3.29637300	-0.89446100	2.15795200	C	-1.19282100	3.47703400	1.31161200
C	3.47070000	-3.87238500	3.81109700	C	-2.23060300	4.61957500	-1.02046300
H	2.80808600	-5.77535900	3.02045000	H	-0.38684800	4.03464300	-1.96792500
H	4.03927900	-1.84583600	4.32370600	C	-2.46038500	4.06450400	1.32315100
H	3.79265900	-4.29108800	4.76829200	H	-0.79943500	3.03419500	2.22934100

C	-2.98332000	4.63552700	0.15742700	H	-4.25174600	-2.56409700	-0.31616400
H	-2.63040400	5.06679800	-1.93433900	H	-4.38592500	-0.95366500	0.42102000
H	-3.04099600	4.07678800	2.24932600	N	-2.74784000	-1.25566500	-0.92393600
H	-3.97542300	5.09448900	0.16881400	C	-1.63654700	-0.43450300	-0.44318200
C	2.06823300	3.22651000	1.62960300	H	-1.07135900	-0.04399300	-1.29731900
C	1.86573300	4.52518600	2.13069900	H	-1.99854300	0.41698800	0.16239900
C	2.99582800	2.38281600	2.26370100	C	-0.73656500	-1.32721200	0.42253900
C	2.57990400	4.96534100	3.24864900	O	0.23978600	-0.59716900	1.11996600
H	1.15189700	5.19879600	1.65187700	H	-0.27010300	-2.08811800	-0.23782900
C	3.71101200	2.82855700	3.37912200	S	-3.39412600	-0.94455200	-2.43488400
H	3.15505200	1.37071200	1.88242300	O	-2.25600200	-0.64328700	-3.32157500
C	3.50218300	4.11935700	3.87433900	O	-4.27621500	-2.08016100	-2.74757700
H	2.41441500	5.97584800	3.63144600	C	-4.40881600	0.52574200	-2.33592100
H	4.42884500	2.16222000	3.86441800	C	-3.82156400	1.78338300	-2.51249300
H	4.05666300	4.46662200	4.75026200	C	-5.77616500	0.40177100	-2.05647800
C	2.14659900	3.26731200	-1.30594400	C	-4.61679900	2.92541200	-2.39868200
C	3.06701500	4.32349700	-1.19095400	H	-2.76006900	1.87491200	-2.74867600
C	1.95797500	2.65223200	-2.55789000	C	-6.55234300	1.55471700	-1.94763200
C	3.77603800	4.76174100	-2.31304500	H	-6.22993200	-0.58381700	-1.93899600
H	3.23668600	4.80890500	-0.22811600	C	-5.98983700	2.83381600	-2.11440800
C	2.66554900	3.09950500	-3.67798400	H	-4.15926900	3.90821200	-2.54014200
H	1.24599200	1.83059500	-2.66662700	H	-7.62055800	1.45932000	-1.73345500
C	3.57684000	4.15316700	-3.55691800	P	1.03355400	2.42859700	0.95317300
H	4.48895700	5.58438700	-2.21247400	P	2.67609200	-1.71020300	-0.74213600
H	2.50395400	2.61916400	-4.64655000	C	2.31326800	-2.24663600	-2.45872700
H	4.13428100	4.49901800	-4.43147500	C	1.03174700	-2.04225200	-2.99660500
C	-8.76019900	1.30519300	-1.09296600	C	3.30103300	-2.86785000	-3.24520300
H	-8.59546600	2.29022300	-1.56133500	C	0.73813700	-2.45954900	-4.29815400
H	-9.49735100	0.77504900	-1.71956300	H	0.25454100	-1.55738000	-2.40577900
H	-9.20601200	1.46600000	-0.10069800	C	3.00218000	-3.28251400	-4.54561500
int-11				H	4.30459100	-3.03106400	-2.84573100
C	-3.71738100	-2.88179100	2.40238700	C	1.72199600	-3.07976900	-5.07381700
C	-4.86458700	-3.64378000	2.10176800	H	-0.26412400	-2.29152100	-4.69994500
C	-3.35074900	-2.75325000	3.75895700	H	3.77509300	-3.76563200	-5.14916200
C	-5.60064700	-4.26836100	3.11318300	H	1.49341300	-3.40320100	-6.09284700
H	-5.18445400	-3.77358900	1.06604300	C	4.43613700	-1.18890400	-0.76278200
C	-4.08529800	-3.37790400	4.76794600	C	5.44934000	-1.84834000	-0.04809900
H	-2.48959400	-2.13704400	4.02705600	C	4.74932500	-0.02781600	-1.49903900
C	-5.21476200	-4.14131600	4.45049500	C	6.75795300	-1.35579600	-0.07644900
H	-6.48150500	-4.86050400	2.85006100	H	5.22539700	-2.74878700	0.52715000
H	-3.78017300	-3.25755600	5.81116700	C	6.05876300	0.45855000	-1.52156500
H	-5.79306600	-4.62710600	5.24102500	H	3.97152100	0.49032700	-2.06849800
C	-2.91345000	-2.22083100	1.33672500	C	7.06468600	-0.20460500	-0.80949300
C	-1.58122200	-2.04636100	1.44922300	H	7.54276100	-1.87909000	0.47603500
H	-1.03954800	-2.44669100	2.31063200	H	6.29373600	1.35670600	-2.09851300
C	-3.66633800	-1.73984500	0.11277400	H	8.08958200	0.17513500	-0.82832100

C	2.53774000	-3.17514400	0.34351600	H	-7.56530500	4.11531300	-2.84657500
C	2.32186400	-4.46809000	-0.16176600	H	-7.44635700	4.05395500	-1.08077800
C	2.62088700	-2.97981700	1.73545200	H	-6.24634500	4.98415500	-2.02200100
C	2.20111200	-5.55100500	0.71492500	int-12			
H	2.24684900	-4.63729100	-1.23767000	P	-2.38496300	0.00783200	0.02509400
C	2.50670000	-4.06702600	2.60445700	P	2.38504200	0.00772300	-0.02512800
H	2.77749400	-1.97737500	2.14180300	C	3.35105000	1.52826200	-0.49380900
C	2.29471300	-5.35368900	2.09580800	C	3.37509700	2.59705900	0.42308300
H	2.03328200	-6.55367600	0.31322700	C	4.03925100	1.67172900	-1.70895400
H	2.57777100	-3.90707700	3.68343200	C	4.06287800	3.77570600	0.12871300
H	2.19918600	-6.20256800	2.77806900	H	2.85510800	2.51220400	1.37928000
C	-0.35125800	2.47030100	2.14564700	C	4.72779500	2.85571400	-2.00244400
C	-0.19269100	1.81409200	3.38125700	H	4.05886100	0.86168500	-2.43832600
C	-1.58322300	3.06855200	1.83489700	C	4.74049100	3.91140800	-1.08861800
C	-1.24579000	1.77860500	4.29728600	H	4.06904300	4.59239400	0.85566300
H	0.75639400	1.33300800	3.63232100	H	5.26040800	2.94456500	-2.95327800
C	-2.63599300	3.02478000	2.75544900	H	5.27902600	4.83450600	-1.31954900
H	-1.72815700	3.57325900	0.87765300	C	3.03507300	-1.30174500	-1.15357500
C	-2.46950700	2.38346700	3.98619900	C	3.79433900	-2.39787500	-0.71516900
H	-1.11080900	1.27340200	5.25721900	C	2.67489900	-1.22771800	-2.51323800
H	-3.58952300	3.49801100	2.50680800	C	4.20481800	-3.38339900	-1.62083400
H	-3.29354900	2.35271300	4.70396500	H	4.06465000	-2.50160400	0.33643200
C	0.61328500	3.56098800	-0.42966200	C	3.09943800	-2.20416200	-3.41733200
C	0.63539200	4.95913400	-0.27878500	H	2.04937000	-0.40567700	-2.87140000
C	0.28317300	3.00497500	-1.67756300	C	3.86794400	-3.28601900	-2.97326700
C	0.31993500	5.78411100	-1.36089100	H	4.79277700	-4.23208500	-1.26090400
H	0.89959000	5.40780400	0.68176300	H	2.81819000	-2.12462600	-4.47086000
C	-0.02841900	3.83598400	-2.75928400	H	4.19453100	-4.05493600	-3.67854600
H	0.27612000	1.91842800	-1.80276000	C	3.08190800	-0.32095800	1.65240800
C	-0.01188400	5.22489300	-2.60103900	C	4.47008700	-0.41818000	1.86715000
H	0.33682000	6.86994800	-1.23576100	C	2.21600800	-0.39315900	2.75452300
H	-0.27839600	3.39501700	-3.72769600	C	4.97306400	-0.61244900	3.15541800
H	-0.25260100	5.87479800	-3.44657600	H	5.16503700	-0.33416800	1.02822500
C	2.47743700	3.18512000	1.79835700	C	2.72265100	-0.58018900	4.04603600
C	2.35434800	4.07955100	2.87495300	H	1.13980900	-0.28615100	2.60020900
C	3.75689400	2.85485200	1.31610600	C	4.10017300	-0.69651900	4.24730500
C	3.49870000	4.63641800	3.45489000	H	6.05269200	-0.69151400	3.30892100
H	1.36958400	4.34406200	3.26581700	H	2.03597000	-0.63087300	4.89518600
C	4.89653100	3.41552000	1.89809300	H	4.49717500	-0.84375600	5.25539500
H	3.86276000	2.15397300	0.48191400	C	-3.03505400	-1.30160000	1.15354800
C	4.76830700	4.30679700	2.96904800	C	-3.79426900	-2.39775100	0.71510900
H	3.39541700	5.33219100	4.29176500	C	-2.67500200	-1.22752400	2.51323500
H	5.88605900	3.15076700	1.51667000	C	-4.20481300	-3.38325300	1.62077000
H	5.65965100	4.74319800	3.42758600	H	-4.06448200	-2.50153200	-0.33651200
Pd	1.68345500	0.29374400	0.07812500	C	-3.09958800	-2.20395100	3.41732300
C	-6.84972700	4.06484800	-2.00758800	H	-2.04951500	-0.40545000	2.87139600

C	-3.86804600	-3.28583100	2.97322700
H	-4.79273200	-4.23195800	1.26081900
H	-2.81842600	-2.12438400	4.47087100
H	-4.19468000	-4.05472700	3.67850600
C	-3.35094000	1.52838500	0.49382800
C	-4.03973300	1.67160600	1.70866500
C	-3.37443100	2.59742900	-0.42279600
C	-4.72834700	2.85556700	2.00210100
H	-4.05973900	0.86139700	2.43784300
C	-4.06229200	3.77604200	-0.12849000
H	-2.85390300	2.51279800	-1.37871300
C	-4.74052000	3.91148400	1.08852900
H	-5.26142300	2.94421500	2.95269600
H	-4.06802200	4.59291800	-0.85523300
H	-5.27910700	4.83456200	1.31942200
C	-3.08199100	-0.32081700	-1.65240000
C	-4.47019100	-0.41796000	-1.86702600
C	-2.21618900	-0.39307700	-2.75459000
C	-4.97328800	-0.61221800	-3.15524800
H	-5.16505800	-0.33393200	-1.02803400
C	-2.72294900	-0.58011000	-4.04605600
H	-1.13997600	-0.28608500	-2.60037500
C	-4.10049600	-0.69636200	-4.24720800
H	-6.05293500	-0.69121300	-3.30866000
H	-2.03634200	-0.63085500	-4.89526200
H	-4.49759200	-0.84359400	-5.25526200
Pd	0.00000700	0.06304700	-0.00004900
C	-0.00007400	-2.06862200	0.00008700
C	-0.09487400	-2.82292400	-1.19032500
C	0.09472700	-2.82302100	1.19042800
C	-0.09931000	-4.22566700	-1.19921700
H	-0.16384700	-2.31364800	-2.15586700
C	0.09918500	-4.22576600	1.19920100
H	0.16368600	-2.31382500	2.15601700
C	-0.00005500	-4.93903200	-0.00003600
H	-0.17891800	-4.76248100	-2.15057600
H	0.17879400	-4.76265700	2.15051600
H	-0.00003600	-6.03322300	-0.00008200
C	0.14068400	2.90459600	-1.19016300
C	0.00020800	2.15891000	-0.00009700
C	-0.14021800	2.90436700	1.19012900
C	-0.13785900	4.30675700	1.19784900
C	0.00022500	5.01793400	0.00019700
C	0.13834300	4.30699000	-1.19758800
H	0.26027500	2.38623600	-2.14870000
H	-0.25972900	2.38581900	2.14857500

H	-0.24705600	4.84658700	2.14451400
H	0.00019800	6.11204500	0.00029400
H	0.24757700	4.84701200	-2.14414000

pro-side

C	2.84502700	-0.15396700	1.94781700
C	3.65321200	-0.80393000	1.10294300
C	1.56279000	0.50531000	1.52731200
H	0.70843900	-0.01571000	2.00873700
H	1.54594000	1.54504500	1.88633300
N	1.44141600	0.51175700	0.06225800
C	1.84373300	-0.72435000	-0.61199400
H	1.28116500	-1.59777300	-0.22990500
H	1.65779200	-0.63047700	-1.68833700
C	3.33369700	-0.96702400	-0.36285200
O	3.60478700	-2.28536400	-0.82288000
H	3.91676600	-0.23083100	-0.95138700
S	0.17898700	1.39393400	-0.59503800
O	0.13745200	2.66267000	0.14917800
O	0.39382300	1.41126800	-2.05048500
C	-1.35012700	0.52118200	-0.27443400
C	-2.07952800	0.81085800	0.88339600
C	-1.78830100	-0.45857100	-1.17600600
C	-3.25508700	0.10150800	1.14076900
H	-1.74424800	1.59135600	1.56857000
C	-2.96326300	-1.15510100	-0.89999900
H	-1.22725100	-0.66360700	-2.08954300
C	-3.71509900	-0.89174200	0.26077100
H	-3.82866300	0.33112900	2.04276200
H	-3.30990900	-1.91622600	-1.60474500
H	4.59019500	-1.24826300	1.45770400
C	-4.97945200	-1.66023300	0.53891200
H	-4.76542300	-2.73534500	0.66512700
H	-5.48024900	-1.30248300	1.45018700
H	-5.68799600	-1.57396900	-0.30176500
H	4.56418300	-2.41989000	-0.80669500
H	3.09144300	-0.07044800	3.01145100

int-Au(I)

C	2.86239700	-0.61977900	0.00180500
C	2.86497300	0.60839800	-0.00047300
H	3.03691300	1.67717500	-0.00219800
Au	0.64317300	0.00086600	-0.00065000
H	3.02849900	-1.68944000	0.00397600
P	-1.68532700	-0.00217700	-0.00062400
C	-2.38697200	1.67749800	0.14216500
H	-2.04524200	2.13976000	1.08042100
H	-2.04643800	2.29123100	-0.70535600

H -3.48731000 1.62166000 0.13797800
C -2.40385000 -0.71552800 -1.51940000
H -2.06612400 -0.13596600 -2.39178200
H -2.06782600 -1.75761700 -1.62964000
H -3.50367900 -0.68743700 -1.46132200
C -2.39734300 -0.95745100 1.38250900
H -2.06281600 -2.00374600 1.31660100
H -2.05460500 -0.53099100 2.33725500
H -3.49738900 -0.91922100 1.33510900

int-Pd(II)

Pd -0.18847400 0.31709700 -0.15261400
C 0.70174400 2.08941500 0.74653100
C 0.54296600 2.34429900 -0.45210800
H 0.49645400 2.76109300 -1.45045500
H 0.92459700 2.07080200 1.80580800
C 2.43665800 -0.76997100 0.20584100
O 2.20581500 -0.73815100 1.41352100
O 1.60413800 -0.36269100 -0.71632300
C -2.46779000 -0.62539200 0.03260700
O -1.49247000 -1.37490900 -0.29885200
O -2.20095900 0.61014800 0.24470700
C 3.74597200 -1.28206000 -0.35822200
H 3.56047900 -2.01048100 -1.16223500
H 4.30585200 -0.44055400 -0.79821800
H 4.34626700 -1.74257900 0.43760200
C -3.84867400 -1.15723000 0.20136500
H -3.94326600 -1.55775100 1.22524400
H -4.59022600 -0.35760100 0.06840500
H -4.02779900 -1.97896700 -0.50640400

int-Pd(0)

P -1.85499400 -0.62284600 0.00402100
P 1.85473900 -0.62319500 -0.00408900
Pd 0.00002700 0.86896300 -0.00007400
C 0.64311500 2.83976100 -0.01691800
C -0.64174000 2.84028400 0.01691800
H -1.53638300 3.46296100 0.03960800
H 1.53839000 3.46152000 -0.03959000
C 3.47034000 0.11063500 -0.51566600
H 4.28923700 -0.62646700 -0.46685100
H 3.38795800 0.48941600 -1.54688600
H 3.70920900 0.95992200 0.14373100
C 2.27992000 -1.35342600 1.63792800
H 1.42237200 -1.92902400 2.01998300
H 3.15861900 -2.01635900 1.57118700
H 2.49426900 -0.54244600 2.35194000
C -2.27974300 -1.35435900 -1.63753000

H -3.15821000 -2.01755900 -1.57041500
H -2.49429600 -0.54397500 -2.35215800
H -1.42193600 -1.92991500 -2.01905800
C -3.47062900 0.11163600 0.51454800
H -3.70880800 0.96093900 -0.14507100
H -4.28979900 -0.62514300 0.46540000
H -3.38862700 0.49050900 1.54576600
C -1.77895900 -2.12205500 1.08001700
H -0.93761900 -2.76019300 0.76846600
H -1.61483800 -1.81608600 2.12539700
H -2.71164700 -2.70737900 1.02059500
C 1.77820700 -2.12324900 -1.07885900
H 1.61459000 -1.81803000 -2.12453700
H 2.71058200 -2.70900200 -1.01869500
H 0.93646400 -2.76071800 -0.76704300

int-oxcyc

P -1.64282400 -1.89047900 -0.02137800
P -2.21547700 1.74323500 0.19166200
C -3.56483100 1.44693100 -1.03357400
C -3.17760800 1.22646300 -2.36912900
C -4.93149600 1.44517600 -0.71277000
C -4.13845600 1.03633900 -3.36572300
H -2.11675200 1.20754400 -2.63221500
C -5.89043300 1.24397300 -1.71199500
H -5.26247000 1.59118300 0.31588600
C -5.49860400 1.04618400 -3.03909400
H -3.82134900 0.87413200 -4.39928600
H -6.95079900 1.24093000 -1.44618800
H -6.25132600 0.89248900 -3.81697300
C -2.93658400 1.67083300 1.88744900
C -3.93162300 2.57626000 2.30401900
C -2.42869700 0.74412000 2.81158600
C -4.42656100 2.52887200 3.60930600
H -4.31605700 3.33120100 1.61458500
C -2.91973400 0.70551700 4.12166000
H -1.63649100 0.05608700 2.50861400
C -3.92316500 1.59237900 4.52022400
H -5.20309400 3.23330100 3.91907700
H -2.51091000 -0.01880400 4.83103600
H -4.30738600 1.56273500 5.54340500
C -1.86510400 3.55661400 0.02793900
C -2.20781300 4.29270800 -1.11676400
C -1.18994900 4.20744800 1.07777300
C -1.88880400 5.65303600 -1.20632600
H -2.73108700 3.81634800 -1.94744400
C -0.87502400 5.56514700 0.98588900

H -0.90594600 3.65362600 1.97636400
C -1.22431400 6.29317700 -0.15735500
H -2.16789400 6.21259000 -2.10324000
H -0.35346000 6.05579000 1.81209300
H -0.97874000 7.35615600 -0.22851500
C -1.08127500 -2.88520300 -1.47905500
C -0.87263400 -4.27294100 -1.42519600
C -0.86280400 -2.21064900 -2.69359400
C -0.45974700 -4.97111200 -2.56494700
H -1.02523500 -4.82059100 -0.49334600
C -0.45800700 -2.91167300 -3.83336500
H -1.00467500 -1.12836000 -2.74668900
C -0.25391700 -4.29404400 -3.77107700
H -0.29656000 -6.05071600 -2.50654500
H -0.29433100 -2.37327100 -4.77077800
H 0.06991800 -4.84207100 -4.66009400
C -3.48395000 -2.09495700 -0.05928600
C -4.16347300 -2.44160700 -1.23947000
C -4.23495600 -1.86064900 1.10816300
C -5.55769000 -2.56302700 -1.24777500
H -3.61012600 -2.62714100 -2.16176800
C -5.62628600 -1.98821600 1.09778000
H -3.73452000 -1.59035400 2.03975000
C -6.29324700 -2.34122000 -0.08043000
H -6.06782200 -2.83861200 -2.17473900
H -6.19042000 -1.81172900 2.01767400
H -7.38175100 -2.44340200 -0.08735400
C -1.13980700 -2.87469400 1.46224100
C -1.85339400 -4.00565800 1.90102000
C 0.00620500 -2.47661200 2.17310900
C -1.42571500 -4.72145500 3.02315900
H -2.75089400 -4.33268600 1.37205500
C 0.43184700 -3.19600100 3.29472000
H 0.57189300 -1.60470600 1.83815800
C -0.28308500 -4.31846800 3.72288800
H -1.99027300 -5.59823500 3.35192900
H 1.32479000 -2.87320900 3.83685100
H 0.04716400 -4.87816000 4.60225200
Pd -0.45049100 0.29496500 -0.14271600
C 2.07410000 1.38152000 -0.77524800
C 0.86784400 1.81466700 -0.36914900
C 3.39342700 2.09650100 -0.92943800
H 3.55674500 2.43899500 -1.96536300
H 3.49552700 2.97117200 -0.26851400
N 4.37434800 1.02548000 -0.55866000
C 3.68414700 -0.26247000 -0.28815900

H 4.25974700 -1.11171000 -0.68178400
H 3.55345000 -0.39807700 0.79931400
C 2.30205500 -0.08985200 -0.96013000
O 1.26361800 -0.85794400 -0.43873300
H 2.45198500 -0.29406700 -2.04854700
S 5.80975300 0.98303600 -1.40401700
O 5.75370100 0.04401100 -2.54541700
O 6.14774100 2.39014600 -1.69537400
C 6.98530300 0.33213200 -0.22666700
C 7.60897500 -0.89416500 -0.47469800
C 7.30518300 1.09195800 0.90375900
C 8.55727000 -1.36636700 0.43320300
H 7.35655400 -1.46773200 -1.36798900
C 8.25556200 0.60260000 1.79953800
H 6.82202900 2.05467100 1.08430500
C 8.89556900 -0.63131500 1.58311400
H 9.04676700 -2.32557400 0.24237000
H 8.50902800 1.19274400 2.68426500
H 0.69613600 2.87548800 -0.15297400
C 9.91205200 -1.16432800 2.55763700
H 10.16811800 -0.42009800 3.32573300
H 9.52762900 -2.06290300 3.07069200
H 10.83847300 -1.46454000 2.04110600

int-LA

P -2.23835200 -1.72682600 -0.02783100
P -1.27034300 1.87004500 0.16039600
C -2.99543000 2.35449500 -0.25241800
C -3.50591100 1.93579200 -1.49405300
C -3.79313300 3.15248600 0.58365100
C -4.78641200 2.32193100 -1.89875600
H -2.89778400 1.30622900 -2.14931200
C -5.07673300 3.53093900 0.17761400
H -3.42417500 3.48204800 1.55626800
C -5.57427800 3.12060600 -1.06309100
H -5.17049800 1.99272300 -2.86777000
H -5.69011400 4.14995000 0.83770100
H -6.57811900 3.41898200 -1.37706800
C -1.02267900 2.09955100 1.96944500
C -0.97277800 3.38475900 2.54153500
C -0.83955900 0.97596800 2.79259300
C -0.76842900 3.53603100 3.91523600
H -1.08399200 4.27327700 1.91594900
C -0.63186200 1.13238300 4.16732100
H -0.84659000 -0.02573300 2.35771800
C -0.60017600 2.41098700 4.73066900
H -0.73369800 4.53889300 4.34900200

H	-0.48764300	0.24975200	4.79575200	Pd	-0.55262200	-0.18964400	-0.66256000
H	-0.43459800	2.53328300	5.80442600	C	3.11038700	0.13610700	-3.64250100
C	-0.23534300	3.21543400	-0.57781900	C	1.88742800	-0.26492200	-3.23687100
C	-0.76729700	4.21251300	-1.41019900	H	1.04137800	-0.43631100	-3.92378900
C	1.14704600	3.20957600	-0.31363300	C	4.15315600	0.44441500	-2.60779400
C	0.07120600	5.18598600	-1.96801600	H	4.99257300	-0.27581600	-2.70844500
H	-1.83584700	4.24106500	-1.63003000	H	4.57837800	1.44452600	-2.78523300
C	1.97871700	4.18132200	-0.87183300	N	3.64568500	0.43206700	-1.19819900
H	1.58710400	2.44243200	0.32795800	C	2.77034400	-0.69715400	-0.89834000
C	1.44256400	5.17314100	-1.70252300	H	3.26497200	-1.66554600	-1.10960200
H	-0.35644000	5.95698700	-2.61461100	H	2.47488100	-0.68012800	0.15703700
H	3.05136300	4.14797500	-0.66567000	C	1.52846400	-0.60411400	-1.79663900
H	2.09502800	5.93169800	-2.14315000	O	0.63550500	-1.60410000	-1.60014400
C	-2.45472000	-2.89456700	-1.43563600	H	0.97026300	0.43550000	-1.43549800
C	-2.65302800	-4.27064700	-1.23372400	S	4.57965900	1.06195900	0.02568200
C	-2.43434000	-2.38694000	-2.74676400	O	5.16563700	2.31104300	-0.49802700
C	-2.83408900	-5.12219200	-2.32800300	O	3.73507800	1.12269400	1.23769000
H	-2.66830000	-4.68548700	-0.22382600	C	5.93367000	-0.05754700	0.37543900
C	-2.62262300	-3.24096500	-3.83682800	C	7.13468400	0.07223700	-0.32989600
H	-2.26517200	-1.32063100	-2.91780400	C	5.76340200	-1.07569800	1.32336800
C	-2.82127700	-4.61007200	-3.62932600	C	8.16931600	-0.83333700	-0.08343800
H	-2.98508700	-6.19186100	-2.15995400	H	7.26831900	0.87914600	-1.05250400
H	-2.60570400	-2.83521600	-4.85171400	C	6.80800900	-1.96912100	1.55438500
H	-2.96086400	-5.27907700	-4.48271600	H	4.83158500	-1.15925900	1.88541000
C	-3.94559100	-1.21409500	0.42548700	C	8.02623100	-1.86701900	0.85663000
C	-5.05106400	-1.54421700	-0.37652100	H	9.10999300	-0.72875900	-0.63076800
C	-4.15077900	-0.46701400	1.60027200	H	6.67812300	-2.76036800	2.29833700
C	-6.33802700	-1.14245300	-0.00335600	C	9.14262300	-2.84073100	1.12659900
H	-4.91790600	-2.12012800	-1.29371800	H	10.01801500	-2.64116800	0.49157200
C	-5.43846400	-0.07574400	1.97213200	H	9.46429800	-2.78893700	2.18067700
H	-3.30589300	-0.19635600	2.23639600	H	8.81447400	-3.87808000	0.94513700
C	-6.53588600	-0.41176400	1.17110100				
H	-7.18925300	-1.40866400	-0.63555300	int-1-L2			
H	-5.58412900	0.49719900	2.89158000	P	1.55850300	2.10861100	-0.06588500
H	-7.54318800	-0.10285500	1.46283600	P	1.71867600	-1.89044900	0.17503000
C	-1.65761400	-2.76358600	1.38128600	C	3.57757200	-1.77798000	0.07799600
C	-2.54216100	-3.33049100	2.31504800	C	4.22117800	-0.72802000	0.75795000
C	-0.27886600	-3.01832200	1.49853200	C	4.37195100	-2.70175600	-0.62460500
C	-2.05194000	-4.13144000	3.35180600	C	5.61505400	-0.61538800	0.75446500
H	-3.61664000	-3.15449000	2.23923600	H	3.62834600	0.01599500	1.29326500
C	0.20435000	-3.82321400	2.53324300	C	5.76611700	-2.58307900	-0.63784100
H	0.41560500	-2.59139200	0.77142200	H	3.90905500	-3.52477600	-1.17161800
C	-0.68035300	-4.37788300	3.46454500	C	6.39327000	-1.54282100	0.05442000
H	-2.74948900	-4.56523800	4.07323300	H	6.09225300	0.20737900	1.29371700
H	1.27779800	-4.01396500	2.61315000	H	6.36350000	-3.31111600	-1.19397500
H	-0.30060800	-5.00219200	4.27779000	H	7.48287500	-1.45167100	0.04378800
				C	3.11118600	2.02452200	-1.09055700

C	4.27304300	2.77191000	-0.83142600	H	-0.50759900	2.41011400	-2.25741400
C	3.10468100	1.16603700	-2.20578500	H	1.05345800	2.90083200	-2.92874700
C	5.39123800	2.66764600	-1.66647900	C	-1.12688000	5.34908700	-0.71168300
H	4.32327900	3.43819300	0.03099600	H	-1.20456500	3.35375100	0.12738900
C	4.21754900	1.07019200	-3.04698200	H	-0.09417000	4.44113800	0.96518000
H	2.22147300	0.55686400	-2.41454700	C	-1.60433600	5.01355800	-2.12839200
C	5.36700800	1.82010300	-2.77832400	H	-0.82801400	4.15990500	-3.97628000
H	6.28719200	3.25351000	-1.44250600	H	0.29437900	5.24477500	-3.14271300
H	4.18805300	0.39829600	-3.90921100	H	-1.97141200	5.69830400	-0.09276800
H	6.24182700	1.74037200	-3.42946100	H	-0.40727600	6.18751000	-0.75908800
Pd	0.27696200	0.05956200	0.04447900	H	-2.03761300	5.90756000	-2.60935700
C	-1.68142200	-0.68868900	-0.11524000	H	-2.41575800	4.26409400	-2.07147800
C	-1.72971200	0.58989700	-0.09665100	C	1.51993400	-2.96177300	1.72313200
C	-2.41596800	-1.97056800	-0.28379800	C	2.00243500	-2.23529800	2.99335000
H	-1.81804000	-2.67540900	-0.88461700	C	0.07367200	-3.45221900	1.91697100
H	-2.56841300	-2.46007600	0.68794500	H	2.17486100	-3.83690600	1.56623500
N	-3.72440700	-1.85231100	-0.95246200	C	1.87505500	-3.13089800	4.23517600
C	-3.73412000	-1.51093100	-2.36785100	H	1.39675500	-1.32241900	3.13895100
H	-3.02896600	-2.16363800	-2.90867000	H	3.04786600	-1.90879700	2.88428000
H	-4.73928400	-1.70148600	-2.78004700	C	-0.05378000	-4.35534000	3.15299100
C	-3.39859300	-0.06381600	-2.67803000	H	-0.58529200	-2.57565400	2.04131800
O	-2.67223600	0.26817800	-3.59122700	H	-0.28165500	-3.99061000	1.02498000
H	-3.91035500	0.69490400	-2.04115900	C	0.44765900	-3.65570200	4.42043800
S	-5.14501800	-1.94909700	-0.08397900	H	2.19808300	-2.57009200	5.12920900
O	-6.19062700	-2.36785200	-1.03284200	H	2.56896000	-3.98614100	4.13587800
O	-4.85790600	-2.77981700	1.09697900	H	-1.10544200	-4.66670100	3.27584200
C	-5.58720200	-0.31774900	0.50755600	H	0.52901700	-5.28081800	2.98975200
C	-6.43923800	0.48436000	-0.25715000	H	0.39972100	-4.34180400	5.28367000
C	-5.06821700	0.13752600	1.72628900	H	-0.22306800	-2.80845700	4.65598700
C	-6.76276500	1.76268300	0.20397700	C	2.10326600	2.81397800	1.56183000
H	-6.85518300	0.11438900	-1.19590600	C	2.54616900	4.14033300	1.73160700
C	-5.40386400	1.41572300	2.16904100	C	2.03275800	1.98426500	2.69452100
H	-4.41899300	-0.50181800	2.32716000	C	2.92272300	4.61150300	2.99301400
C	-6.25232900	2.25126500	1.41800100	H	2.59572500	4.82179700	0.87974300
H	-7.43114800	2.39015300	-0.39177700	C	2.41283400	2.45395600	3.95692000
H	-5.00250400	1.77189000	3.12199000	H	1.66647700	0.96021900	2.58543500
H	-2.35254700	1.47822100	-0.14847100	C	2.86083000	3.76893500	4.10871900
C	-6.60945300	3.62441800	1.92166600	H	3.26372000	5.64453800	3.10425500
H	-7.19795100	3.55940900	2.85304200	H	2.35140900	1.78993600	4.82347300
H	-5.70414800	4.20774400	2.15794000	H	3.15509300	4.14025000	5.09422500
H	-7.20103000	4.18661600	1.18451300	C	1.32700500	-3.05446600	-1.21895000
C	0.70063400	3.58781500	-0.88432400	C	1.45098200	-4.45364500	-1.13637700
C	0.21315300	3.24613000	-2.30584400	C	0.88717800	-2.49381100	-2.43192400
C	-0.45491300	4.14603300	-0.03226000	C	1.14271200	-5.26451400	-2.23446500
H	1.47756200	4.36824500	-0.97321600	H	1.79269000	-4.92786500	-0.21421000
C	-0.45953900	4.45261600	-2.97797900	C	0.59062900	-3.30261700	-3.53382000

H	0.76518700	-1.40967600	-2.50911300	C	5.35989200	-0.26385200	-0.58990400
C	0.71476800	-4.69236100	-3.43672200	C	6.42130300	0.48189300	-0.06926900
H	1.24058000	-6.35023200	-2.14779200	C	4.55472100	0.24586900	-1.61655900
H	0.25357900	-2.84377600	-4.46735600	C	6.66822700	1.75873700	-0.57954900
H	0.47535500	-5.32789600	-4.29371500	H	7.05584400	0.06973300	0.71717400
int-1-L3							
P	-1.54815200	-1.94740200	-0.16532300	C	4.81880900	1.52111900	-2.11289500
P	-1.61490800	2.06777800	0.14101700	H	3.73886800	-0.34880600	-2.03115900
C	-3.47147300	1.91103700	0.22291700	C	5.87494600	2.30086100	-1.60384100
C	-4.01348700	1.11814300	1.25256600	H	7.49981500	2.34199300	-0.17513800
C	-4.36764500	2.51582200	-0.67811300	H	4.19445100	1.91913800	-2.91780900
C	-5.39473700	0.95673500	1.39644800	H	2.21736900	1.56225900	1.11542900
H	-3.34484900	0.60830800	1.94828800	C	6.14641800	3.67259200	-2.16168700
C	-5.75068400	2.34463900	-0.54429300	H	6.95347700	4.18121500	-1.61462000
H	-4.00397000	3.12549700	-1.50485800	H	6.43848000	3.61304500	-3.22420700
C	-6.27134800	1.57089200	0.49630700	H	5.24411000	4.30474100	-2.11529000
H	-5.78551500	0.33964400	2.21030600	C	-0.50036900	-3.10498100	-1.24068200
H	-6.42292600	2.82284400	-1.26233400	C	-1.14959800	-4.44511200	-1.62748400
H	-7.35194100	1.44038700	0.60091300	C	0.04262200	-2.38526400	-2.48997300
C	-3.10014600	-1.80995000	-1.18247000	H	0.36250600	-3.32113800	-0.58798100
C	-4.19524100	-2.68804900	-1.07725700	C	-0.17291400	-5.33401200	-2.41500900
C	-3.15726600	-0.79483300	-2.15531500	H	-2.04360400	-4.25626000	-2.24741700
C	-5.30606400	-2.55423600	-1.91767200	H	-1.49524900	-4.98674000	-0.73260000
H	-4.19413700	-3.49288900	-0.34012400	C	1.01540300	-3.27435800	-3.27931300
C	-4.26004400	-0.66942300	-3.00658000	H	-0.79947900	-2.10443300	-3.14762800
H	-2.32747200	-0.08964000	-2.24688800	H	0.54099800	-1.44614800	-2.19778700
C	-5.34139200	-1.54796000	-2.88800600	C	0.38153000	-4.61909700	-3.65176100
H	-6.14690500	-3.24592400	-1.81393300	H	-0.67755200	-6.27136800	-2.70700700
H	-4.27662700	0.12415200	-3.75876000	H	0.66597100	-5.62378700	-1.75530100
H	-6.20871400	-1.44742300	-3.54629200	H	1.34943900	-2.74325700	-4.18754400
Pd	-0.27920900	0.04316000	0.41533000	H	1.92207900	-3.45075900	-2.67153300
C	1.66438600	-0.62148400	0.86510100	H	1.11679400	-5.26033100	-4.16804400
C	1.64374000	0.65664800	0.93957900	H	-0.44152200	-4.44585200	-4.37021100
C	2.43505700	-1.88776500	0.96334400	C	-2.05220000	-3.04719400	1.27943400
H	1.99934500	-2.52530400	1.75075200	C	-0.83398300	-3.58067300	2.05871800
H	2.34533900	-2.46533500	0.03429300	C	-3.01270700	-2.31994100	2.23977700
N	3.87034100	-1.75782500	1.27533300	H	-2.58061000	-3.91693300	0.85442000
C	4.26151900	-1.43588300	2.63863700	C	-1.26277000	-4.48547900	3.22415600
H	3.70876500	-2.07621000	3.34618800	H	-0.25720400	-2.72633700	2.45538400
H	5.33334900	-1.66146800	2.77342900	H	-0.15664700	-4.13872100	1.39373800
C	4.07062200	0.01361500	3.03904600	C	-3.44643100	-3.22400100	3.40265000
O	3.73534200	0.35084400	4.15377900	H	-2.50152300	-1.42847400	2.64516000
H	4.30958800	0.76675600	2.25128900	H	-3.89991300	-1.95479200	1.69985100
S	5.01894100	-1.89201500	0.07266900	C	-2.24132600	-3.77966200	4.16853000
O	6.25569100	-2.36761500	0.71537600	H	-0.36950400	-4.82230300	3.77806700
O	4.40998600	-2.68782800	-1.00659000	H	-1.74010900	-5.39681200	2.81854000
				H	-4.10862000	-2.66129400	4.08320900

H	-4.04715700	-4.06365700	3.00622000	H	-0.18140500	2.31333300	-2.69357500
H	-2.57443800	-4.47031800	4.96245800	H	0.02897600	3.93447700	-2.02036800
H	-1.71932200	-2.94723200	4.67625400	C	-3.41114100	2.68293100	-3.52699100
C	-1.32743500	2.87256800	-1.55158100	H	-2.43161200	1.09285400	-2.42850300
C	-1.61171400	4.38435100	-1.67446500	H	-3.76046700	1.85518500	-1.55452600
C	0.06785400	2.55039700	-2.12687400	C	-2.25720100	3.00279300	-4.48190200
H	-2.05745500	2.33740000	-2.18531600	H	-0.34335800	4.04170800	-4.46920700
C	-1.49327900	4.85606100	-3.13241400	H	-1.63280600	4.87365800	-3.58962300
H	-0.88378800	4.94504700	-1.06529900	H	-4.12926700	1.99602100	-4.00762400
H	-2.60613800	4.64164300	-1.28005500	H	-3.96975900	3.61105700	-3.30346300
C	0.19985800	3.03035600	-3.57983200	H	-2.63476400	3.49930100	-5.39263700
H	0.84585900	3.03425800	-1.51033700	H	-1.78732200	2.05759800	-4.81198000
H	0.25705700	1.46659800	-2.06821600	C	-2.61855100	2.58934700	1.42170700
C	-0.12028300	4.52203900	-3.72531600	C	-4.04923900	2.87472700	0.92854300
H	-1.68099300	5.94245600	-3.18668700	C	-2.63623900	1.51873100	2.53054900
H	-2.28186700	4.37204800	-3.73816400	H	-2.26489300	3.52448600	1.88539000
H	1.21771000	2.81796200	-3.95063000	C	-4.96251900	3.28698600	2.09477500
H	-0.49163900	2.44644800	-4.21557200	H	-4.47256300	1.97691500	0.44950400
H	-0.07619200	4.82247800	-4.78650600	H	-4.04806800	3.67111800	0.16830700
H	0.65367500	5.11290800	-3.20067000	C	-3.55583300	1.92076600	3.69312700
C	-1.33300300	3.46520200	1.39844100	H	-2.98309100	0.56188400	2.10651200
C	-1.77366300	3.08698800	2.82588000	H	-1.61700300	1.33688900	2.90693400
C	0.12974300	3.94869200	1.42204800	C	-4.97581600	2.23706900	3.21112300
H	-1.97415700	4.29611000	1.05616800	H	-5.98618900	3.46164500	1.72014700
C	-1.57039700	4.24968900	3.81027600	H	-4.61232400	4.25192000	2.50648100
H	-1.19068800	2.21065000	3.16503600	H	-3.57666100	1.11586300	4.44842400
H	-2.83191000	2.78809700	2.84168300	H	-3.13591400	2.81076800	4.19801400
C	0.32225200	5.12701400	2.38833500	H	-5.60052100	2.58076500	4.05382300
H	0.77271700	3.11519700	1.74624700	H	-5.44575400	1.31042600	2.83197600
H	0.47056500	4.23448100	0.41573400	C	0.05941200	3.43399100	0.67279600
C	-0.12941600	4.76863000	3.80728400	C	-0.33307300	4.92521200	0.68051500
H	-1.86211500	3.92823800	4.82516500	C	0.67522500	3.03662900	2.02992400
H	-2.25415600	5.07479100	3.53680400	H	0.84526000	3.30596400	-0.08783300
H	1.38198900	5.43585500	2.38820900	C	0.86505500	5.81758500	1.04566900
H	-0.25684600	5.99693700	2.02646900	H	-1.13821600	5.10172300	1.41507700
H	-0.03402700	5.64158100	4.47607600	H	-0.73190700	5.23336000	-0.29855000
H	0.53995600	3.98761400	4.21366500	C	1.86745100	3.93208800	2.40102800
int-1-L4				H	-0.08942300	3.12290600	2.82217900
P	-1.27616200	2.20479200	0.11498400	H	0.98823200	1.97935500	2.01003900
P	-1.72652800	-1.96994600	-0.10834300	C	1.48867500	5.41696000	2.38658200
Pd	-0.23303700	-0.00623100	-0.22429600	H	0.54679200	6.87438200	1.07050800
C	-1.87610400	2.97014700	-1.50824000	H	1.62997600	5.74111800	0.25070400
C	-0.70980900	3.25969100	-2.47735200	H	2.25238400	3.64449400	3.39496700
C	-2.90758900	2.06663400	-2.21379300	H	2.69314900	3.75812000	1.68695800
H	-2.36233400	3.92928500	-1.25916300	H	2.37335000	6.04137800	2.60076600
C	-1.20230500	3.87601300	-3.79590900	H	0.76289400	5.61487200	3.19767900

C -1.01118400 -3.49225100 -0.98154900
C -0.65498800 -3.14321900 -2.44383000
C 0.18845600 -4.15312600 -0.27307300
H -1.82144500 -4.23975300 -0.99782300
C -0.12633300 -4.35819200 -3.21911700
H 0.11619000 -2.35367900 -2.44761500
H -1.52838000 -2.72211700 -2.96761200
C 0.73011600 -5.35412400 -1.06630500
H 0.99622500 -3.42002500 -0.13300000
H -0.09985900 -4.49105100 0.73289900
C 1.07700600 -4.99037000 -2.51377100
H 0.14441200 -4.05342300 -4.24493400
H -0.93037600 -5.11124400 -3.31831700
H 1.61392800 -5.76706400 -0.54950300
H -0.03008300 -6.15764500 -1.07121900
H 1.41959700 -5.88550600 -3.06152900
H 1.91871400 -4.27278700 -2.52894500
C -2.14538300 -2.50533000 1.65485200
C -2.80291000 -3.88576300 1.84850900
C -0.94909400 -2.32439400 2.61460500
H -2.88945700 -1.74340700 1.94658600
C -3.19630600 -4.12179600 3.31609000
H -2.10563900 -4.68084700 1.53366500
H -3.69508500 -3.98248900 1.21240300
C -1.35553300 -2.56400600 4.07567000
H -0.14189500 -3.02750900 2.34806900
H -0.52874900 -1.31177600 2.49788600
C -2.00899000 -3.93721100 4.26674500
H -3.62493500 -5.13304200 3.42766900
H -3.99727600 -3.41159700 3.59429400
H -0.47211300 -2.46395500 4.73002000
H -2.06667800 -1.77674400 4.38858200
H -2.33261300 -4.06677300 5.31412100
H -1.25961100 -4.72711500 4.07132000
C -3.41249700 -1.80095500 -0.99215200
C -4.09947000 -3.07184500 -1.53596400
C -4.41505900 -0.98396400 -0.15683000
H -3.14188200 -1.18244000 -1.86689600
C -5.36787800 -2.72443400 -2.33326600
H -4.37383600 -3.73929800 -0.70178000
H -3.42224200 -3.64354500 -2.18616200
C -5.68320100 -0.63778700 -0.95048600
H -4.70920200 -1.56309300 0.73609200
H -3.94018600 -0.06264000 0.20951300
C -6.35772600 -1.89276800 -1.51252900
H -5.84661400 -3.65413000 -2.68710100

H -5.08060100 -2.15822400 -3.23889500
H -6.38421400 -0.07994100 -0.30548400
H -5.41940800 0.03821900 -1.78402900
H -7.23274600 -1.61834600 -2.12692200
H -6.74252700 -2.50555200 -0.67588000
C 1.78483700 0.42173800 -0.69903600
C 1.62519400 -0.84490300 -0.60364800
C 2.71153400 1.53472900 -1.02730600
H 2.28035600 2.14902000 -1.83657700
H 2.82640200 2.21291500 -0.17210800
N 4.06071500 1.13016500 -1.47086600
C 4.19603600 0.43536700 -2.74311100
H 3.56871500 0.93099100 -3.50219600
H 5.24142300 0.51073700 -3.08797700
C 3.85842400 -1.04240000 -2.70830300
O 3.30007100 -1.62105100 -3.61661000
H 4.21018600 -1.59098000 -1.80352500
S 5.38563700 1.37119600 -0.48738300
O 6.56418300 1.43129200 -1.36892700
O 5.06914200 2.51920700 0.37891600
C 5.58662300 -0.05742100 0.57355300
C 6.46048600 -1.08216700 0.19012200
C 4.85957700 -0.13865000 1.76511600
C 6.59257400 -2.20162800 1.01049000
H 7.03684900 -1.00079800 -0.73305400
C 5.00582000 -1.26877000 2.57250800
H 4.19428400 0.67137700 2.06931100
C 5.86818100 -2.31775800 2.21149600
H 7.27730800 -3.00149500 0.71463500
H 4.44034000 -1.33222000 3.50597500
H 2.09424600 -1.82048900 -0.67116600
C 6.03146100 -3.53357800 3.08449500
H 7.06902900 -3.61805400 3.45034600
H 5.36345100 -3.50047400 3.95750800
H 5.81724900 -4.45670000 2.52041800

int-2-L4

P 0.90429200 -2.58039700 -0.27417200
P 1.69470400 2.20523300 -0.08506800
Pd 1.15943700 -0.16867200 -0.11557400
C -0.53209400 -3.14862700 -1.35603400
C -1.88472500 -3.27563100 -0.62435700
C -0.70398900 -2.22981000 -2.58593000
H -0.24457100 -4.15550600 -1.70823800
C -2.97353800 -3.81043600 -1.56827200
H -2.18913600 -2.28876900 -0.24003700
H -1.80991900 -3.93882300 0.24782700

C	-1.78449900	-2.76017200	-3.53917800	C	2.85537200	2.06203400	2.47742500
H	-0.99021600	-1.22320600	-2.23300700	H	2.51892200	3.91293600	1.41786900
H	0.24342000	-2.10739800	-3.12979800	C	0.95777200	3.96428600	3.71087900
C	-3.12696300	-2.94849800	-2.82557300	H	0.05049900	2.43247000	2.47424300
H	-3.93244500	-3.87009500	-1.02531100	H	0.06420500	4.04049700	1.74073900
H	-2.71719000	-4.84508300	-1.86301900	C	3.13910400	2.69345100	3.84765300
H	-1.89618100	-2.07001600	-4.39319000	H	2.34174000	1.09526400	2.62087200
H	-1.45284000	-3.72726200	-3.96067100	H	3.80455000	1.83826900	1.96430900
H	-3.86684900	-3.39781000	-3.51038300	C	1.84432100	3.06435400	4.57818100
H	-3.52756400	-1.95867300	-2.53960200	H	0.00642600	4.17923400	4.22714100
C	2.43773800	-3.39711700	-1.02856300	H	1.46093700	4.93830700	3.56467700
C	2.47922200	-3.45157900	-2.56826200	H	3.74136200	1.99871400	4.45803400
C	3.73904600	-2.76056800	-0.49640100	H	3.75416000	3.60200400	3.70916000
H	2.38765300	-4.43909100	-0.66664300	H	2.07333400	3.56147900	5.53658200
C	3.72201800	-4.20778500	-3.06433200	H	1.29041600	2.14062600	4.82838300
H	2.49360700	-2.42480800	-2.97598400	C	3.30878200	2.43336200	-1.04746700
H	1.58065300	-3.94367600	-2.96828400	C	4.23001600	3.57857400	-0.58177500
C	4.98271600	-3.51486000	-0.98833300	C	4.10338500	1.11825100	-1.16660800
H	3.78918100	-1.71553000	-0.84515500	H	2.94931600	2.68526200	-2.06096200
H	3.74168600	-2.72124300	0.60195000	C	5.43813700	3.73286800	-1.51906200
C	5.02100400	-3.60941800	-2.51661700	H	4.59752500	3.36616900	0.43643000
H	3.73376500	-4.20986300	-4.16791700	H	3.67974100	4.52951800	-0.52729400
H	3.64713400	-5.26558000	-2.75110000	C	5.32186200	1.27213300	-2.08838300
H	5.89133000	-3.01566700	-0.60995800	H	4.43832700	0.79591300	-0.16492900
H	4.98333900	-4.53337700	-0.55772100	H	3.44992100	0.31713900	-1.55408700
H	5.88784600	-4.20878100	-2.84423900	C	6.22839900	2.42658200	-1.64847800
H	5.16230000	-2.59770400	-2.94021600	H	6.09078200	4.54183400	-1.14818000
C	0.66411000	-3.47418200	1.36099500	H	5.08558500	4.04847500	-2.51845200
C	0.47603400	-5.00389000	1.28016000	H	5.88912900	0.32617700	-2.11616100
C	1.75133000	-3.16164800	2.41179900	H	4.97072200	1.45798600	-3.12031900
H	-0.27576300	-3.03401900	1.73727000	H	7.06223700	2.55063900	-2.36067100
C	0.05472900	-5.56207100	2.65021600	H	6.68456900	2.17992600	-0.67171500
H	1.42553400	-5.47741500	0.97411200	C	0.46126200	3.31395100	-0.96179100
H	-0.27111600	-5.28542200	0.52332600	C	0.85874000	4.79877500	-1.07875600
C	1.32765200	-3.68733900	3.79195800	C	0.07473400	2.74627500	-2.34345700
H	2.69651300	-3.64993600	2.12028000	H	-0.43417700	3.25821600	-0.31926600
H	1.95868900	-2.08106900	2.45959200	C	-0.26578200	5.62199600	-1.72630700
C	1.05465800	-5.19604300	3.75388000	H	1.76664100	4.88937300	-1.69942500
H	-0.05917300	-6.65811900	2.58564900	H	1.10462200	5.21678000	-0.08997100
H	-0.93991600	-5.15659000	2.91049100	C	-1.03685500	3.57838200	-3.00094400
H	2.11128800	-3.46013900	4.53556200	H	0.96007300	2.74288100	-3.00437500
H	0.41684800	-3.14926800	4.10938700	H	-0.24667000	1.69582700	-2.24669000
H	0.68388800	-5.54367400	4.73372000	C	-0.66139400	5.06125300	-3.09645500
H	2.00560200	-5.73130700	3.57215600	H	0.05278200	6.67464400	-1.81857700
C	1.97025200	2.97447300	1.60297800	H	-1.14838100	5.61767800	-1.06062400
C	0.66467400	3.33785600	2.33877000	H	-1.26069200	3.17229700	-4.00239800

H	-1.96135500	3.47764800	-2.40478100	H	-1.31893800	-4.96889500	4.39707000
H	-1.49955700	5.64056700	-3.52050700	C	-3.96562200	-0.87798000	0.08373400
H	0.18675600	5.17934900	-3.79661100	C	-4.98000600	-1.02275800	-0.87712200
C	-0.48069900	-0.00226900	1.02180100	C	-4.22605400	-0.10573200	1.23209300
C	-0.48966200	-0.38471100	2.30014500	C	-6.22733500	-0.41433600	-0.69133600
C	-1.70773400	0.55768000	0.33892900	H	-4.80526300	-1.61143900	-1.77981000
N	-2.70410700	0.91256700	1.36507200	C	-5.47449300	0.49247300	1.41872900
C	-2.99705500	-0.17009800	2.31146000	H	-3.45224200	0.02532500	1.99215700
C	-1.75582500	-0.50914300	3.18006500	C	-6.47964500	0.34228000	0.45597100
O	-1.86185000	-1.73936800	3.73551800	H	-7.00546600	-0.53888900	-1.44949700
H	-1.67484600	0.32844000	3.93589300	H	-5.66084500	1.08235100	2.32026000
S	-3.91787600	1.97972000	0.95589500	H	-7.45517300	0.81417100	0.60112200
O	-4.55808100	2.39343300	2.21555800	C	-2.49217600	-2.77542000	-1.54781500
O	-3.30541500	3.00896200	0.09287600	C	-3.04703100	-4.05487700	-1.37110800
C	-5.15548300	1.12312500	-0.01712100	C	-2.08880000	-2.38220000	-2.83606400
C	-6.25122800	0.53814800	0.62560900	C	-3.19309800	-4.91972100	-2.46006000
C	-5.00224300	1.02506200	-1.40689200	H	-3.36615000	-4.38654100	-0.38067400
C	-7.19502100	-0.15733300	-0.13404700	C	-2.24405000	-3.24497900	-3.92606900
H	-6.37681800	0.63618400	1.70518500	H	-1.64300700	-1.39468200	-2.98653600
C	-5.95567000	0.32762900	-2.14740600	C	-2.79376600	-4.51707300	-3.73931300
H	-4.15605600	1.49785900	-1.90826200	H	-3.62067200	-5.91440800	-2.30679500
C	-7.06558200	-0.27717800	-1.52720500	H	-1.92607100	-2.92364700	-4.92159100
H	-8.05335500	-0.61085600	0.36883400	H	-2.90721600	-5.19638000	-4.58856900
H	-5.84019800	0.25658600	-3.23267500	C	0.61924900	3.28915800	0.12817000
H	0.41401800	-0.74293400	2.79898400	C	0.92391200	3.97636100	-1.06155300
H	-3.27579500	-1.09372600	1.76883200	C	1.45077400	3.47378200	1.24599500
H	-3.83389200	0.11944700	2.95960100	C	2.02610600	4.83252000	-1.12629300
H	-1.45992400	1.45928800	-0.22999200	H	0.30103400	3.84340900	-1.94964400
H	-2.12430200	-0.17645900	-0.37704500	C	2.55932800	4.32533800	1.17524400
C	-8.08493500	-1.02149000	-2.34824000	H	1.24072800	2.95297900	2.18260400
H	-8.87408300	-1.45738400	-1.71844700	C	2.85124900	5.00701400	-0.00960900
H	-8.56320000	-0.35216000	-3.08346300	H	2.24402700	5.36203700	-2.05789100
H	-7.61144400	-1.83643000	-2.92111400	H	3.19476400	4.45626200	2.05536700
TS-endo				H	3.71684100	5.67259500	-0.06318900
P	-0.77115000	2.06265400	0.14927100	C	-1.28011900	2.03546900	1.93165600
P	-2.26628500	-1.57147100	-0.15678000	C	-2.18579500	2.94868700	2.49737700
C	-2.02456900	-2.65288100	1.32658300	C	-0.72119000	1.03874500	2.75215600
C	-0.70518900	-2.96019000	1.70445400	C	-2.51999100	2.86655600	3.85325900
C	-3.08652200	-3.18966900	2.07594800	H	-2.64660700	3.72618700	1.88640000
C	-0.45227800	-3.79363400	2.79827800	C	-1.04818700	0.96494500	4.10964500
H	0.13182600	-2.54025400	1.13946700	H	-0.02998900	0.30899400	2.32164200
C	-2.83142400	-4.01753700	3.17421300	C	-1.95146400	1.87797900	4.66322600
H	-4.12066500	-2.96364700	1.80781500	H	-3.23095200	3.58120100	4.27682000
C	-1.51545300	-4.32275900	3.53718200	H	-0.60201200	0.18503000	4.73247900
H	0.57963600	-4.02318100	3.07730300	H	-2.21549100	1.81667700	5.72247100
H	-3.66767100	-4.42663500	3.74781500	C	-2.11334300	2.95733200	-0.75501000

C	-2.33466000	4.34008000	-0.60482500	C	-5.39290400	0.12413100	-0.19486000
C	-2.93273600	2.23272300	-1.63601500	C	-4.75395500	-0.64493200	-2.80875700
C	-3.36350500	4.97295200	-1.30737000	H	-2.80979500	0.21498100	-2.42658400
H	-1.69784200	4.93347500	0.05469500	C	-6.33722100	-0.54265000	-0.98227000
C	-3.96192400	2.86830600	-2.33922400	H	-5.65960600	0.41480400	0.82275800
H	-2.75762400	1.16432800	-1.77837800	C	-6.02195600	-0.92647600	-2.28965900
C	-4.18095500	4.23854100	-2.17425800	H	-4.49770900	-0.94505700	-3.82827200
H	-3.52409300	6.04689900	-1.17946500	H	-7.32515400	-0.76259600	-0.56863300
H	-4.58926100	2.28852200	-3.02135500	H	-6.76232000	-1.44838700	-2.90192500
H	-4.98293200	4.73727600	-2.72526700	C	-3.28733000	1.09454000	2.03538000
Pd	-0.32363200	-0.11187800	-0.59647600	C	-4.32671800	1.83950900	2.62318600
C	1.59695000	-0.02578600	-1.27213200	C	-2.58850500	0.16330400	2.82215200
C	1.57692600	-1.29688000	-1.51775900	C	-4.66313200	1.64494600	3.96600000
C	2.63626200	1.01331700	-1.51923500	H	-4.87663600	2.57864500	2.03670500
H	2.30072800	1.68758500	-2.32685600	C	-2.92867800	-0.03029100	4.16506900
H	2.78932800	1.64898100	-0.63887800	H	-1.76587800	-0.40582000	2.38349000
N	3.91349000	0.40433000	-1.91404500	C	-3.96690200	0.70920200	4.73909500
C	3.86476500	-0.65434500	-2.91386400	H	-5.47256100	2.23047900	4.41028400
H	3.31191600	-0.28438000	-3.79399000	H	-2.37312700	-0.75668800	4.76409300
H	4.89163500	-0.86962700	-3.24811200	H	-4.23017600	0.56209100	5.79005000
C	3.24030500	-1.99329500	-2.49212600	C	-3.15470100	3.08222500	-0.06536400
O	2.88992600	-2.78819800	-3.39255500	C	-3.92824300	3.51284300	-1.15638800
H	3.63290500	-2.38567700	-1.52370500	C	-2.54686900	4.04838600	0.75997600
S	5.27323400	0.65173400	-0.98385600	C	-4.10212900	4.87860700	-1.40651300
O	6.42912400	0.32972500	-1.83742200	H	-4.40622800	2.78604600	-1.81607800
O	5.14295100	2.00391400	-0.41371200	C	-2.72810600	5.41119300	0.51005100
C	5.28957300	-0.50170200	0.38838700	H	-1.93429200	3.73823400	1.61086500
C	5.96940800	-1.71919100	0.25660900	C	-3.50650900	5.83083700	-0.57439700
C	4.62190300	-0.17612500	1.57310900	H	-4.71241900	5.19654200	-2.25624400
C	5.96330900	-2.61817600	1.32179400	H	-2.25497000	6.14789000	1.16486600
H	6.50738000	-1.95521400	-0.66313200	H	-3.64615700	6.89727900	-0.77054900
C	4.62520800	-1.09202800	2.62803100	C	0.78637800	-2.44792000	-1.47643300
H	4.11587300	0.78478200	1.68231400	C	1.81485100	-3.37372400	-1.23342500
C	5.28911500	-2.32551900	2.52219100	C	0.73621400	-1.79996500	-2.72546500
H	6.49847700	-3.56672700	1.22164800	C	2.77009600	-3.64528700	-2.21960200
H	4.10672600	-0.83671700	3.55615700	H	1.87863000	-3.88828400	-0.27249800
H	0.93223800	-2.17051400	-1.40210500	C	1.68457800	-2.08187300	-3.71249800
C	5.28972800	-3.31494600	3.65713800	H	-0.04950600	-1.06579700	-2.92633500
H	4.77715400	-4.24750600	3.36500700	C	2.70711400	-3.00276700	-3.45982500
H	6.31877200	-3.59314500	3.93951500	H	3.56761300	-4.36470200	-2.01465100
H	4.78446200	-2.91281500	4.54732300	H	1.63060500	-1.57115900	-4.67764000
TS-exo				H	3.45739300	-3.21379500	-4.22642000
P	-0.49050500	-1.98630100	-0.22016900	C	-1.90957900	-3.11403600	-0.58258800
P	-2.81674200	1.29714300	0.26052200	C	-1.90235100	-4.04137300	-1.63695000
C	-4.11664700	0.40980100	-0.70827900	C	-3.06025400	-3.00642200	0.22122600
C	-3.80468200	0.01198100	-2.02070700	C	-3.02140600	-4.84711600	-1.87938000

H -1.02320800 -4.14361900 -2.27612500
C -4.17079600 -3.81935200 -0.01638000
H -3.09010500 -2.28537500 1.04239300
C -4.15561500 -4.74112500 -1.07017500
H -3.00054800 -5.56389400 -2.70494800
H -5.05461100 -3.72774200 0.62052500
H -5.02761400 -5.37274000 -1.26011500
C 0.18549000 -2.63312100 1.37270500
C 0.00203500 -3.95622800 1.80998700
C 0.92602400 -1.74644500 2.17491700
C 0.55392600 -4.38222800 3.02264800
H -0.57227300 -4.66172800 1.20514300
C 1.48366400 -2.17634000 3.38296100
H 1.06001800 -0.70885600 1.85288800
C 1.29664900 -3.49549300 3.80972200
H 0.40306600 -5.41369200 3.35273700
H 2.05795700 -1.47593600 3.99524700
H 1.72548600 -3.83142100 4.75774400
Pd -0.69757000 0.50131100 -0.24963700
C 1.36440400 2.10027700 -0.82108800
C 0.11573500 2.31566700 -0.54706300
C 2.44782900 1.08458500 -0.93015200
H 2.21860800 0.26877800 -1.62807400
H 2.65023200 0.63729100 0.06213500
N 3.64817600 1.80685500 -1.43343800
C 3.70804100 3.17929400 -0.94833400
H 4.48352300 3.73061200 -1.50103500
H 3.91392900 3.25384900 0.13714600
C 2.34880600 3.82602100 -1.23283300
O 1.96130800 4.81023100 -0.55952200
H 2.07797100 3.74992500 -2.31541000
S 5.05516700 0.94343800 -1.64759900
O 5.99482200 1.83461200 -2.34706400
O 4.66313000 -0.33269000 -2.27037300
C 5.74600500 0.57736400 -0.03731400
C 6.60683600 1.50224300 0.56964900
C 5.39776200 -0.61276900 0.60978200
C 7.11119600 1.22634900 1.83912900
H 6.89078800 2.41877000 0.04919100
C 5.91407800 -0.86995900 1.88224800
H 4.74376600 -1.33786500 0.12242900
C 6.77368800 0.04042100 2.51863800
H 7.78713900 1.94445200 2.31201800
H 5.64545200 -1.80156100 2.38746100
H -0.41085600 3.27348900 -0.49625300
C 7.33222300 -0.23612700 3.88925900

H 6.98028100 -1.19987300 4.28499800
H 7.04060100 0.55534200 4.60022700
H 8.43504100 -0.25427900 3.86923900

TS-endo-side

P -0.71065900 2.09190700 -0.18072900
P -2.50470700 -1.43144200 0.02102100
C -1.89824400 -2.29107900 1.54346600
C -0.51157500 -2.47994000 1.68115700
C -2.75076700 -2.75902500 2.55966100
C 0.01227400 -3.12910500 2.80341000
H 0.16705200 -2.11868200 0.90500800
C -2.22458500 -3.40384200 3.68380400
H -3.83138100 -2.62030400 2.48028100
C -0.84316200 -3.59092700 3.80856600
H 1.09426200 -3.26277200 2.88662300
H -2.89914100 -3.76195100 4.46647800
H -0.43529000 -4.09300700 4.69022000
C -4.10835000 -0.68071500 0.56847100
C -5.32686900 -0.93185900 -0.08361000
C -4.08857600 0.24389600 1.63070400
C -6.49749400 -0.27687200 0.31872700
H -5.37438000 -1.64221500 -0.91125700
C -5.25951100 0.88817200 2.03627400
H -3.15297100 0.45896400 2.15241700
C -6.46913100 0.63238800 1.37921200
H -7.43691800 -0.48636400 -0.20044300
H -5.22482200 1.59725000 2.86792300
H -7.38459700 1.14057200 1.69402800
C -3.04664100 -2.80226200 -1.10375500
C -3.34710600 -4.09921100 -0.65542600
C -3.14900100 -2.51945400 -2.47839100
C -3.74204700 -5.08899100 -1.56232600
H -3.27075100 -4.34881600 0.40474900
C -3.55645300 -3.50576700 -3.38150000
H -2.90469500 -1.51885400 -2.84663900
C -3.85053400 -4.79534900 -2.92516700
H -3.96536800 -6.09579900 -1.19869500
H -3.63513400 -3.26765300 -4.44578800
H -4.15911400 -5.57097800 -3.63133400
C 0.75979300 3.14332300 -0.59530200
C 1.01814100 3.40798600 -1.95420900
C 1.65221400 3.63340100 0.37062800
C 2.13263800 4.15742600 -2.33427600
H 0.34328900 3.02339800 -2.72459400
C 2.77565400 4.37744100 -0.01395000
H 1.48061500 3.44005500 1.43109600

C 3.01838300 4.64354400 -1.36370600
H 2.31415600 4.35929100 -3.39355600
H 3.46011100 4.75301500 0.75171700
H 3.89404100 5.22677900 -1.66114800
C -0.84342000 2.23087800 1.65907300
C -1.66276300 3.16776100 2.31055400
C -0.09798300 1.32351800 2.43501600
C -1.73225800 3.19706700 3.70798100
H -2.25839000 3.87827600 1.73493700
C -0.16091900 1.36251900 3.83071600
H 0.54002100 0.58376300 1.94508900
C -0.98190800 2.29725900 4.47121500
H -2.37826400 3.92921100 4.20030200
H 0.42776500 0.65290000 4.41823500
H -1.03887600 2.32181900 5.56286500
C -2.10386500 3.10912700 -0.85236600
C -2.07872500 4.51634000 -0.83931500
C -3.21814200 2.45594300 -1.40483500
C -3.15025900 5.24877500 -1.35789400
H -1.21850200 5.04795900 -0.42605400
C -4.29009100 3.19069300 -1.92305000
H -3.24256300 1.36437100 -1.43527900
C -4.25865300 4.58794700 -1.89983700
H -3.11729900 6.34161100 -1.34067600
H -5.14909100 2.66664500 -2.35050700
H -5.09404200 5.16321200 -2.30826300
Pd -0.67111100 -0.12185100 -0.95822700
C 1.09273300 -0.28263200 -1.96581400
C 0.65303400 -1.38337600 -2.48466500
C 2.48618100 0.20778400 -1.71375900
H 2.95474900 0.55086100 -2.65314200
H 2.50950700 1.03905000 -1.00383600
N 3.27845300 -0.90995300 -1.18217000
C 3.29013200 -2.12375400 -1.98972300
H 3.59153100 -1.84592700 -3.01325800
H 4.05084500 -2.82006900 -1.60078800
C 1.96524100 -2.91215700 -2.05847800
O 1.44892700 -3.43534500 -1.04910100
H 1.84016600 -3.39581900 -3.05757400
S 3.75896800 -0.94856700 0.41595600
O 3.18331500 0.24376900 1.06657700
O 3.47793500 -2.28226700 0.97532300
C 5.53651100 -0.74984000 0.39318200
C 6.07886300 0.52791700 0.19745400
C 6.36040500 -1.86335800 0.57006600
C 7.46305200 0.67626100 0.16955800

H 5.42907200 1.39727700 0.07664000
C 7.74756400 -1.69275500 0.53743000
H 5.92699600 -2.85002800 0.74120100
C 8.32200800 -0.42834900 0.33605500
H 7.88988300 1.67218700 0.02058800
H 8.39375600 -2.56346000 0.67718100
H -0.22502600 -1.93520300 -2.80845100
C 9.81556400 -0.24169800 0.30240100
H 10.13809500 0.18179700 -0.66398500
H 10.14263000 0.46511400 1.08372100
H 10.34747400 -1.19213300 0.45494800

TS-endo-MeOH

P 0.78549000 -2.26141600 -0.17694700
P 2.28303600 1.44779800 0.20675900
C 1.79548400 2.80636700 1.37830900
C 0.83284400 3.73556300 0.94061600
C 2.29591900 2.92419300 2.68501800
C 0.38664000 4.75598800 1.78220700
H 0.42795800 3.68293300 -0.07188900
C 1.84084200 3.94370800 3.53136000
H 3.04791400 2.22591300 3.05630300
C 0.88641500 4.86163800 3.08572500
H -0.35793100 5.46476700 1.40967400
H 2.24273400 4.01849200 4.54565200
H 0.53429500 5.65655200 3.74875400
C 3.76972500 0.69502300 1.01550000
C 5.08724500 0.93824100 0.59258600
C 3.55582400 -0.19984000 2.08072600
C 6.16419500 0.30667100 1.22554600
H 5.28589300 1.61916500 -0.23675600
C 4.63361000 -0.81840100 2.72024700
H 2.53899100 -0.41586300 2.41663800
C 5.94216300 -0.56914200 2.29192600
H 7.18280700 0.50444500 0.88048600
H 4.44777600 -1.50515200 3.55023300
H 6.78523600 -1.05998600 2.78560200
C 2.97167500 2.38573100 -1.23119600
C 3.66467200 3.60116500 -1.08539100
C 2.78709700 1.85853600 -2.52098000
C 4.16502500 4.26910700 -2.20672100
H 3.81552700 4.03258300 -0.09294600
C 3.29320700 2.52561200 -3.64202500
H 2.23549300 0.92243300 -2.64761700
C 3.98175300 3.73247500 -3.48662600
H 4.70039000 5.21405900 -2.07982500
H 3.14162100 2.10326000 -4.63900000

H 4.37245400 4.25816300 -4.36217900
C -0.47508400 -3.44696700 -0.84442500
C -0.52392200 -3.65870100 -2.23534800
C -1.42734600 -4.08033500 -0.03010300
C -1.49666400 -4.48982900 -2.79432600
H 0.20180900 -3.16941900 -2.89108900
C -2.40975500 -4.90386800 -0.59467700
H -1.41344400 -3.93581200 1.05193000
C -2.44705400 -5.11246200 -1.97546300
H -1.51635600 -4.64809100 -3.87611600
H -3.14610100 -5.38599300 0.05402500
H -3.21258700 -5.75783600 -2.41446700
C 0.81198600 -2.63801200 1.63689300
C 1.65357600 -3.59755600 2.22333700
C -0.05978500 -1.90475100 2.46362800
C 1.61697000 -3.82259900 3.60409800
H 2.35033600 -4.17333600 1.61235500
C -0.10211300 -2.13847100 3.84109300
H -0.70599900 -1.13918900 2.02485200
C 0.73861200 -3.09794000 4.41563200
H 2.28189200 -4.57002600 4.04549100
H -0.78807000 -1.56181600 4.46745400
H 0.71289100 -3.27648600 5.49399700
C 2.35012600 -2.97537100 -0.86416900
C 2.54761600 -4.36578000 -0.97229900
C 3.36260000 -2.11253600 -1.31178600
C 3.73834600 -4.87376200 -1.49807100
H 1.76817700 -5.06025700 -0.65120000
C 4.55385900 -2.62235600 -1.83991700
H 3.21502600 -1.03332300 -1.25616200
C 4.74530400 -4.00341800 -1.93157200
H 3.87799500 -5.95559600 -1.57347900
H 5.33006800 -1.93441300 -2.18534900
H 5.67430200 -4.40343900 -2.34686900
Pd 0.38813500 0.02779600 -0.50997200
C -1.52416700 0.07227200 -1.24453000
C -1.45999000 1.35962100 -1.27170300
C -2.58948400 -0.89348200 -1.63899500
H -2.30498000 -1.38926700 -2.58352200
H -2.70207500 -1.69547500 -0.89998700
N -3.88164200 -0.21935100 -1.82779300
C -3.89478800 1.01611700 -2.59689700
H -3.40336400 0.84031900 -3.56865800
H -4.94078000 1.28585400 -2.81220800
C -3.24671900 2.23691000 -1.94527100
O -2.95968200 3.21512300 -2.67703700

H -3.52189400 2.40125800 -0.88101400
S -5.19342500 -0.68026400 -0.90663200
O -6.38671100 -0.14923000 -1.58605700
O -5.06050900 -2.13117900 -0.69358900
C -5.10078000 0.10279800 0.70201300
C -5.70366900 1.35259000 0.89514300
C -4.42193800 -0.53693200 1.74330000
C -5.60811300 1.96495300 2.14334500
H -6.25065600 1.83503900 0.08314400
C -4.33594600 0.09476700 2.98655700
H -3.97582900 -1.52178200 1.59432600
C -4.92133700 1.35209000 3.20856600
H -6.08200300 2.93863100 2.29695700
H -3.80817200 -0.40625200 3.80247200
H -0.85038300 2.23625000 -1.06824800
C -4.83628500 2.03023800 4.55009600
H -5.84033800 2.15972000 4.98908000
H -4.22549900 1.45284000 5.25925900
H -4.39807300 3.03788700 4.45645200
C -0.53272300 5.42936700 -2.61040900
H 0.30084900 6.04273600 -2.23011300
H -1.11045500 6.05531600 -3.31983000
H -0.09486300 4.58946700 -3.18444900
O -1.31259400 4.99397300 -1.51606400
H -2.01643800 4.40122300 -1.88138300

TS-endo-PhB(OH)2

P 2.77641600 -1.21416100 -0.80094300
P 1.40454500 2.27838400 0.65359500
C 0.34685100 2.69551300 2.12414900
C -1.03413900 2.87852800 1.91795000
C 0.84291900 2.74348500 3.43707100
C -1.89507400 3.09523100 2.99586300
H -1.44786300 2.85890500 0.90708600
C -0.02239400 2.96309200 4.51651700
H 1.90855500 2.61082600 3.63264000
C -1.39216600 3.13617200 4.30193000
H -2.96474800 3.22030900 2.80855300
H 0.38340300 2.99891000 5.53140100
H -2.06583800 3.30334600 5.14673000
C 3.12239800 2.63143400 1.25399000
C 3.81155800 3.82678200 0.98926400
C 3.77450600 1.62369700 1.98860500
C 5.11841800 4.01091800 1.45499300
H 3.33804000 4.62314900 0.41279000
C 5.07449600 1.81528800 2.46541500
H 3.26409400 0.67848100 2.18935100

C	5.75181500	3.00964000	2.19692600	H	5.30425100	2.68078800	-2.61552200
H	5.64186900	4.94546000	1.23489500	H	7.08098700	1.29766000	-3.69787700
H	5.56228700	1.02303200	3.03935200	Pd	0.86262500	0.05763400	-0.25254800
H	6.77249000	3.15656200	2.56041100	C	-0.70291300	-1.22020400	-0.59301700
C	1.02597600	3.65039500	-0.52642600	C	-1.42372700	-0.26635900	-0.12667500
C	0.77338500	4.97008500	-0.10852100	C	-0.95383900	-2.54892700	-1.21432100
C	0.97781500	3.35146900	-1.89891100	H	-0.60309400	-2.54851000	-2.25967000
C	0.48993300	5.96722900	-1.04592000	H	-0.38527800	-3.33910400	-0.70608300
H	0.79300700	5.22411600	0.95392300	N	-2.38237200	-2.88926000	-1.20941700
C	0.69825900	4.35189000	-2.83646900	C	-3.27831700	-1.86682500	-1.71821500
H	1.15054600	2.32491300	-2.23399200	H	-2.93237000	-1.56117300	-2.71896600
C	0.45397700	5.66104000	-2.41138200	H	-4.28446900	-2.30001600	-1.84724400
H	0.29417400	6.98848400	-0.70777100	C	-3.45749400	-0.62118900	-0.87453600
H	0.66367300	4.10364700	-3.90066800	O	-3.80688400	0.42739700	-1.49475400
H	0.22972900	6.44282500	-3.14220200	H	-3.74840600	-0.72906200	0.17988600
C	2.47003200	-2.70459900	-1.86327600	S	-2.95899400	-4.11766400	-0.22847200
C	2.05499600	-2.48639900	-3.19106500	O	-4.28793800	-4.46629000	-0.75530100
C	2.59237300	-4.02342200	-1.40030000	O	-1.89516200	-5.13268200	-0.18894100
C	1.77811800	-3.56284100	-4.03584100	C	-3.18424900	-3.50454100	1.43823200
H	1.94586700	-1.46580900	-3.57017800	C	-4.44054200	-3.03705800	1.83536900
C	2.30415800	-5.10205500	-2.24708100	C	-2.09637500	-3.48969400	2.32078400
H	2.91442200	-4.22271900	-0.37633700	C	-4.59893200	-2.53288500	3.12819400
C	1.89875300	-4.87664100	-3.56462800	H	-5.28843300	-3.07501900	1.14929200
H	1.46220000	-3.37589900	-5.06588300	C	-2.27527000	-2.98136600	3.60606200
H	2.40325400	-6.12375900	-1.87019500	H	-1.12537500	-3.88279300	2.01443200
H	1.67690800	-5.71979300	-4.22433700	C	-3.52366700	-2.48860900	4.03112800
C	3.54081500	-1.91408100	0.73463200	H	-5.58198300	-2.17175900	3.44196100
C	4.92605300	-1.99192100	0.95338200	H	-1.42850600	-2.97247600	4.29810300
C	2.66953000	-2.36190100	1.74610700	H	-1.71742800	0.59066800	0.46007300
C	5.42666100	-2.51472400	2.15159300	C	-3.68918800	-1.92708700	5.41799300
H	5.62785000	-1.64076200	0.19529700	H	-3.28946600	-2.61839400	6.17781800
C	3.17148000	-2.89440100	2.93650200	H	-3.13180100	-0.98010500	5.52319400
H	1.58805500	-2.28767600	1.60215000	H	-4.74474400	-1.72553400	5.65165500
C	4.55347500	-2.97035100	3.14354300	C	-5.74822400	2.12197400	-1.43343300
H	6.50785800	-2.56408700	2.30721000	C	-6.74322900	1.13225400	-1.57106700
H	2.47985700	-3.24266800	3.70835100	C	-6.07351600	3.41728400	-1.88064300
H	4.94775400	-3.37853900	4.07806100	C	-7.99796400	1.41739800	-2.12126200
C	4.17524900	-0.42477400	-1.72754700	H	-6.53516500	0.10785900	-1.24306100
C	5.17490700	-1.19663400	-2.35130000	C	-7.32473400	3.71651200	-2.43444400
C	4.23554600	0.97274500	-1.83702800	H	-5.32856100	4.21500400	-1.79259900
C	6.21477700	-0.57910900	-3.05088700	C	-8.29347000	2.71481000	-2.55679700
H	5.14360100	-2.28718400	-2.29623500	H	-8.74775500	0.62568200	-2.21494600
C	5.27633900	1.59055400	-2.53953900	H	-7.54450100	4.73410600	-2.77207200
H	3.45878100	1.58497500	-1.37853900	H	-9.27209600	2.94227800	-2.98963300
C	6.26889300	0.81654100	-3.14598600	B	-4.31486800	1.81601900	-0.73912500
H	6.98457300	-1.19200300	-3.52776200	O	-3.26275900	2.75940700	-0.99713700

H -3.21346100 2.99433400 -1.93321600
O -4.34776700 1.55531600 0.67227100
H -5.21321000 1.23598000 0.95767400

TS-proton

P 2.30800800 -0.41651100 -0.16957800
C 1.62710000 -1.52510200 1.13745100
C 0.40060600 -2.17589100 0.91049900
C 2.27938300 -1.70742400 2.36839500
C -0.15580600 -2.99863200 1.89267400
H -0.13053900 -2.04779300 -0.03443600
C 1.71841100 -2.53343300 3.34887800
H 3.23123900 -1.21317700 2.57053000
C 0.50235600 -3.18149100 3.11405700
H -1.11697300 -3.48339300 1.70497000
H 2.24049800 -2.67129500 4.29952700
H 0.06645500 -3.82702100 3.88127800
C 4.07751700 -0.18223900 0.28697400
C 5.09987300 -1.02366300 -0.17828300
C 4.40182700 0.88183800 1.14791100
C 6.42440400 -0.80622500 0.21701400
H 4.87457300 -1.84970800 -0.85525000
C 5.72446100 1.09063700 1.54650900
H 3.61570500 1.55315800 1.50447700
C 6.73917700 0.24720600 1.08025500
H 7.21297000 -1.46517400 -0.15610400
H 5.96357400 1.91981100 2.21764600
H 7.77543000 0.41497200 1.38589000
C 2.27135400 -1.44672800 -1.69519400
C 2.49987800 -2.83460700 -1.64850600
C 2.01093200 -0.83464000 -2.93348400
C 2.47461300 -3.59182400 -2.82292400
H 2.69358400 -3.33211000 -0.69572500
C 1.98588600 -1.59783700 -4.10494800
H 1.83471100 0.24161700 -2.97834800
C 2.21739600 -2.97562700 -4.05242300
H 2.65362000 -4.66925600 -2.77494400
H 1.78014500 -1.11095100 -5.06192000
H 2.19401900 -3.57140100 -4.96890700
Pd 1.32279700 1.64116500 -0.47082900
C -0.58742600 1.39365000 0.63864100
C -0.52494300 1.43965900 1.98975400
C -1.69383800 0.63025900 -0.05928800
H -2.36304200 1.35474000 -0.56796400
H -1.27350200 -0.01547000 -0.84146600
N -2.44461200 -0.20942800 0.88635000
C -2.79904600 0.42010700 2.15681100

H -3.37362700 1.35285100 1.99967000
H -3.40616300 -0.26835800 2.75649600
C -1.51057500 0.76040200 2.90848400
O -1.87548600 1.59510100 3.99777900
H -1.05608800 -0.18091600 3.27658900
S -3.43652700 -1.40618700 0.27799700
O -2.72387700 -1.98804200 -0.87313400
O -3.79969300 -2.27167200 1.41358600
C -4.93655800 -0.65024300 -0.33588800
C -4.98649400 -0.19295400 -1.65988000
C -6.03183600 -0.49740600 0.52048800
C -6.14643700 0.42998600 -2.11692800
H -4.13562700 -0.33554200 -2.32844300
C -7.18438600 0.12966300 0.04209300
H -5.99415400 -0.87512700 1.54375000
C -7.26249700 0.60557800 -1.27724800
H -6.18963200 0.78296500 -3.15114700
H -8.04299700 0.24498500 0.70894300
H 0.27020000 2.00827000 2.48653600
C -8.50347200 1.28415200 -1.79323600
H -8.89647500 0.76479700 -2.68333700
H -9.29731300 1.31304300 -1.03275500
H -8.28502700 2.32096600 -2.10085300
H -1.11431400 1.67182800 4.59286800
O 0.24657400 3.50387700 -0.66033100
C 0.59468400 4.55711500 0.21487100
H 1.65262600 4.85853900 0.10944500
H -0.02869000 5.44602700 -0.00332700
H -0.30371300 2.52331300 0.05047000
H 0.42278100 4.28964900 1.27649600
O 2.92893100 2.00112100 -1.66534800
C 3.34949800 3.33115100 -1.69546100
H 3.79769700 3.68009800 -0.73807000
H 4.14086100 3.44760600 -2.46732300
H 2.54729300 4.05082200 -1.96467400

TS-β-H

P -2.42658000 -0.21309100 -0.23387900
C -1.77572500 0.53595300 -1.78604700
C -0.45848400 0.23532800 -2.18121000
C -2.52925900 1.43591200 -2.55703100
C 0.08466000 0.81170200 -3.33162100
H 0.15181700 -0.45638600 -1.59619200
C -1.97902700 2.01579500 -3.70632300
H -3.55122600 1.68962700 -2.26924300
C -0.67425700 1.70454100 -4.09753600
H 1.11091300 0.57023400 -3.61825900

H -2.57891000 2.71290400 -4.29765300
H -0.24653200 2.15798400 -4.99579000
C -4.20988200 0.25828800 -0.19737000
C -5.19969500 -0.46831500 -0.88027200
C -4.58119300 1.39463800 0.54282800
C -6.53604700 -0.06022500 -0.82628600
H -4.93375400 -1.35709800 -1.45684400
C -5.91725800 1.80405600 0.58885400
H -3.82053700 1.96022500 1.08887200
C -6.89697500 1.07610800 -0.09433600
H -7.29865800 -0.63478300 -1.35899700
H -6.19323500 2.69051900 1.16617100
H -7.94298800 1.39170800 -0.05282400
C -2.42472500 -2.03167200 -0.54955700
C -2.37321900 -2.58468000 -1.84052100
C -2.49553800 -2.89161000 0.56213100
C -2.39005000 -3.97275200 -2.01405100
H -2.31893300 -1.93705200 -2.71792400
C -2.51821200 -4.27747700 0.38317700
H -2.54044000 -2.47289500 1.57100700
C -2.46225800 -4.82106700 -0.90481900
H -2.34698200 -4.39087400 -3.02338900
H -2.57396800 -4.93469600 1.25513800
H -2.47288100 -5.90550800 -1.04385900
Pd -1.40844000 0.31166900 1.89896900
C 0.30354600 1.11144700 1.19549700
C 0.41372600 2.34521400 0.67136200
C 1.52437200 0.22731700 1.34826700
H 1.78591200 0.14557300 2.42022300
H 1.32128600 -0.79365400 1.00226000
N 2.70264200 0.74024900 0.62521500
C 2.91573500 2.18194900 0.73419700
H 3.03714600 2.42730600 1.80321800
H 3.84286300 2.47605400 0.22285300
C 1.71561400 2.96091100 0.19409600
O 1.87128900 4.30140400 0.66046000
H 1.74925600 2.95106300 -0.91359800
S 3.30436000 -0.04589400 -0.71300500
O 2.57801100 -1.32517800 -0.83481800
O 3.32567600 0.86851600 -1.87378500
C 5.00671400 -0.41972600 -0.30915100
C 5.27627000 -1.41592100 0.63973700
C 6.04083100 0.26606900 -0.94796500
C 6.60040500 -1.71172400 0.95001900
H 4.46269800 -1.95742700 1.12740900
C 7.36456200 -0.04525000 -0.62130000

H 5.81758300 1.02893500 -1.69533600
C 7.66767800 -1.03226700 0.32855100
H 6.81456900 -2.48953500 1.68847600
H 8.17596800 0.49099000 -1.12063500
H -0.46857500 2.98582800 0.54401000
C 9.09138700 -1.36921900 0.68379600
H 9.28157400 -1.19293500 1.75616300
H 9.30342400 -2.43510700 0.49483200
H 9.80794400 -0.76823300 0.10530900
H 1.17180100 4.84110200 0.26291200
O -3.07218600 -0.51929000 3.10912200
C -2.25685600 -0.17402700 4.01561900
H -2.41475200 0.76256400 4.58375900
H -1.60528500 -0.92668500 4.49994400
H -0.71176800 0.64297400 3.31095300

TS-1

P -1.45098700 0.00895000 -0.05433800
C -2.31914300 1.55545500 -0.53687000
C -3.38205700 2.09699100 0.20392200
C -1.85900900 2.24219500 -1.67717300
C -3.98448800 3.29414800 -0.19907200
H -3.74764400 1.59265300 1.10002400
C -2.46968000 3.43147400 -2.08071300
H -1.01855500 1.84627300 -2.25339600
C -3.53393500 3.96074000 -1.34164200
H -4.81092800 3.70490100 0.38701600
H -2.10658200 3.95103200 -2.97138800
H -4.00715700 4.89545600 -1.65426600
C -1.99145200 -1.27706600 -1.26435900
C -2.68477000 -0.97362600 -2.44740400
C -1.65268700 -2.61815600 -0.99604000
C -3.03230000 -1.99106400 -3.34338000
H -2.96682100 0.05483400 -2.67795900
C -2.00412000 -3.62956000 -1.89288800
H -1.11726700 -2.87843500 -0.08038500
C -2.69328800 -3.31894800 -3.07072200
H -3.57624300 -1.73915500 -4.25774600
H -1.73816400 -4.66605200 -1.66869000
H -2.96735700 -4.11170600 -3.77187400
C -2.19169100 -0.55258800 1.53297900
C -3.49483800 -1.08024100 1.59196500
C -1.43185500 -0.46438300 2.71125600
C -4.02793900 -1.50077200 2.81283800
H -4.09662200 -1.16626000 0.68401100
C -1.96915000 -0.88789900 3.93161000
H -0.41281800 -0.07092500 2.67192700

C	-3.26676500	-1.40478700	3.98384500	C	-1.28377500	2.61101500	-1.24614700
H	-5.04177800	-1.90824300	2.84918400	C	-1.13085100	4.33549600	0.94628800
H	-1.36801000	-0.81760500	4.84189600	H	-2.05256000	2.75112400	2.08153800
H	-3.68550700	-1.73879400	4.93699200	C	-0.74100300	3.88831200	-1.39865900
Pd	0.90531800	0.20018500	0.04721500	H	-1.33104800	1.94119500	-2.10978500
C	3.09719700	0.30270800	0.00058500	C	-0.66224300	4.75489100	-0.30099900
C	3.53616800	0.69087700	-1.28744400	H	-1.07286800	5.00508100	1.80870300
C	3.75497200	0.89210100	1.10312200	H	-0.37606000	4.20800700	-2.37820600
C	4.57147300	1.61385100	-1.46749500	H	-0.23529400	5.75427800	-0.42042600
H	3.06479500	0.25346000	-2.17413000	C	-3.95750800	0.56875300	-0.95093400
C	4.79360200	1.81341400	0.93734800	C	-4.65232800	1.77584500	-1.15361900
H	3.45760700	0.61396700	2.11893000	C	-4.41239600	-0.60230800	-1.58225500
C	5.20013600	2.18072100	-0.35151500	C	-5.78537300	1.80689600	-1.97153500
H	4.88959200	1.89378300	-2.47623500	H	-4.31312100	2.69742500	-0.67579500
H	5.28762800	2.24803000	1.81154500	C	-5.54777600	-0.56316700	-2.39917500
H	6.00993600	2.90379700	-0.48623300	H	-3.86231800	-1.53700400	-1.42806800
B	2.76149900	-1.69338000	0.21948800	C	-6.23524000	0.63821200	-2.59618500
O	3.00288400	-1.97177100	1.57310400	H	-6.31744000	2.75016800	-2.12235300
H	2.35297500	-1.56142600	2.16013400	H	-5.89261800	-1.47845200	-2.88830800
O	1.36096000	-1.82453700	-0.19149400	H	-7.11978500	0.66643900	-3.23853000
H	1.28131600	-2.06254200	-1.13058300	Pd	-0.87354100	-1.30720500	-0.31996800
O	3.61894300	-2.29828800	-0.70962000	O	-2.38170400	-2.74386700	-0.53312900
C	5.00470100	-2.38950600	-0.45690900	C	-3.06394500	-3.12906800	0.61706100
H	5.22006100	-2.88836200	0.50437500	H	-3.67705600	-4.03827200	0.42333200
H	5.46876600	-2.97963300	-1.26329700	H	-2.39858500	-3.39042200	1.47214700
H	5.48449300	-1.39342000	-0.44212300	H	-3.77318400	-2.36010700	1.00167800
O	0.80284400	2.18889900	0.25746600	C	0.44632400	-2.82086700	-0.91748400
C	0.51211400	2.66395200	1.53879600	C	0.85239600	-2.77777300	-2.26076000
H	1.22542300	2.31637300	2.31737900	C	0.52575400	-4.03356100	-0.21176800
H	0.56933600	3.77318300	1.53607700	C	1.28455400	-3.94509700	-2.90564200
H	-0.51001000	2.40441800	1.89107800	H	0.83634200	-1.83307500	-2.81154400
TS-2				C	0.97119600	-5.19300000	-0.85443000
P	-2.46265000	0.47748200	0.12851900	H	0.22630500	-4.08234800	0.83885300
C	-3.09592600	0.35836600	1.85724700	C	1.34748000	-5.15299800	-2.20359200
C	-4.42309000	0.65465300	2.20882900	H	1.58318000	-3.90385600	-3.95719600
C	-2.19900000	-0.05685200	2.85862700	H	1.02131900	-6.13441400	-0.29943900
C	-4.84258800	0.54008600	3.53847400	H	1.69607600	-6.06117600	-2.70295900
H	-5.13871700	0.97325600	1.44837200	C	1.35918500	-1.10258200	0.06393600
C	-2.61920200	-0.16090900	4.18742100	C	0.72418700	-0.02218600	-0.12755600
H	-1.16557200	-0.30076600	2.59722300	H	0.75133000	1.06252800	-0.11625900
C	-3.94339400	0.13438100	4.52955600	C	2.57037300	-1.80108400	0.59848700
H	-5.87949800	0.76941700	3.79853000	H	2.26058600	-2.55037100	1.34321000
H	-1.91136700	-0.48194500	4.95626900	H	3.09175800	-2.35026800	-0.19598100
H	-4.27490300	0.04450900	5.56753700	N	3.51893900	-0.89300500	1.23932200
C	-1.76933300	2.18577800	0.00506400	C	3.13019900	-0.16020200	2.43933500
C	-1.68423300	3.05798200	1.10074500	H	2.87194200	0.89770000	2.25786900

H	2.21967800	-0.64324600	2.83443000	S	4.29686700	0.42515300	-0.91192700
C	4.15667300	-0.24769200	3.55032100	O	3.31994600	-0.66685200	-1.07315400
O	4.27685000	0.60478200	4.40078800	O	4.45874500	1.40128400	-2.00753200
H	4.75754100	-1.18810100	3.56771800	C	5.90551300	-0.26650400	-0.56718900
S	4.81273400	-0.28108400	0.35533200	C	6.02811900	-1.26256600	0.41140900
O	5.74881700	0.22727600	1.37382800	C	7.00870700	0.16369900	-1.30703900
O	5.23068200	-1.34453600	-0.56841200	C	7.28055800	-1.82204800	0.64650400
C	4.26646700	1.11428500	-0.61500600	H	5.16026700	-1.59711900	0.98281400
C	4.27082200	2.39334700	-0.04417600	C	8.25660300	-0.41355500	-1.05671000
C	3.84246900	0.91065500	-1.93317900	H	6.89507500	0.93715800	-2.06797100
C	3.83360400	3.47466400	-0.80911300	C	8.41520100	-1.41049300	-0.08178600
H	4.62566900	2.54616600	0.97642600	H	7.38375300	-2.59814500	1.41003300
C	3.41369200	2.00698700	-2.68129900	H	9.12292800	-0.07927400	-1.63350300
H	3.85571100	-0.08797900	-2.37319500	C	9.75771600	-2.03399200	0.18953500
C	3.40145800	3.30369600	-2.13669600	H	10.04978600	-1.89602900	1.24422400
H	3.83744900	4.47487700	-0.36755000	H	9.72920200	-3.12169900	0.00754000
H	3.08671200	1.85233400	-3.71303300	H	10.54336900	-1.59974500	-0.44546500
C	2.97440400	4.48638600	-2.96379100	P	-0.83408900	-2.27773400	0.24999500
H	2.30245300	4.18788300	-3.78218100	P	-3.07515900	0.94417000	-0.25220400
H	2.47044700	5.24786500	-2.34928000	C	-3.52550200	1.39530500	-1.98374900
H	3.85445000	4.97185400	-3.42251100	C	-2.49772300	1.66430000	-2.90404000
TS-3				C	-4.86362600	1.49423500	-2.40659700
C	1.12555800	3.17301500	0.64431100	C	-2.80005200	2.03457100	-4.21794000
C	1.50929800	3.75928200	1.86843300	H	-1.45391100	1.57787100	-2.59142200
C	0.46405300	3.98852300	-0.30334500	C	-5.16223600	1.86119600	-3.72220700
C	1.24631100	5.10690200	2.13149100	H	-5.67944800	1.28611200	-1.71121500
H	2.00626500	3.16533500	2.63598600	C	-4.13276500	2.13253600	-4.62977100
C	0.21162700	5.33217100	-0.04141400	H	-1.98983500	2.23924900	-4.92273700
H	0.15467100	3.56212300	-1.26017100	H	-6.20624800	1.93481000	-4.03835100
C	0.60044100	5.89987200	1.18003200	H	-4.36978700	2.41576400	-5.65882200
H	1.54973700	5.53624000	3.08992200	C	-4.51653600	-0.04827200	0.33422000
H	-0.29153600	5.94406300	-0.79464100	C	-5.28920100	0.32884800	1.44445700
H	0.39905200	6.95436700	1.38564000	C	-4.81530500	-1.25318100	-0.32973900
C	1.40775000	1.74907200	0.33819500	C	-6.34401700	-0.48248700	1.87894600
C	0.75272800	1.07814200	-0.65348300	H	-5.07648200	1.25760300	1.97724200
H	0.78338100	0.98347900	-1.74781600	C	-5.87304300	-2.05559300	0.10311500
C	2.53574500	1.00449500	1.07594400	H	-4.22582100	-1.56438800	-1.19553800
H	2.59521800	1.30437200	2.13039600	C	-6.63919500	-1.67385000	1.21093800
H	2.33295200	-0.07077200	1.05626300	H	-6.93877700	-0.17539700	2.74347400
N	3.86691800	1.23722000	0.49550800	H	-6.09693100	-2.98547300	-0.42631400
C	4.68341800	2.39644300	0.83493600	H	-7.46465400	-2.30479500	1.55122100
H	4.39649100	2.72561100	1.84753900	C	-3.17327600	2.51690600	0.70719300
H	5.75125100	2.12502800	0.89567900	C	-3.92258200	3.62614400	0.28036600
C	4.55570200	3.60623000	-0.07860300	C	-2.46250400	2.59591200	1.91835400
O	5.40928500	4.46374100	-0.12371300	C	-3.96161000	4.78978600	1.05511800
H	3.62280600	3.67915800	-0.68359100	H	-4.47901900	3.59074300	-0.65834300

C	-2.51174300	3.75704700	2.69495500	C	2.67234700	5.49810200	-1.69914900
H	-1.86408400	1.74480300	2.25515100	H	0.99255000	4.21656800	-1.29987700
C	-3.25959300	4.85747000	2.26299100	C	4.06446800	5.60016800	-1.80462100
H	-4.54510800	5.64787700	0.71076000	H	5.94406300	4.53392100	-1.68018000
H	-1.95668800	3.80411900	3.63536400	H	2.04458800	6.38064200	-1.84833200
H	-3.29167100	5.76916300	2.86551200	H	4.52969600	6.56019500	-2.04376100
C	0.83437400	-3.07284200	0.28285000	C	2.22106600	1.81935600	-0.86062000
C	1.62832400	-2.92512300	1.43583500	C	0.97776800	1.49732500	-1.32297400
C	1.35032400	-3.78005700	-0.81449000	H	0.51666500	2.20267000	-2.02387600
C	2.90389000	-3.49049000	1.49286000	C	3.04282700	0.75345400	-0.16260700
H	1.24701300	-2.37672400	2.30127400	H	3.88577900	1.18334000	0.38640100
C	2.63412100	-4.33463000	-0.75686200	H	2.41565500	0.18756600	0.54329600
H	0.75556200	-3.90806100	-1.72090400	N	3.54848500	-0.14720600	-1.21894400
C	3.41165000	-4.19651000	0.39549300	C	2.50319600	-0.98088600	-1.79273800
H	3.50298400	-3.38053400	2.40077500	H	2.94103900	-1.61282200	-2.58263400
H	3.02169500	-4.88437200	-1.61878900	H	2.02983200	-1.63288500	-1.03633800
H	4.41126400	-4.63647000	0.44039100	C	1.40306700	-0.19456200	-2.49042900
C	-1.72322600	-3.11853200	-1.13095800	O	0.24397200	-0.74092600	-2.53956800
C	-2.51636100	-4.26491800	-0.95968900	H	1.72709400	0.43231100	-3.34148400
C	-1.59778000	-2.55947400	-2.41635400	S	5.06726700	-0.85448300	-1.01284200
C	-3.16410300	-4.84357000	-2.05637400	O	5.37291800	-1.52553200	-2.28410100
H	-2.64340300	-4.71111900	0.02783600	O	5.94918400	0.21575300	-0.51981800
C	-2.23788500	-3.14643900	-3.51130700	C	4.94730000	-2.10026200	0.26260400
H	-0.99842500	-1.65589200	-2.56084300	C	4.64630500	-3.41929000	-0.09261700
C	-3.02468100	-4.28944100	-3.33275700	C	5.14087700	-1.73775300	1.60270200
H	-3.78201700	-5.73331800	-1.90865400	C	4.52975400	-4.38120400	0.91292900
H	-2.12772800	-2.70353800	-4.50463900	H	4.51917200	-3.69732800	-1.14028800
H	-3.53264000	-4.74487800	-4.18705000	C	5.01966800	-2.71376700	2.58994000
C	-1.59353700	-2.85679400	1.82561200	H	5.39760400	-0.71117000	1.86982200
C	-1.42206500	-4.17551100	2.28890500	C	4.71161900	-4.04875100	2.26563300
C	-2.34200700	-1.95374800	2.59749600	H	4.29908500	-5.41369200	0.63755400
C	-2.00693100	-4.58112600	3.49097100	H	5.17591600	-2.43572900	3.63600400
H	-0.82549100	-4.88953100	1.71671800	P	-2.29055600	-1.55698000	-0.71441600
C	-2.92417900	-2.36277100	3.80214000	P	-1.16676400	1.57380000	0.96626500
H	-2.46503100	-0.92337000	2.25915700	C	-1.86454200	3.14565900	0.30086000
C	-2.76015800	-3.67667700	4.24878400	C	-2.00072000	3.34122000	-1.08236900
H	-1.86944700	-5.60821400	3.83945400	C	-2.32825500	4.14231000	1.18200400
H	-3.50316200	-1.64840700	4.39310200	C	-2.56941400	4.51998900	-1.57901100
H	-3.21303800	-3.99647500	5.19113500	H	-1.67663300	2.56538000	-1.77746500
Pd	-0.77986000	0.10431100	-0.14624200	C	-2.88964500	5.31893200	0.68260000
TS-4				H	-2.25879000	4.00093800	2.26290100
C	2.86302900	3.11810900	-1.18083800	C	-3.00902700	5.51163400	-0.69900200
C	4.26633100	3.24064400	-1.27981400	H	-2.67181800	4.65692800	-2.65860000
C	2.07855100	4.27324300	-1.39531300	H	-3.24165600	6.08644600	1.37682900
C	4.85613100	4.46633300	-1.59604700	H	-3.45321300	6.43211000	-1.08709100
H	4.90699300	2.36981400	-1.13608500	C	-2.48048000	1.08606700	2.18174900

C -2.19880000 0.73443700 3.51257500
C -3.82074600 1.10288300 1.75377300
C -3.23429700 0.40094100 4.39183400
H -1.17423600 0.72715100 3.88391800
C -4.85179200 0.77089000 2.63622700
H -4.07033100 1.39103000 0.73158100
C -4.56225800 0.41619800 3.95766400
H -2.99580000 0.13503200 5.42502600
H -5.88711800 0.79481800 2.28718400
H -5.37031300 0.15933600 4.64771000
C 0.28439900 2.01711800 2.01675700
C 0.72171700 3.33926300 2.19743800
C 0.99030800 0.97479900 2.64715700
C 1.82891000 3.61243200 3.00866700
H 0.21103300 4.16766300 1.70593800
C 2.08707400 1.25311600 3.46642100
H 0.68731700 -0.06440200 2.49802100
C 2.50907100 2.57422400 3.65036200
H 2.15846500 4.64692200 3.13578700
H 2.61851300 0.43201800 3.95429800
H 3.37059600 2.79237100 4.28693800
C -2.01249000 -2.76642400 -2.08671300
C -0.95256400 -3.68418300 -1.96185200
C -2.78810800 -2.77750700 -3.25625900
C -0.68581600 -4.60133700 -2.98003600
H -0.33353800 -3.69105400 -1.06119700
C -2.51550600 -3.69708300 -4.27625000
H -3.61541800 -2.07687600 -3.38115900
C -1.46721200 -4.61054500 -4.14157200
H 0.13692100 -5.31224600 -2.86566300
H -3.13309800 -3.69786300 -5.17841900
H -1.25835800 -5.32927000 -4.93845700
C -3.96675600 -0.87185400 -1.05103100
C -5.14551500 -1.35231600 -0.45923100
C -4.04540500 0.19410300 -1.96635600
C -6.37987400 -0.77902700 -0.78290300
H -5.11340700 -2.16578200 0.26668800
C -5.28089900 0.75988500 -2.29206800
H -3.13516200 0.58635000 -2.42771000
C -6.45160900 0.27470800 -1.69917400
H -7.28979200 -1.15952000 -0.31129900
H -5.32690200 1.58623400 -3.00617000
H -7.41824300 0.72056700 -1.94832200
C -2.38837000 -2.66215200 0.75310000
C -3.17149500 -3.83307000 0.73157100
C -1.61926500 -2.37709000 1.89164100

C -3.20237000 -4.68023800 1.84116200
H -3.75116500 -4.09449300 -0.15649500
C -1.64772400 -3.23145200 2.99955300
H -0.98668100 -1.48902200 1.91140100
C -2.44278300 -4.37985600 2.97829500
H -3.81702200 -5.58387700 1.81445200
H -1.04249800 -2.99701500 3.87905600
H -2.46506400 -5.04792500 3.84348400
Pd -0.55030500 0.14062200 -0.78030100
C 4.60216600 -5.08926800 3.34764800
H 5.58435900 -5.26652500 3.81899900
H 3.92042900 -4.75910800 4.14856100
H 4.23720000 -6.04878300 2.95350800

TS-5

P 0.80348400 0.80027700 -0.08560700
C -0.13745200 2.38158500 -0.33637700
C -0.20297800 3.05537900 -1.56606100
C -0.78696100 2.94004400 0.78006000
C -0.90208300 4.26348400 -1.67509300
H 0.29839600 2.65590200 -2.44818400
C -1.47851000 4.14790000 0.66864400
H -0.74772300 2.43632600 1.74889200
C -1.53886500 4.81437300 -0.56058000
H -0.93860900 4.77742900 -2.63945700
H -1.97274500 4.57009200 1.54762200
H -2.07905100 5.76096200 -0.64700800
C 1.88164200 1.29135200 1.32787200
C 2.66999700 2.45637800 1.25508100
C 1.85625500 0.56002800 2.52428800
C 3.44093900 2.85576800 2.34853900
H 2.67824300 3.06231200 0.34610000
C 2.62321200 0.96783000 3.62206300
H 1.22469300 -0.32459100 2.60430900
C 3.42172100 2.11036300 3.53385500
H 4.05400300 3.75814500 2.27740400
H 2.59092800 0.38864100 4.54863500
H 4.02275900 2.42786800 4.39025300
C 1.87417200 0.65806400 -1.58066200
C 3.26883100 0.81235300 -1.55536900
C 1.24970900 0.30611200 -2.79307700
C 4.02023100 0.64049400 -2.72390300
H 3.78594200 1.05498300 -0.62625700
C 2.00171100 0.14640900 -3.95929800
H 0.16927000 0.14355500 -2.82680600
C 3.39078300 0.31486300 -3.92791400
H 5.10622600 0.76077300 -2.68645800

H	1.50037200	-0.12043600	-4.89340600	H	0.84796400	4.98297400	2.13441100
H	3.98068400	0.18324200	-4.83892400	H	3.27848200	5.26879400	-1.42312800
Pd	-0.41190300	-1.11930700	0.18241000	H	2.07105500	6.37939800	0.45986400
C	-2.54236500	-0.32243200	0.15211500	C	3.13673700	0.15563700	-1.28064600
C	-2.98056500	-0.00973700	1.46292500	C	4.33594100	-0.55739700	-1.11934500
C	-3.05011000	0.49711600	-0.88045700	C	2.68741700	0.43020400	-2.58823000
C	-3.87011100	1.03619000	1.72762500	C	5.07803200	-0.96334300	-2.23542500
H	-2.63395700	-0.62007200	2.30547900	H	4.69912600	-0.81148700	-0.12241300
C	-3.94431500	1.54788000	-0.63592500	C	3.43651700	0.03659200	-3.69950900
H	-2.75528100	0.29894100	-1.91683000	H	1.74079000	0.95563400	-2.74289700
C	-4.35699400	1.82015100	0.67255600	C	4.63708800	-0.66204800	-3.52638100
H	-4.18911500	1.24210400	2.75418300	H	6.00802500	-1.51948900	-2.08864200
H	-4.32157200	2.15333600	-1.46577700	H	3.07570400	0.26911000	-4.70519200
H	-5.05642200	2.63761500	0.87124600	H	5.22099800	-0.97633500	-4.39569100
B	-2.73286700	-2.33266200	-0.33406400	C	2.98795600	0.31148100	1.66907200
O	-2.63976600	-2.39594000	-1.73597800	C	4.26336800	0.86970200	1.87839700
H	-3.41160500	-2.03200700	-2.18930600	C	2.39474800	-0.42786100	2.70428600
O	-1.57245400	-2.94500900	0.27413400	C	4.93572000	0.66852900	3.08612300
H	-1.73783100	-3.17950900	1.20120200	H	4.73466500	1.47237300	1.09797100
O	-3.91899400	-2.68190100	0.33589900	C	3.06514300	-0.62174100	3.91827500
C	-5.18690200	-2.35959400	-0.19099900	H	1.39386300	-0.84307200	2.56081200
H	-5.32515500	-2.75310800	-1.21538500	C	4.33853900	-0.07952400	4.10863400
H	-5.95905700	-2.81288800	0.45098800	H	5.92788200	1.10415200	3.23309800
H	-5.35906400	-1.26805700	-0.21498800	H	2.58708000	-1.19678200	4.71592500
C	1.31683100	-2.19232000	0.36930800	H	4.86467200	-0.23172600	5.05506400
C	1.58167400	-2.81115200	1.60796200	C	-3.16121000	0.14296000	1.25802400
C	2.10877900	-2.57071000	-0.72944500	C	-4.36866800	-0.54739500	1.06301800
C	2.60310700	-3.76127900	1.74500700	C	-2.72758800	0.38092200	2.57797000
H	0.98038300	-2.56610300	2.48925900	C	-5.13370300	-0.96638600	2.15860000
C	3.12938100	-3.52481400	-0.59715100	H	-4.72088000	-0.77317700	0.05542900
H	1.93376200	-2.12949300	-1.71368200	C	-3.49951000	-0.02507200	3.66898900
C	3.38536800	-4.12031000	0.64165600	H	-1.77491100	0.88694000	2.75807500
H	2.78468200	-4.22388500	2.72038000	C	-4.70786200	-0.70073800	3.46240300
H	3.72578700	-3.80186400	-1.47225100	H	-6.06972700	-1.50462900	1.98563500
H	4.18361200	-4.86075100	0.74639300	H	-3.15031400	0.17906900	4.68487500
TS-6				H	-5.30965000	-1.02521300	4.31563400
P	-2.01658800	0.62304400	-0.11177000	C	-2.05235500	2.48500100	-0.10102200
P	2.01916400	0.61720300	0.11718300	C	-2.72520000	3.26426600	0.85318200
C	2.05604600	2.47911100	0.13386200	C	-1.37091100	3.13803700	-1.14627800
C	1.36955100	3.11667600	1.18528500	C	-2.72036300	4.66219900	0.76084800
C	2.73896500	3.27191500	-0.80192300	H	-3.27017700	2.79095000	1.67149400
C	1.38042200	4.50748500	1.30634100	C	-1.37738000	4.53071000	-1.24353900
H	0.82945500	2.52033800	1.92628700	H	-0.83870500	2.55245300	-1.90136500
C	2.73834000	4.66806100	-0.68592700	C	-2.05208300	5.29958000	-0.28727400
H	3.28810900	2.81049700	-1.62427000	H	-3.25310900	5.25213900	1.51200900
C	2.06462800	5.28994100	0.36805000	H	-0.84917900	5.01824100	-2.06733600

H	-2.05536300	6.39045000	-0.36062200	H	-3.98047800	-0.51830600	-4.36380200
C	-2.95592500	0.33910500	-1.68568900	H	-7.30005600	-0.04019700	-1.64264300
C	-4.21905100	0.91592100	-1.91803500	H	-6.41599500	-0.75738400	-3.86404900
C	-2.35281700	-0.40482400	-2.71189300	C	-3.58710700	1.33863400	1.67950500
C	-4.87013800	0.72872100	-3.13957600	C	-4.63225400	2.18888600	2.08668500
H	-4.69717100	1.52224000	-1.14460100	C	-3.11915100	0.35950700	2.57103200
C	-3.00186700	-0.58503900	-3.93952000	C	-5.20473500	2.04674000	3.35388400
H	-1.36066900	-0.83425800	-2.55045400	H	-5.00145000	2.96999400	1.41858200
C	-4.26346000	-0.02411600	-4.15293500	C	-3.69388400	0.22008700	3.83868800
H	-5.85290700	1.17900400	-3.30443400	H	-2.29122000	-0.28830700	2.27808500
H	-2.51623500	-1.16384800	-4.72983900	C	-4.73863100	1.06154600	4.23162100
H	-4.77283800	-0.16538900	-5.11016200	H	-6.01662700	2.71306400	3.65763500
Pd	-0.00018800	-0.80133700	0.00688400	H	-3.31468400	-0.54412200	4.52223800
C	0.94713100	-2.66218100	-0.27808100	H	-5.18509200	0.95610800	5.22410300
C	1.16882300	-2.96225000	-1.64435800	C	-2.91574400	3.30284100	-0.32103300
C	1.80891500	-3.27925100	0.65744600	C	-3.62640300	3.83710000	-1.40631100
C	2.20719900	-3.80630600	-2.05117600	C	-2.21857500	4.17658700	0.53481200
H	0.51124900	-2.53709200	-2.40797600	C	-3.64828100	5.22088300	-1.62553200
C	2.84392000	-4.12664000	0.25206400	H	-4.17166200	3.18132300	-2.08764200
H	1.66167000	-3.10977100	1.72645200	C	-2.25034400	5.55524900	0.31925800
C	3.05411500	-4.39778800	-1.10633700	H	-1.64466200	3.77665600	1.37572900
H	2.35094300	-4.00633100	-3.11756000	C	-2.96582000	6.08219700	-0.76372200
H	3.49097600	-4.58326800	1.00776700	H	-4.20703000	5.62240400	-2.47531800
H	3.86033100	-5.06555200	-1.42210300	H	-1.70912400	6.22148600	0.99652600
C	-0.95655400	-2.65794200	0.28771300	H	-2.98616700	7.16180400	-0.93520400
C	-1.18029100	-2.95897000	1.65338500	C	0.71871300	-2.52932200	-0.93433200
C	-1.82168200	-3.26824100	-0.64917000	C	1.52660000	-3.59613600	-0.50785800
C	-2.22416900	-3.79706400	2.05850300	C	1.04569800	-1.86663600	-2.13254700
H	-0.52048800	-2.53899200	2.41796400	C	2.63347700	-3.99302000	-1.26634400
C	-2.86181000	-4.11011800	-0.24551100	H	1.29948800	-4.12412400	0.42039700
H	-1.67350500	-3.09738800	-1.71785900	C	2.14710700	-2.26934000	-2.89198000
C	-3.07422200	-4.38197800	1.11241800	H	0.43529500	-1.02468200	-2.47187200
H	-2.36967900	-3.99774400	3.12452200	C	2.94529200	-3.33348800	-2.45864700
H	-3.51144000	-4.56154900	-1.00212700	H	3.25627600	-4.82171500	-0.91840600
H	-3.88472200	-5.04516200	1.42686200	H	2.38941800	-1.74165900	-3.81809600
TS-oxcyc				H	3.81419000	-3.64250100	-3.04602700
P	-0.75440400	-1.92304700	0.01084700	C	-2.16970800	-2.84958500	-0.74018000
P	-2.80708100	1.48576700	0.01115400	C	-2.03095900	-3.68617500	-1.85917200
C	-4.00509300	0.74696700	-1.18422400	C	-3.44723600	-2.67934400	-0.17386400
C	-3.51290600	0.33060800	-2.43403800	C	-3.14506400	-4.34207400	-2.39713200
C	-5.37556900	0.60684900	-0.90917700	H	-1.05219000	-3.83588300	-2.31874800
C	-4.37672400	-0.20084900	-3.39566200	C	-4.55471600	-3.34318400	-0.70589800
H	-2.44497300	0.41875200	-2.65233700	H	-3.57970000	-2.02844100	0.69416400
C	-6.23603500	0.06656300	-1.87049100	C	-4.40734800	-4.17581200	-1.82191000
H	-5.78251900	0.91440100	0.05576500	H	-3.01949200	-4.99048200	-3.26864200
C	-5.74057900	-0.33514900	-3.11510400	H	-5.53861300	-3.20500200	-0.24982100

H	-5.27551000	-4.69141700	-2.24125400	C	-2.85757300	2.59545200	0.08267100
C	-0.58218000	-2.70848500	1.67631300	C	-3.64394500	2.16462400	-1.00125600
C	-1.00850300	-4.02322100	1.93813300	C	-3.43883500	3.42657500	1.05450800
C	0.01016800	-1.96347900	2.71187500	C	-4.97672800	2.56869800	-1.11946200
C	-0.84224800	-4.58205500	3.20896400	H	-3.20922900	1.50395600	-1.75680200
H	-1.47254400	-4.61938000	1.14931800	C	-4.77634800	3.82091700	0.94044700
C	0.17882000	-2.52938600	3.98066400	H	-2.85530200	3.77003300	1.91067200
H	0.33431200	-0.93215200	2.54035400	C	-5.54710600	3.39642600	-0.14637900
C	-0.24707400	-3.83718900	4.23287800	H	-5.57329100	2.22819900	-1.97006000
H	-1.17905500	-5.60503000	3.39828800	H	-5.21638500	4.46437400	1.70726300
H	0.64071900	-1.93883000	4.77666700	H	-6.59209100	3.70625700	-0.23299100
H	-0.11946000	-4.27495300	5.22675100	C	-0.54781100	2.29865300	1.88319800
Pd	-0.69012200	0.56675300	-0.17263700	C	-0.23949600	3.57382700	2.39195900
C	1.40052400	1.83264600	-0.43820300	C	-0.41990100	1.18220700	2.72764500
C	0.20412800	2.24255300	-0.75748700	C	0.17210600	3.72615800	3.71921500
C	2.74482300	2.21361100	-1.00205500	H	-0.31447900	4.45532000	1.75108000
H	2.85954300	1.90389000	-2.04893400	C	-0.01055500	1.33706300	4.05646700
H	2.87198700	3.31018000	-0.96512400	H	-0.62891000	0.18285400	2.33743100
N	3.81141100	1.61012000	-0.17828900	C	0.28485500	2.60932100	4.55497600
C	3.33976900	1.52072700	1.19861500	H	0.40878500	4.72306400	4.10102800
H	4.01417900	0.90029300	1.80794700	H	0.08539500	0.45818300	4.69963500
H	3.31400300	2.53150000	1.63924200	H	0.61032500	2.73109800	5.59169700
C	1.91575000	0.92070900	1.25941700	C	-0.19127100	3.36534000	-0.77979500
O	1.17970300	1.22102500	2.25251100	C	-0.83402900	4.35898900	-1.53556600
H	1.93154700	-0.13276800	0.90618200	C	1.21657200	3.32680300	-0.76998900
S	4.65745200	0.28789000	-0.78715100	C	-0.08379900	5.29132700	-2.26460400
O	4.23369500	-0.97423400	-0.14492200	H	-1.92398800	4.41597600	-1.56262500
O	4.58514700	0.38051000	-2.25826300	C	1.96138100	4.25985700	-1.49272800
C	6.34186600	0.60177700	-0.28139700	H	1.74286100	2.56412600	-0.19148400
C	6.95235100	-0.23754200	0.65132500	C	1.31261200	5.24607600	-2.24692400
C	7.03946000	1.66823300	-0.86500000	H	-0.60051700	6.05869400	-2.84782900
C	8.28113400	0.00509200	1.01287200	H	3.05319900	4.20247400	-1.47024600
H	6.40003500	-1.07124600	1.08756900	H	1.89456100	5.97419200	-2.81845600
C	8.36151000	1.89225100	-0.49244300	C	-2.66877200	-2.92146400	-1.43419300
H	6.55646400	2.31384700	-1.60173900	C	-2.83473900	-4.30739100	-1.27100300
C	9.00558400	1.06793700	0.45258400	C	-2.78894100	-2.36799200	-2.72213500
H	8.76158800	-0.64965400	1.74475300	C	-3.12149600	-5.11990500	-2.37298900
H	8.91057500	2.72307700	-0.94451800	H	-2.74326500	-4.76073200	-0.28159000
H	-0.23600900	3.06579100	-1.32694400	C	-3.08503400	-3.18089200	-3.82006200
C	10.43567700	1.33302500	0.84078200	H	-2.64495300	-1.29374900	-2.86747300
H	11.09646100	1.30016500	-0.04186300	C	-3.24975100	-4.55961100	-3.64813200
H	10.54376900	2.33893400	1.28080000	H	-3.24646300	-6.19703800	-2.23184600
H	10.80145700	0.59764000	1.57202100	H	-3.17883800	-2.73594000	-4.81439000
TS-LA				H	-3.47338900	-5.19705600	-4.50789800
P	-2.28476600	-1.78170900	-0.03116400	C	-3.94647100	-1.28634200	0.60361300
P	-1.09780800	2.03012000	0.13796400	C	-5.14602500	-1.70136300	0.00123200

C -4.00830200 -0.42365700 1.71471700
C -6.37877600 -1.26726800 0.50263400
H -5.12816300 -2.36872400 -0.86234400
C -5.24003900 -0.00161700 2.21943600
H -3.08805500 -0.08037300 2.19371100
C -6.43043500 -0.41993500 1.61253000
H -7.30280700 -1.59930200 0.02133800
H -5.26972400 0.66333200 3.08671000
H -7.39440200 -0.08365600 2.00371700
C -1.62014100 -2.89936800 1.28384500
C -2.41309000 -3.44643400 2.30700200
C -0.24919100 -3.21521500 1.24198200
C -1.84446100 -4.29004800 3.26794000
H -3.47997600 -3.22025400 2.35965800
C 0.31344400 -4.06540000 2.19743200
H 0.37897800 -2.79390800 0.45261200
C -0.48249200 -4.60200100 3.21588900
H -2.47315300 -4.70707900 4.05949600
H 1.37949200 -4.30354000 2.14955600
H -0.04097600 -5.26062100 3.96874100
Pd -0.69984600 -0.12054100 -0.71165500
C 3.37054700 -0.38655100 -3.76973600
C 2.11148800 -0.56289300 -3.77908500
H 1.27383900 -0.71994200 -4.45651800
C 4.36314700 -0.07895100 -2.72211000
H 5.06252000 -0.92930600 -2.59981600
H 4.96188700 0.80394000 -2.99196500
N 3.64431100 0.20784400 -1.45646100
C 2.56233900 -0.72109300 -1.12425900
H 2.89412400 -1.77257100 -1.20852400
H 2.24563600 -0.54755200 -0.08875100
C 1.35658000 -0.53232400 -2.05921700
O 0.41709800 -1.43280300 -2.00582800
H 1.03650900 0.52863400 -2.21578800
S 4.50020700 0.95168000 -0.22733400
O 5.21421300 2.08087400 -0.84866700
O 3.54336500 1.21358800 0.86404800
C 5.72926100 -0.19030200 0.39370000
C 7.01606100 -0.18537100 -0.15385300
C 5.37950100 -1.09373600 1.40692500
C 7.95754600 -1.10329800 0.31795900
H 7.28655200 0.53327600 -0.92940000
C 6.33372200 -2.00089800 1.86273300
H 4.37955500 -1.07945300 1.84414600
C 7.63618800 -2.02415100 1.32837100
H 8.96500500 -1.09785900 -0.10652900

H 6.06467400 -2.70328700 2.65668400
C 8.65297200 -3.00521400 1.84814500
H 9.59302700 -2.95704300 1.27971100
H 8.88438800 -2.80362300 2.90835300
H 8.26907200 -4.03750100 1.79820900

TS-TM

P 2.37857700 -1.19240500 -0.20040500
C 1.21158200 -2.54792000 -0.64196100
C 0.70518900 -3.44852500 0.30859900
C 0.74938400 -2.62669800 -1.96982800
C -0.22562200 -4.42408600 -0.06835200
H 1.02200000 -3.39157000 1.35125000
C -0.17312700 -3.60675000 -2.34359900
H 1.11518400 -1.92236700 -2.72182200
C -0.66116500 -4.51114300 -1.39340900
H -0.61041000 -5.11829800 0.68341600
H -0.51417800 -3.66100800 -3.38085300
H -1.38346700 -5.27806400 -1.68554700
C 3.80783300 -1.42459800 -1.35964100
C 4.02892200 -2.61914800 -2.06810300
C 4.74382700 -0.38072600 -1.47865700
C 5.15650500 -2.75995800 -2.88384200
H 3.32748100 -3.45100500 -1.98913600
C 5.87078700 -0.52806300 -2.29279400
H 4.59441000 0.55274600 -0.93463900
C 6.07916200 -1.71613100 -3.00034000
H 5.31291100 -3.69509600 -3.42846800
H 6.58779800 0.29336500 -2.37457200
H 6.95882600 -1.82881700 -3.63980200
C 3.12111800 -1.65941200 1.42439400
C 3.76469800 -2.89758900 1.60565600
C 3.09848300 -0.73850700 2.48359700
C 4.36132800 -3.20834000 2.82947900
H 3.80602600 -3.62279700 0.78922000
C 3.70042200 -1.05112900 3.70786800
H 2.61205100 0.23074500 2.34526100
C 4.32968400 -2.28619300 3.88303100
H 4.85744900 -4.17379500 2.96028000
H 3.67657600 -0.32457600 4.52435200
H 4.80056700 -2.53124200 4.83892000
Pd 1.44838400 0.98797200 -0.13642800
C -0.28280400 0.19628700 0.48656300
C -0.49806100 -0.17229000 1.76074200
C -1.35796100 0.05661600 -0.56618700
H -1.05950400 -0.71028900 -1.30234100
H -1.47590900 0.99028800 -1.13033000

N -2.68294500 -0.33357900 -0.02672900
C -2.63409200 -1.28389100 1.08823800
H -2.17566600 -2.21189500 0.70934400
H -3.65515200 -1.53585800 1.41266300
C -1.78679200 -0.77710200 2.26250000
O -1.45108400 -1.86121100 3.12967700
H -2.36126100 -0.02031500 2.83119100
S -3.88099100 0.83853000 0.03569200
O -3.69684800 1.69036300 -1.15563400
O -3.94763100 1.51138700 1.35193600
C -5.38622500 -0.10382800 -0.16818300
C -5.61962800 -0.75295700 -1.38821900
C -6.33058700 -0.13193400 0.85873900
C -6.81371400 -1.44600800 -1.56416700
H -4.87865900 -0.71627600 -2.18973900
C -7.52397700 -0.83332700 0.66209300
H -6.13742600 0.38781600 1.79852000
C -7.78557900 -1.50026400 -0.54452100
H -7.00114200 -1.95560200 -2.51353900
H -8.26507500 -0.85931800 1.46539500
H 0.27447100 -0.05857900 2.52892600
H -2.25626900 -2.13296300 3.59656700
C 0.58120800 3.02427500 -0.17696200
C 0.15135100 3.33993800 -1.49070900
C -0.24653300 3.47107900 0.87839400
C -1.01973500 4.06246100 -1.73676600
H 0.76278700 3.03078900 -2.34590300
C -1.42527800 4.18841000 0.64826400
H 0.04648800 3.26129500 1.91179100
C -1.81427500 4.48534100 -0.66318400
H -1.31892900 4.29384500 -2.76346400
H -2.04324600 4.51530100 1.48964300
H -2.73632500 5.04346200 -0.84965500
B 2.54291200 3.38803200 0.12361500
O 2.74861000 3.41080300 1.51746800
H 2.56998800 2.55423500 1.92954100
O 3.18810600 2.28132000 -0.57259800
H 3.24571200 2.44709900 -1.52697600
O 2.77148600 4.60882000 -0.54123400
C 2.33058000 5.82817000 0.01353600
H 2.69413300 5.97319100 1.04629500
H 2.71604300 6.65463300 -0.60546500
H 1.22708600 5.89843800 0.02759700
C -9.06823700 -2.25848000 -0.75873300
H -9.73078500 -2.19239300 0.11639900
H -9.61395200 -1.86999200 -1.63507200

H -8.86616500 -3.32467900 -0.95766800
TS-RE
P -1.16348800 2.22684000 0.01361800
P -2.63652600 -1.51557300 -0.43173300
C -4.20523400 -0.85515900 -1.18619900
C -4.06960800 -0.06696700 -2.34539700
C -5.49403900 -1.09978000 -0.68665600
C -5.19243300 0.44932800 -2.99489500
H -3.07554300 0.13762700 -2.75333800
C -6.61919300 -0.57148200 -1.33306200
H -5.63598800 -1.71227000 0.20534900
C -6.47408900 0.19994600 -2.48871000
H -5.06596800 1.05256200 -3.89798800
H -7.61540400 -0.77528900 -0.93043800
H -7.35429300 0.60638900 -2.99411200
C -3.22578400 -2.63896500 0.91247800
C -3.05623200 -4.03308400 0.90200200
C -3.77556200 -2.03608200 2.06172700
C -3.44841100 -4.80550000 2.00222200
H -2.61007600 -4.53003100 0.03927100
C -4.18063500 -2.81003800 3.15163200
H -3.88751300 -0.94918300 2.10860000
C -4.01790200 -4.20003800 3.12520200
H -3.30506500 -5.88925100 1.97625900
H -4.61535100 -2.32371400 4.02919400
H -4.32669300 -4.80648200 3.98096800
C -2.09779500 -2.62022300 -1.82016700
C -2.96350000 -3.56526500 -2.40282100
C -0.81213700 -2.45707400 -2.35962100
C -2.54046300 -4.34227200 -3.48385100
H -3.97799000 -3.69282800 -2.01688800
C -0.39099100 -3.23075900 -3.44806400
H -0.14077300 -1.71020900 -1.92774900
C -1.25219400 -4.17766600 -4.00817300
H -3.22205700 -5.07544000 -3.92389100
H 0.61273200 -3.08922200 -3.85786600
H -0.92487300 -4.78374200 -4.85743600
C 0.10049900 2.93410000 -1.13123100
C 1.20927700 3.67328500 -0.68472600
C 0.02410900 2.59297100 -2.49711000
C 2.19719700 4.08776400 -1.58714000
H 1.32255700 3.91799300 0.37252200
C 1.00713000 3.01425100 -3.39545800
H -0.81126500 1.99148700 -2.86592700
C 2.09714500 3.76785300 -2.94347700
H 3.05103900 4.66440700 -1.22096400

H 0.92333000 2.74800500 -4.45267800
H 2.86775000 4.09700200 -3.64571700
C -2.78036000 2.93445000 -0.57773500
C -2.91513100 3.87298400 -1.61300400
C -3.93281500 2.52888300 0.12122700
C -4.17419300 4.39153500 -1.94120800
H -2.04036900 4.21714800 -2.16743900
C -5.18529300 3.05778100 -0.19733100
H -3.84982600 1.79891700 0.93142200
C -5.31069400 3.99015100 -1.23419800
H -4.26086500 5.12179600 -2.75073100
H -6.06776800 2.73571300 0.36190000
H -6.29131400 4.40115100 -1.48897300
C -1.01578800 3.20249800 1.58566400
C -0.97607900 4.60948100 1.59315700
C -1.04722000 2.51998600 2.81158100
C -0.94526400 5.31119900 2.80058000
H -0.97726700 5.16610700 0.65269400
C -1.02686000 3.22404200 4.02171500
H -1.09826100 1.42843600 2.81623700
C -0.96948900 4.61982800 4.01836500
H -0.91046900 6.40414800 2.79113300
H -1.05500400 2.67655100 4.96772600
H -0.94982800 5.17165300 4.96218000
Pd -0.73210700 -0.16605200 0.39800200
C 1.29786000 -0.06439900 0.96978000
C 1.79747500 0.57802200 2.05310300
C 2.16234600 -0.16671500 -0.27739100
H 1.85975800 0.61264600 -0.99665500
H 2.03691600 -1.12409900 -0.79330700
N 3.60648100 0.03698600 -0.03037100
C 3.88925600 1.21706100 0.79232600
H 3.53152300 2.09169700 0.22671700
H 4.97565700 1.33638400 0.92230900
C 3.16720700 1.19480600 2.14790000
O 3.02355600 2.52963400 2.64672800
H 3.76887300 0.61084100 2.87272400
S 4.55853700 -1.31739200 0.24661500
O 4.00548600 -2.39871700 -0.59159500
O 4.74009400 -1.59069800 1.68878000
C 6.14819100 -0.83958200 -0.41734600
C 6.27155400 -0.62084500 -1.79632400
C 7.25292600 -0.74937100 0.43041600
C 7.52062200 -0.29658600 -2.31768800
H 5.40346400 -0.70253000 -2.45392800
C 8.49918200 -0.42282400 -0.11289700

H 7.14241900 -0.93401200 1.50015200
C 8.65514700 -0.19008600 -1.48783700
H 7.62222200 -0.12355900 -3.39279400
H 9.36607500 -0.35021300 0.54919300
H 1.22589900 0.62332400 2.98522200
H 3.89936100 2.84155000 2.92318000
C 0.30845300 -1.70130800 1.40508900
C -0.10598000 -1.81670900 2.75819600
C 0.81420100 -2.87035800 0.79456200
C -0.02457800 -3.02446300 3.44991800
H -0.48161800 -0.93504800 3.28558100
C 0.91403200 -4.07917000 1.49662500
H 1.14029900 -2.85388600 -0.24618600
C 0.49634000 -4.16924500 2.82680900
H -0.36331700 -3.07308500 4.48946900
H 1.31831200 -4.95997200 0.98784400
H 0.57288000 -5.11345100 3.37280700
C 9.99376300 0.16945300 -2.07524100
H 10.78930800 0.15071300 -1.31621200
H 10.27034700 -0.52676900 -2.88449500
H 9.96830100 1.17915300 -2.51976400

TS-endo(T-shape)

P 2.14974700 0.68701300 -0.03867900
P -0.98037700 -1.56719300 0.12457900
C -0.40012200 -2.41194300 -1.41310300
C -0.71473500 -1.79487400 -2.63995500
C 0.35655800 -3.59449300 -1.42525800
C -0.30723800 -2.36354900 -3.84871700
H -1.28308100 -0.86056500 -2.65092500
C 0.77435600 -4.15528300 -2.63833800
H 0.63178000 -4.08722000 -0.49190900
C 0.43965600 -3.54734300 -3.85108700
H -0.56735800 -1.87506100 -4.79164400
H 1.36618200 -5.07447400 -2.62987900
H 0.76551300 -3.98959300 -4.79638100
C -0.30751500 -2.52803000 1.55858200
C -0.66489000 -3.87307900 1.77404100
C 0.51526500 -1.88667000 2.49741600
C -0.18495000 -4.56287300 2.88996200
H -1.32797200 -4.38668700 1.07391700
C 0.98763100 -2.57645000 3.62031600
H 0.77946100 -0.83668400 2.35369200
C 0.64321700 -3.91636200 3.81557500
H -0.46621500 -5.60850400 3.04183300
H 1.62325100 -2.05989400 4.34450200
H 1.01124200 -4.45628500 4.69228900

C	-2.77009100	-2.03857000	0.24974700
C	-3.43757600	-2.81733100	-0.70804100
C	-3.48264500	-1.58497300	1.37541200
C	-4.79177900	-3.13533800	-0.54225200
H	-2.90908700	-3.18468900	-1.58970700
C	-4.82942000	-1.91144300	1.54288400
H	-2.98214200	-0.97012700	2.12934600
C	-5.49023900	-2.68618000	0.58139000
H	-5.29824900	-3.74331500	-1.29701600
H	-5.36776200	-1.55416100	2.42498600
H	-6.54654200	-2.93757100	0.70949900
C	2.57535000	2.01747200	-1.25988600
C	3.75030500	2.78532700	-1.18852500
C	1.66646100	2.26446300	-2.30484600
C	4.00836100	3.77550000	-2.14191700
H	4.47164500	2.62007200	-0.38588900
C	1.93101200	3.24806900	-3.26323900
H	0.74248400	1.68227700	-2.36604900
C	3.10193400	4.00832800	-3.18175500
H	4.92420600	4.36853200	-2.06972200
H	1.21517500	3.42446400	-4.07064000
H	3.30610100	4.78404200	-3.92478300
C	3.10485100	-0.77320300	-0.66285900
C	3.48575900	-0.88197700	-2.01121300
C	3.39445100	-1.84119500	0.20794600
C	4.14965900	-2.02386700	-2.47371600
H	3.27084900	-0.07305100	-2.71235000
C	4.06574300	-2.97592600	-0.25489700
H	3.10654700	-1.78739900	1.25983400
C	4.44644700	-3.07190300	-1.59806000
H	4.44074500	-2.08775600	-3.52577200
H	4.29124800	-3.78969900	0.43981900
H	4.97178400	-3.96002800	-1.95944700
C	3.05430500	1.17605200	1.49968500
C	4.42802700	0.94473300	1.69811700
C	2.32529600	1.82993300	2.50867100
C	5.05443200	1.36456600	2.87551700
H	5.01774200	0.43362100	0.93427700
C	2.95474100	2.25395800	3.68365500
H	1.25423800	2.00517800	2.37503700
C	4.32065200	2.02103000	3.86982100
H	6.12274400	1.17784500	3.01521000
H	2.37246500	2.76150400	4.45738400
H	4.81319400	2.34653900	4.79013800
Pd	-0.32032800	0.67473300	0.13298800
C	-1.96333200	1.90559400	0.11877200

C	-1.16016400	2.88604400	0.42986700
C	-3.39222300	4.19473500	1.01865500
C	-2.06075100	4.66471700	0.40755800
O	-1.36618400	5.50706400	1.02924800
H	-2.08830800	4.70058400	-0.71200600
H	-0.11906600	3.04228300	0.72659200
H	-3.17852200	3.87246400	2.05445700
H	-4.03569500	5.08884400	1.08915600
C	-4.10254300	3.11834500	0.24075600
C	-3.38775100	1.96700100	-0.19457800
C	-4.04817700	0.98478800	-0.95167200
C	-5.40279400	1.11353400	-1.26484900
C	-6.11277700	2.23528300	-0.82574900
C	-5.46044000	3.22828800	-0.08635600
H	-3.48590500	0.11837200	-1.30112700
H	-5.90191300	0.33973800	-1.85404400
H	-7.17403500	2.34433600	-1.06579900
H	-6.01665700	4.11110000	0.24232700

TS-L2-endo(Y-shape)

P	-2.16709900	1.78207700	-0.00774200
P	-1.02186100	-2.11376800	-0.15735100
C	-2.83142700	-2.48264600	-0.39420500
C	-3.59928000	-1.63233300	-1.20989900
C	-3.46211900	-3.59586700	0.19032400
C	-4.95066100	-1.89660600	-1.45227300
H	-3.14163900	-0.74991100	-1.65910100
C	-4.81712400	-3.85389600	-0.04367100
H	-2.90162400	-4.27374700	0.83588900
C	-5.56541600	-3.00847900	-0.86809900
H	-5.52599400	-1.22314200	-2.09318200
H	-5.28796600	-4.72324700	0.42374500
H	-6.62422800	-3.21178900	-1.05010700
C	-3.76946300	1.25444800	0.77399700
C	-5.04023100	1.65385200	0.32554500
C	-3.69143900	0.40971400	1.89690000
C	-6.19716000	1.22688400	0.98676000
H	-5.14368900	2.29539100	-0.55049200
C	-4.84697300	-0.00792700	2.56432300
H	-2.71516700	0.06534100	2.24793000
C	-6.10535000	0.39873600	2.10966200
H	-7.17642300	1.54488100	0.61809600
H	-4.76194500	-0.66224200	3.43625200
H	-7.01095100	0.06668800	2.62465400
Pd	-0.34438900	0.11824100	0.18467800
C	1.62223500	-0.10383100	0.73847000
C	1.69918900	1.18620700	0.74813600

C 2.55173300 -1.14505400 1.26663300
H 2.04857000 -1.73785500 2.04953800
H 2.84483900 -1.85828200 0.48619800
N 3.75461300 -0.53284600 1.85005300
C 3.53988400 0.59157000 2.75209300
H 2.80948500 0.28396100 3.51924900
H 4.48438800 0.81061000 3.27434600
C 3.04383800 1.91087200 2.14309800
O 2.42497200 2.70615600 2.88669600
H 3.68232600 2.30171000 1.31861600
S 5.24864600 -0.81513200 1.16613000
O 6.24699800 -0.40599600 2.16814900
O 5.22429900 -2.20825000 0.68823500
C 5.47720500 0.23201300 -0.27108300
C 6.11947900 1.46558800 -0.12837900
C 5.00843900 -0.19490100 -1.52024600
C 6.27727600 2.28351000 -1.24950900
H 6.50193800 1.78197500 0.84351800
C 5.17262500 0.63733000 -2.62639600
H 4.53375200 -1.17122300 -1.63202100
C 5.80522900 1.88965200 -2.51251300
H 6.78308500 3.24640900 -1.13879800
H 4.80896700 0.30403600 -3.60254300
H 1.22788200 2.10038600 0.39519900
C 5.97835700 2.76867300 -3.72255600
H 6.60742300 2.27322300 -4.48172000
H 5.00724100 2.97747100 -4.20179000
H 6.44819500 3.72858200 -3.46342900
C -1.86547000 3.43213500 0.88021100
C -1.48609500 3.21401800 2.35752000
C -0.81852200 4.30704300 0.16540500
H -2.83599800 3.95889700 0.85075800
C -1.25074500 4.54537700 3.08703600
H -0.56238200 2.61130900 2.41279500
H -2.27160500 2.64100800 2.87570400
C -0.57777000 5.62942900 0.90979100
H 0.13678300 3.75907000 0.09495200
H -1.13145200 4.51803500 -0.86844400
C -0.19628800 5.39942700 2.37545000
H -0.94489700 4.34358900 4.12804200
H -2.20212400 5.10655700 3.14281500
H 0.20875400 6.20398900 0.39079200
H -1.49596000 6.24407900 0.86314100
H -0.06785700 6.36488200 2.89469000
H 0.77813300 4.88025100 2.42281000
C -0.26695500 -2.99986300 -1.64509300

C -0.69335400 -2.35751000 -2.97918500
C 1.26811100 -3.08220100 -1.56739800
H -0.68240400 -4.02267400 -1.61319700
C -0.11009600 -3.11837200 -4.17952300
H -0.33939600 -1.31094900 -3.00372600
H -1.78985500 -2.32515300 -3.06538500
C 1.85240700 -3.84728900 -2.76441500
H 1.67852700 -2.05759000 -1.55803000
H 1.58839500 -3.56134100 -0.62987400
C 1.41520500 -3.23488700 -4.09876100
H -0.40928100 -2.61456400 -5.11469100
H -0.55283500 -4.13093700 -4.21480900
H 2.95330300 -3.86244700 -2.68927800
H 1.52172500 -4.90135200 -2.71866800
H 1.79971900 -3.83459800 -4.94165200
H 1.86244500 -2.22848500 -4.20032500
C -2.60913000 2.32667000 -1.72350700
C -3.40742400 3.45351800 -2.00327900
C -2.07555800 1.60150000 -2.80327700
C -3.67850700 3.82528900 -3.32333200
H -3.81763100 4.05817700 -1.19160500
C -2.34804100 1.97252500 -4.12501700
H -1.43229700 0.74027900 -2.60520500
C -3.15318600 3.08385900 -4.38787800
H -4.30052200 4.70267200 -3.52077700
H -1.92356500 1.39289600 -4.94922200
H -3.36585000 3.37796800 -5.41931800
C -0.59735900 -3.18753600 1.29281900
C -0.28187100 -4.55425300 1.18707600
C -0.62049600 -2.60084600 2.57103400
C 0.00924500 -5.30836000 2.32933600
H -0.26482300 -5.04808900 0.21360500
C -0.34322200 -3.35777600 3.71337000
H -0.84942100 -1.53601500 2.67068400
C -0.02272100 -4.71419100 3.59469700
H 0.25887700 -6.36800300 2.22675700
H -0.36955900 -2.88291100 4.69786700
H 0.20405400 -5.30599400 4.48569900

TS-L2-endo(T-shape)

P 0.08697900 -2.59232900 0.12602400
P 2.41411500 1.46272000 -0.22660000
Pd 1.02947700 -0.38395700 0.38248500
C 1.36246900 -3.82660500 -0.50178000
C 1.90049300 -3.43284700 -1.88999900
C 2.52028500 -3.98834900 0.50155400
H 0.83822400 -4.79254400 -0.60624700

C	2.94494000	-4.44098300	-2.39149700	C	-5.34280900	0.90593400	-2.51009500
H	2.35770400	-2.42802400	-1.82993100	H	-3.48946700	1.97011600	-2.18460300
H	1.07617300	-3.36013300	-2.61713200	C	-6.57843500	0.49285100	-1.97739000
C	3.56445600	-4.99590600	-0.00117500	H	-7.84530100	0.55249500	-0.22370200
H	3.00181100	-3.00418700	0.64977700	H	-5.08862300	0.64860600	-3.54207500
H	2.14201500	-4.30260700	1.48731500	H	0.39191700	0.52134000	3.56338300
C	4.09157600	-4.62460900	-1.39142600	H	-3.35250900	0.04499800	2.30401800
H	3.33633300	-4.11186800	-3.36948100	H	-4.09626200	1.57498900	2.82966200
H	2.45202600	-5.41555900	-2.56465100	H	-1.23271200	1.73626100	-0.21547000
H	4.39590300	-5.05913500	0.72169300	H	-2.03947000	0.18620100	0.11532300
H	3.10726000	-6.00198800	-0.04008400	C	-7.53810500	-0.30875100	-2.81588500
H	4.79526300	-5.39416500	-1.75273400	H	-8.46428400	-0.53681600	-2.26854000
H	4.66705100	-3.68290900	-1.32169800	H	-7.80678000	0.23482200	-3.73729300
C	4.08010800	0.91677500	-0.92278500	H	-7.08126600	-1.26236300	-3.13070900
C	5.01323600	2.04677300	-1.39128600	C	-0.67887900	-3.44767800	1.58394800
C	4.80450000	-0.01135700	0.07176200	C	-0.64895800	-4.84028800	1.78820100
H	3.79861200	0.30464800	-1.79824000	C	-1.33606400	-2.64823300	2.53613600
C	6.30889900	1.48268900	-1.99595300	C	-1.26432300	-5.40888300	2.90899900
H	5.27001300	2.68695100	-0.52984000	H	-0.14846100	-5.49836500	1.07556800
H	4.50806000	2.69253200	-2.12666900	C	-1.95599400	-3.21656600	3.65298400
C	6.10415400	-0.56786700	-0.52774400	H	-1.35226400	-1.56509700	2.41502500
H	5.04263600	0.55136200	0.99200700	C	-1.92169100	-4.60108300	3.84324600
H	4.13937900	-0.83864600	0.37161900	H	-1.22885500	-6.49264400	3.05063500
C	7.03179500	0.54907400	-1.01897300	H	-2.45375600	-2.56238600	4.37392800
H	6.97003100	2.31467500	-2.29378800	H	-2.40004800	-5.05026400	4.71794500
H	6.06745300	0.92808900	-2.92164000	C	-1.24062700	-2.69463700	-1.16737300
H	6.61859000	-1.19435500	0.22100100	C	-2.14113000	-3.77146800	-1.25095900
H	5.85536600	-1.23308500	-1.37520600	C	-1.32242700	-1.66991800	-2.12691400
H	7.93083000	0.11891700	-1.49298700	C	-3.09385700	-3.82323000	-2.27331100
H	7.38563600	1.13580800	-0.15081900	H	-2.10628600	-4.57858200	-0.51585800
C	-0.46816500	0.68006300	1.48833900	C	-2.27169800	-1.72550600	-3.15322800
C	-0.27934600	0.75431300	2.74470400	H	-0.63363000	-0.82203400	-2.06686500
C	-1.59627400	1.08246000	0.58738200	C	-3.16064700	-2.80237600	-3.22808000
N	-2.60942800	1.81124000	1.37298900	H	-3.78770800	-4.66701000	-2.32312500
C	-3.14513200	1.10534100	2.53160800	H	-2.31685500	-0.92218500	-3.89355000
C	-2.25513900	1.19540600	3.76661300	H	-3.90599800	-2.84575700	-4.02699600
O	-2.35083700	0.36138600	4.67527600	C	2.87571300	2.67080700	1.09580000
H	-1.85186800	2.21683200	3.95547200	C	3.18897500	4.02020800	0.84859300
S	-3.59916500	2.89628800	0.56683400	C	2.97535800	2.18588200	2.41238000
O	-4.35720800	3.61458600	1.60357900	C	3.58476500	4.86054100	1.89370700
O	-2.72766700	3.65301800	-0.34706300	H	3.12508900	4.42504300	-0.16325900
C	-4.76912000	1.98072800	-0.43202000	C	3.38166100	3.02502900	3.45550100
C	-5.99389800	1.59391100	0.12213900	H	2.73259100	1.14116200	2.62264500
C	-4.43705300	1.64529100	-1.75133900	C	3.68298100	4.36574800	3.19894400
C	-6.88625800	0.85193400	-0.65474500	H	3.82107800	5.90760100	1.68493600
H	-6.25832900	1.87986700	1.14163400	H	3.45502000	2.62956700	4.47222400

H	3.99251900	5.02534500	4.01426000	H	4.72115100	0.06595200	3.24249400
C	1.64053600	2.47522900	-1.56501400	C	3.29158600	1.40095800	2.38063500
C	0.70894200	3.48205400	-1.24663100	O	2.83178700	2.16187900	3.25853800
C	1.85697800	2.17012100	-2.92269000	H	3.86637800	1.82011900	1.52301700
C	0.03305800	4.17657100	-2.25491300	S	5.16949700	-1.34135400	0.91600500
H	0.49923900	3.72984000	-0.20372300	O	6.25788400	-1.31855100	1.90726500
C	1.17915300	2.86597900	-3.92869800	O	4.92676900	-2.56635100	0.13326300
H	2.55436500	1.38085300	-3.21054000	C	5.49195700	-0.01711100	-0.24814400
C	0.26735100	3.87407700	-3.60001400	C	6.40650000	0.98551000	0.08486100
H	-0.68655100	4.95267900	-1.98248900	C	4.82236200	-0.00111900	-1.47896000
H	1.36757200	2.61589100	-4.97642900	C	6.64044100	2.02157400	-0.82298400
H	-0.26060200	4.41828200	-4.38767000	H	6.93689700	0.95516700	1.03796700
TS-L3-endo(Y-shape)							
P	-1.18445500	-2.12310700	-0.17113900	C	5.06810800	1.04151500	-2.37009300
P	-1.95334600	1.92681700	-0.02672700	H	4.12591400	-0.79766100	-1.74613400
C	-3.75041300	1.60138800	-0.38860300	C	5.97686100	2.07158100	-2.05935000
C	-4.41400800	0.64336400	0.40140600	H	7.35801700	2.80460000	-0.56373400
C	-4.48575000	2.23280500	-1.40924100	H	4.54849500	1.05359500	-3.33237600
C	-5.76464300	0.34448700	0.20043900	H	1.27632800	1.88837000	0.87131000
H	-3.86436400	0.11361300	1.18053100	C	6.22972900	3.18525900	-3.04042700
C	-5.83525600	1.92613500	-1.61992500	H	6.94134900	3.92331300	-2.64260500
H	-4.02052100	2.97166500	-2.06129100	H	6.63715400	2.79104600	-3.98695100
C	-6.48265200	0.98620100	-0.81365400	H	5.29283900	3.71018100	-3.29197100
H	-6.25347100	-0.40132000	0.83338300	C	0.08757900	-3.24780200	-0.99927900
H	-6.38113200	2.43042800	-2.42226600	C	-0.40777900	-4.65968000	-1.36181200
H	-7.53741300	0.74990600	-0.97861900	C	0.74074100	-2.57220100	-2.21951200
C	-2.59388600	-2.17242800	-1.37675200	H	0.86349000	-3.35034600	-0.22231000
C	-3.61734600	-3.13780000	-1.34275400	C	0.72843400	-5.51708100	-1.94337800
C	-2.61097000	-1.21974500	-2.41176100	H	-1.21963100	-4.58504700	-2.10615900
C	-4.62603400	-3.14457200	-2.31232600	H	-0.83235800	-5.16557000	-0.48021100
H	-3.63946600	-3.89923900	-0.56117400	C	1.87589400	-3.43090600	-2.79709000
C	-3.60965600	-1.23617000	-3.39034300	H	-0.02202100	-2.41247600	-3.00254100
H	-1.83466200	-0.45114000	-2.44842400	H	1.12021800	-1.57464500	-1.94336100
C	-4.62398900	-2.19752300	-3.34109800	C	1.39581500	-4.84379000	-3.14710300
H	-5.41558700	-3.89967400	-2.26320000	H	0.33487600	-6.50862000	-2.22664300
H	-3.59898200	-0.48872500	-4.18830200	H	1.48663100	-5.69468900	-1.15834300
H	-5.41189200	-2.20667100	-4.09922500	H	2.29827700	-2.93653800	-3.68892000
Pd	-0.37155700	0.02103500	0.35082400	H	2.69593300	-3.49647400	-2.05814300
C	1.56242800	-0.35147100	0.91419800	H	2.23883600	-5.45659200	-3.51021200
C	1.73005800	0.92066600	1.07300600	H	0.66982200	-4.78498200	-3.97948300
C	2.46477300	-1.49825900	1.22704400	C	-1.78064200	-3.13125800	1.30109700
H	1.99991600	-2.15082200	1.98555500	C	-0.63595300	-3.47251900	2.27541800
H	2.63570300	-2.12761300	0.34482300	C	-2.92674600	-2.43108300	2.05618900
N	3.75908900	-1.03464700	1.74751700	H	-2.16571000	-4.08100400	0.89346900
C	3.71965900	-0.01637700	2.79019600	C	-1.13616100	-4.31969600	3.45524600
H	3.03567500	-0.35650600	3.58582300	H	-0.20005900	-2.53447600	2.66247400
				H	0.17363100	-4.00988800	1.75792900

C	-3.42731800	-3.27588700	3.23680500	P	-1.87862900	-2.21541100	0.00807800
H	-2.56330100	-1.45784700	2.43189400	Pd	-1.12160800	0.08765700	0.21018300
H	-3.76340000	-2.21445600	1.37491600	C	-0.86193100	2.77368100	-2.14225300
C	-2.29156500	-3.64109000	4.19790800	C	0.54166900	2.30078800	-2.57050200
H	-0.29899000	-4.51919100	4.14605500	C	-1.94121500	2.13260300	-3.03832500
H	-1.47143700	-5.30377600	3.07858400	H	-0.91874900	3.86680100	-2.27891400
H	-4.22338200	-2.72919700	3.77100200	C	0.80568200	2.57149500	-4.05843100
H	-3.89072100	-4.20222700	2.84943600	H	0.62518000	1.21621300	-2.37847200
H	-2.66559600	-4.29428600	5.00506900	H	1.31852800	2.78754900	-1.95953900
H	-1.91903000	-2.72131700	4.68608800	C	-1.67123400	2.39555900	-4.52751600
C	-1.39691400	2.94839200	-1.52274400	H	-1.96215800	1.04251200	-2.85566400
C	-1.78645800	4.44106400	-1.53716300	H	-2.94092900	2.51382700	-2.77728900
C	0.10900400	2.79302000	-1.81963400	C	-0.27022000	1.94019000	-4.94789500
H	-1.92931000	2.44867400	-2.35179000	H	1.80460400	2.19049300	-4.33241400
C	-1.41621800	5.09930200	-2.87570500	H	0.82934700	3.66337400	-4.23207300
H	-1.25286200	4.96609100	-0.72747900	H	-2.43985100	1.88878400	-5.13617500
H	-2.86022100	4.57906300	-1.33889300	H	-1.77796700	3.47767500	-4.72866200
C	0.48730300	3.45544100	-3.15248400	H	-0.08815700	2.18885800	-6.00764700
H	0.69836900	3.25168100	-1.00634300	H	-0.20649300	0.83882300	-4.86911000
H	0.38139100	1.72474600	-1.83768200	C	-2.89719100	3.12467500	-0.00290700
C	0.07230400	4.93018700	-3.19855200	C	-3.32384100	2.94241500	1.46632600
H	-1.68389000	6.16977700	-2.84839600	C	-3.10380300	4.58137000	-0.45392800
H	-2.02020600	4.64661300	-3.68392800	H	-3.54625400	2.47476100	-0.61686600
H	1.57360500	3.35624500	-3.32121200	C	-4.77146300	3.40239500	1.69309300
H	-0.00834000	2.91171900	-3.97829500	H	-2.65580600	3.53094000	2.11972400
H	0.30247000	5.36294700	-4.18747200	H	-3.20760000	1.88732300	1.76594900
H	0.66955100	5.49885100	-2.46155500	C	-4.55142700	5.04236300	-0.21957100
C	-2.07235400	3.16512000	1.40887800	H	-2.41940900	5.23861600	0.11106400
C	-2.80010600	2.59287600	2.64052900	H	-2.84994100	4.70174400	-1.51883600
C	-0.69079500	3.70293600	1.82906300	C	-4.98481800	4.85017600	1.23743100
H	-2.67389800	4.00475700	1.02000800	H	-5.03292400	3.29199100	2.75962200
C	-2.91038900	3.63452600	3.76533400	H	-5.45577000	2.73878700	1.13249500
H	-2.24794900	1.70930200	3.01078100	H	-4.65526000	6.10055000	-0.51579600
H	-3.80948100	2.24741100	2.37303700	H	-5.22604800	4.46585400	-0.87942900
C	-0.80461900	4.75870800	2.93868500	H	-6.04192200	5.14080600	1.36472300
H	-0.07747000	2.86777100	2.20621500	H	-4.39426100	5.52521500	1.88462200
H	-0.15081600	4.12510200	0.96780700	C	-3.57064800	-2.40458800	0.80171900
C	-1.54663600	4.20905200	4.16076300	C	-3.51423500	-2.02426200	2.29559400
H	-3.40523100	3.17959000	4.64083100	C	-4.63627600	-1.56243400	0.07156900
H	-3.56819700	4.45724300	3.42852800	H	-3.86651000	-3.46406700	0.72066800
H	0.20562000	5.09963600	3.22375400	C	-4.88904200	-2.14587700	2.96722100
H	-1.33865700	5.64567300	2.55023000	H	-3.15574800	-0.98219700	2.38264800
H	-1.66849400	4.99593500	4.92514300	H	-2.78024500	-2.65067400	2.82750600
H	-0.93649100	3.41232900	4.62539500	C	-6.00998800	-1.67656200	0.74957400
TS-L3-endo(T-shape)				H	-4.31743100	-0.50366000	0.06237200
P	-1.17452500	2.41549600	-0.32302800	H	-4.72272200	-1.87285500	-0.98165900

C	-5.95051600	-1.31592700	2.23759000	H	3.15090200	1.42492800	2.45826500
H	-4.81476500	-1.83378700	4.02318500	H	4.47234000	0.26535600	2.63392600
H	-5.19755800	-3.20781800	2.97637600	H	1.79250200	-0.27085900	-0.54200200
H	-6.73504100	-1.03025800	0.22546300	H	1.89694900	1.32926900	0.20555600
H	-6.38085300	-2.71267100	0.64086600	C	9.24016200	1.24568400	-1.44921300
H	-6.93961300	-1.45902200	2.70588600	H	10.06954800	1.09513800	-0.74296900
H	-5.70706000	-0.24220400	2.34248200	H	9.54411400	0.83726200	-2.42807000
C	-2.12884100	-2.76813600	-1.77943300	H	9.09739900	2.33050500	-1.58835300
C	-0.82326800	-2.66111700	-2.59023600	C	-0.06625000	3.59536500	0.58424600
C	-2.77491700	-4.15202500	-1.96591600	C	0.51101900	4.73811500	-0.00090800
H	-2.82303400	-2.00350100	-2.17258800	C	0.19034100	3.34353800	1.94585000
C	-1.05499300	-2.97754300	-4.07484800	C	1.32052900	5.59661300	0.75104800
H	-0.07853000	-3.36909300	-2.18515600	H	0.33437600	4.97355700	-1.05180500
H	-0.39165200	-1.65240600	-2.47847500	C	0.99211800	4.20693200	2.69984800
C	-3.00121100	-4.46991900	-3.45289200	H	-0.23293600	2.45654000	2.42081400
H	-2.11717900	-4.92344600	-1.52783800	C	1.56323800	5.33551500	2.10329700
H	-3.73416900	-4.21243200	-1.42740300	H	1.76159400	6.47654400	0.27444700
C	-1.70836600	-4.35082100	-4.26689700	H	1.17682800	3.98819500	3.75521200
H	-0.09622900	-2.92834800	-4.61933600	H	2.19654800	6.00759500	2.68883700
H	-1.70535300	-2.19877100	-4.51484100	C	-0.86831700	-3.58907200	0.73896300
H	-3.42766900	-5.48289800	-3.55458200	C	0.53259300	-3.50266600	0.63848400
H	-3.75484400	-3.77151900	-3.86179400	C	-1.41935200	-4.72085200	1.36926400
H	-1.91058900	-4.53349800	-5.33643600	C	1.35870300	-4.51133900	1.14434200
H	-1.00132700	-5.13735000	-3.94321700	H	0.99132100	-2.63692100	0.16039900
C	0.70430200	-0.06110300	1.31402700	C	-0.59353500	-5.72703100	1.88297600
C	0.59810100	-0.34688300	2.55015600	H	-2.50065700	-4.83386400	1.46536300
C	1.87291500	0.24760200	0.41991300	C	0.79719500	-5.62683900	1.77278500
N	3.14065200	-0.13186400	1.05812100	H	2.44332100	-4.40806100	1.05674900
C	3.39439500	0.35170700	2.40729900	H	-1.04378300	-6.59580900	2.37140300
C	2.65342000	-0.37679600	3.52919100	H	1.43976700	-6.41339400	2.17794100
O	2.54333800	0.14986700	4.64230500	TS-L4-endo(Y-shape)			
H	2.59363600	-1.48156600	3.40262700	P	-0.86628700	2.30220600	0.08732000
S	4.07709100	-1.37455300	0.46314000	P	-2.00968100	-1.81475000	-0.07102900
O	4.42644900	-2.28989400	1.56735000	Pd	-0.26026500	0.02959000	-0.29214900
O	3.38349200	-1.91503100	-0.72105900	C	-1.48053800	3.10242100	-1.51020200
C	5.59878200	-0.61435800	-0.08905600	C	-0.34868000	3.30328400	-2.53986300
C	6.76111400	-0.75245900	0.67212700	C	-2.62154100	2.29192400	-2.15776200
C	5.60053300	0.11058700	-1.28899800	H	-1.87086100	4.09662900	-1.23208200
C	7.93896000	-0.14439700	0.22732900	C	-0.86243800	3.97033300	-3.82534900
H	6.75082500	-1.33399800	1.59519300	H	0.08711400	2.31952300	-2.79084400
C	6.78412700	0.70693900	-1.71476800	H	0.46640400	3.91200600	-2.12149600
H	4.69097000	0.20371400	-1.88636700	C	-3.14397400	2.96060400	-3.43755600
C	7.97253500	0.59324900	-0.96576900	H	-2.24089100	1.28389800	-2.40248500
H	8.85016900	-0.25162600	0.82180800	H	-3.45028000	2.14753200	-1.45132500
H	6.79029300	1.27174900	-2.65128200	C	-2.02248200	3.19293700	-4.45437000
H	-0.09222500	-0.58973600	3.35084600	H	-0.03145800	4.07064500	-4.54484200

H	-1.19655600	4.99794700	-3.59012500	C	-0.05296600	-5.53959200	-0.93388200
H	-3.94203700	2.33985300	-3.88028900	H	0.54507300	-3.61798900	-0.14587500
H	-3.61022000	3.92939700	-3.17816000	H	-0.64308000	-4.45901300	0.84248500
H	-2.40804500	3.72725600	-5.33990100	C	0.27098500	-5.31011100	-2.41324800
H	-1.65163200	2.21540000	-4.81484800	H	-0.59337300	-4.33444100	-4.15856800
C	-2.10576100	2.78562200	1.45746800	H	-1.76805200	-5.17393000	-3.13473000
C	-3.50749100	3.25755700	1.02810800	H	0.78650100	-6.04879400	-0.42940700
C	-2.21004400	1.69843400	2.54321000	H	-0.92239000	-6.21852800	-0.85333500
H	-1.62178900	3.65774200	1.92548400	H	0.45159900	-6.27410300	-2.91986600
C	-4.31404800	3.75235700	2.23976300	H	1.20599300	-4.72743800	-2.49944100
H	-4.05777200	2.43052800	0.55160900	C	-2.41460500	-2.23118100	1.72574000
H	-3.43717800	4.06485100	0.28303700	C	-3.21757800	-3.51722500	2.00286300
C	-3.02595700	2.18454300	3.75045400	C	-1.16081800	-2.15512000	2.62503100
H	-2.68874400	0.80286900	2.11470100	H	-3.05336500	-1.37868900	2.01547700
H	-1.20588700	1.38680300	2.87216400	C	-3.56314200	-3.65375700	3.49494300
C	-4.41348500	2.68585200	3.33563300	H	-2.63522000	-4.40037100	1.68969200
H	-5.32171200	4.06143700	1.91176500	H	-4.14495600	-3.52824600	1.41129100
H	-3.82973800	4.65635600	2.65362500	C	-1.52056000	-2.29717800	4.11085000
H	-3.11710300	1.37141700	4.49130000	H	-0.45161300	-2.95461500	2.35224800
H	-2.47808400	3.00335200	4.25302000	H	-0.63493500	-1.20174400	2.45023100
H	-4.95524100	3.08459200	4.21076900	C	-2.31699100	-3.57796800	4.38322900
H	-5.01087600	1.83420900	2.96029300	H	-4.10042500	-4.60284100	3.66582400
C	0.59393400	3.40084300	0.57770600	H	-4.26132300	-2.84473900	3.78014600
C	0.31992900	4.91833600	0.62368700	H	-0.60055700	-2.27891500	4.72054700
C	1.24859600	2.93081500	1.89225500	H	-2.12086200	-1.42314000	4.42497300
H	1.32146100	3.22946600	-0.22922800	H	-2.60133700	-3.63427200	5.44830300
C	1.60373200	5.70626800	0.93301800	H	-1.67395200	-4.45582700	4.18450900
H	-0.42790400	5.14617500	1.40291100	C	-3.68732600	-1.47601300	-0.91187200
H	-0.10413800	5.27026200	-0.32966200	C	-4.55053800	-2.67346300	-1.36176700
C	2.52683700	3.72425100	2.20393500	C	-4.54326300	-0.49440900	-0.09062400
H	0.53769900	3.06212800	2.72733500	H	-3.37260400	-0.94254700	-1.82716400
H	1.47384000	1.85264000	1.84001500	C	-5.79249300	-2.20481200	-2.13836700
C	2.26513400	5.23411900	2.23193300	H	-4.87608900	-3.25435700	-0.48247000
H	1.37163700	6.78395300	0.98936700	H	-3.97667100	-3.36168400	-1.99864700
H	2.31564100	5.58375900	0.09586100	C	-5.78336600	-0.02537400	-0.86495400
H	2.94606000	3.38913600	3.16852600	H	-4.87651700	-0.98581000	0.84029200
H	3.29147800	3.50162400	1.43752600	H	-3.93943700	0.37330000	0.21180600
H	3.20668600	5.78344700	2.40475400	C	-6.63468800	-1.20838700	-1.33629300
H	1.60233700	5.47308900	3.08470400	H	-6.40053300	-3.08084900	-2.42367000
C	-1.50545500	-3.44831000	-0.89335200	H	-5.46864800	-1.72971100	-3.08315300
C	-1.17317200	-3.22561500	-2.38509400	H	-6.38241000	0.65205400	-0.23186800
C	-0.37197300	-4.22815300	-0.19738700	H	-5.46423000	0.56630700	-1.74231400
H	-2.40286400	-4.08634200	-0.83792500	H	-7.48851000	-0.85318900	-1.93892300
C	-0.85939900	-4.54387600	-3.10798100	H	-7.06484700	-1.72108600	-0.45562000
H	-0.29730300	-2.55969100	-2.46791200	C	1.71656800	0.20698200	-0.84903400
H	-2.00192700	-2.71081300	-2.89719600	C	1.74523600	-1.07737800	-0.97289900

C	2.74060000	1.23713700	-1.19676000	H	-0.89642000	-4.20422300	-3.55623600
H	2.34694700	1.91560700	-1.97322800	H	-3.11442900	-4.80263600	-2.61855300
H	2.98378200	1.86693700	-0.33270900	H	-3.09069100	-3.38023800	-1.56664900
N	3.97735200	0.62321900	-1.70308400	C	3.16302100	-2.72510700	-1.32791800
C	3.83690600	-0.41602000	-2.71457300	C	2.99432400	-2.24132000	-2.78284000
H	3.18342000	-0.03728900	-3.51819600	C	4.46399400	-2.16123100	-0.72356300
H	4.82409600	-0.60398600	-3.16672900	H	3.24147300	-3.82670700	-1.34830000
C	3.28538200	-1.77222200	-2.26019500	C	4.23260100	-2.53469400	-3.64380300
O	2.76305200	-2.51971200	-3.11288000	H	2.79642400	-1.15346400	-2.78515200
H	3.79734900	-2.20545000	-1.37212100	H	2.12228300	-2.72120900	-3.24955400
S	5.41198100	0.81884300	-0.87870700	C	5.69273700	-2.45924900	-1.59583500
O	6.49167100	0.57463000	-1.84947700	H	4.36250600	-1.06857500	-0.60085200
O	5.32557900	2.12625200	-0.20519700	H	4.63217600	-2.57394600	0.28078500
C	5.55734000	-0.43123700	0.39768000	C	5.51162500	-1.95984200	-3.03107300
C	6.28203700	-1.60072200	0.13661900	H	4.07523500	-2.13414800	-4.66026900
C	4.94066600	-0.22932400	1.63638300	H	4.34444700	-3.62941700	-3.75455500
C	6.37307300	-2.57756400	1.12697600	H	6.58768200	-2.00441000	-1.13693800
H	6.77577600	-1.74081800	-0.82647000	H	5.87125300	-3.55066800	-1.61088500
C	5.04178300	-1.22095400	2.61471300	H	6.38810000	-2.22641000	-3.64675500
H	4.39634000	0.69300200	1.84608800	H	5.45324600	-0.85536700	-3.02970100
C	5.75321300	-2.40939000	2.37920000	C	1.96551100	-3.29156900	1.35887300
H	6.94153800	-3.48988100	0.92488600	C	2.55483500	-4.70870200	1.22281900
H	4.56164300	-1.06309200	3.58415400	C	2.76174400	-2.47793000	2.40186400
H	1.19053100	-1.98707500	-0.76102500	H	0.94525000	-3.38779100	1.76948900
C	5.86727500	-3.47623500	3.43549200	C	2.58536000	-5.43038100	2.57990200
H	6.91942700	-3.62375600	3.73345700	H	3.58495600	-4.64169100	0.83199000
H	5.29025700	-3.21970400	4.33580700	H	1.98335300	-5.30765500	0.49549200
H	5.50497000	-4.44691000	3.05764300	C	2.77884200	-3.19555100	3.75972700
TS-L4-endo(T-shape)				H	3.80144600	-2.33811400	2.06388700
P	1.64170300	-2.35958900	-0.25194500	H	2.33047800	-1.46973000	2.50609900
P	1.13041700	2.37845000	-0.10581200	C	3.33709600	-4.61910000	3.64168000
Pd	1.09989900	-0.03667600	0.12849800	H	3.04543600	-6.42699600	2.46237300
C	0.31531800	-3.41119600	-1.12300600	H	1.54779900	-5.60378200	2.92075300
C	-0.70222200	-4.08401000	-0.17831900	H	3.37178400	-2.61085100	4.48437200
C	-0.44654500	-2.58636700	-2.18442000	H	1.74916500	-3.23974600	4.16086700
H	0.87144200	-4.21307500	-1.64195300	H	3.29093300	-5.13180300	4.61809900
C	-1.71776100	-4.93835900	-0.95459600	H	4.40736500	-4.56640900	3.36718800
H	-1.23934800	-3.30797300	0.39607600	C	0.81614600	3.43914300	1.41999000
H	-0.19626400	-4.72558400	0.55681700	C	-0.65981600	3.44337400	1.86519600
C	-1.44739400	-3.44409700	-2.97145900	C	1.72892400	2.99787900	2.58346300
H	-0.98954700	-1.77356400	-1.67317200	H	1.08387900	4.47381000	1.14730700
H	0.24769700	-2.09487000	-2.88054200	C	-0.86878900	4.30156800	3.12220800
C	-2.44462000	-4.14155300	-2.04168600	H	-0.98626200	2.41195000	2.07736200
H	-2.44394800	-5.37755600	-0.24877100	H	-1.31015200	3.81707800	1.06038900
H	-1.18594600	-5.78788100	-1.42218000	C	1.51209100	3.85401200	3.83961300
H	-1.98013500	-2.81357800	-3.70431800	H	1.51970800	1.93968600	2.82173500

H 2.78745000 3.04442300 2.28212000
C 0.04272600 3.86432200 4.27348800
H -1.92795500 4.25157900 3.42908600
H -0.66400700 5.36081300 2.87818200
H 2.15325800 3.48224300 4.65766900
H 1.83857600 4.89057600 3.63405300
H -0.09605600 4.52540600 5.14653100
H -0.24718900 2.84824100 4.60015000
C 2.80059600 2.97750900 -0.77978100
C 3.20878100 4.43151200 -0.46791300
C 3.95163300 2.02026800 -0.41222300
H 2.65307400 2.89717200 -1.87242800
C 4.50869200 4.81313500 -1.19492100
H 3.36753500 4.54370200 0.61828500
H 2.41174500 5.13699300 -0.74342800
C 5.25623900 2.39782700 -1.12745200
H 4.11543500 2.04257900 0.68029800
H 3.66631800 0.98487600 -0.65957500
C 5.65448100 3.85310100 -0.85743200
H 4.78762800 5.84930100 -0.93569400
H 4.33119100 4.80149900 -2.28648100
H 6.06484000 1.71363100 -0.81667600
H 5.12528900 2.25276000 -2.21620200
H 6.55941000 4.11736100 -1.43164800
H 5.91829800 3.96520700 0.21086100
C -0.13093200 2.99134400 -1.36691900
C -0.15121300 4.50099800 -1.67086500
C -0.05993300 2.18170800 -2.67768900
H -1.09198300 2.73830900 -0.88606200
C -1.31302900 4.86232600 -2.61010800
H 0.79667900 4.79255700 -2.15476900
H -0.22800700 5.08759700 -0.74176500
C -1.20495100 2.55061300 -3.63281500
H 0.90527800 2.37425700 -3.18103100
H -0.08450000 1.10194600 -2.45455400
C -1.25752300 4.05667100 -3.91262200
H -1.29494900 5.94459700 -2.82677300
H -2.27112600 4.66121700 -2.09593400
H -1.09942100 1.98788700 -4.57655200
H -2.16401900 2.23203900 -3.18404500
H -2.12485700 4.29749300 -4.55147000
H -0.35730200 4.35228400 -4.48349700
C -0.64058300 -0.28422800 1.42473000
C -0.42400100 -0.55682500 2.64511400
C -1.88191700 -0.07173600 0.60695000
N -3.03722800 0.16861200 1.49008600

C -3.35192900 -0.86949800 2.46412900
C -2.55958900 -0.75188500 3.75859200
O -2.46329800 -1.69616200 4.53768000
H -2.35367700 0.29662900 4.07546200
S -4.27711500 1.15141000 0.94534300
O -5.10030400 1.47197000 2.12195900
O -3.64595000 2.24333500 0.18372100
C -5.29504800 0.21687100 -0.19304200
C -6.45313500 -0.41263300 0.27308300
C -4.90954800 0.11299700 -1.53687400
C -7.22438000 -1.16258800 -0.61832300
H -6.76006500 -0.30788000 1.31496700
C -5.69240900 -0.64058700 -2.40931200
H -4.01761700 0.62508300 -1.90219800
C -6.85997000 -1.29257300 -1.96811200
H -8.13247000 -1.65121400 -0.25512300
H -5.39615900 -0.71840100 -3.45918300
H 0.29849000 -0.74372300 3.42963100
H -3.21691700 -1.87982200 2.04130300
H -4.40914900 -0.77964700 2.76477600
H -1.76810700 0.78943300 -0.05993900
H -2.06363500 -0.95875200 -0.02594000
C -7.69316000 -2.09496200 -2.93168100
H -8.55348400 -2.56400300 -2.43264200
H -8.07505000 -1.45695200 -3.74677300
H -7.09299600 -2.88998400 -3.40517300

TS-endo-1d

P 2.14974700 0.68701300 -0.03867900
P -0.98037700 -1.56719300 0.12457900
C -0.40012200 -2.41194300 -1.41310300
C -0.71473500 -1.79487400 -2.63995500
C 0.35655800 -3.59449300 -1.42525800
C -0.30723800 -2.36354900 -3.84871700
H -1.28308100 -0.86056500 -2.65092500
C 0.77435600 -4.15528300 -2.63833800
H 0.63178000 -4.08722000 -0.49190900
C 0.43965600 -3.54734300 -3.85108700
H -0.56735800 -1.87506100 -4.79164400
H 1.36618200 -5.07447400 -2.62987900
H 0.76551300 -3.98959300 -4.79638100
C -0.30751500 -2.52803000 1.55858200
C -0.66489000 -3.87307900 1.77404100
C 0.51526500 -1.88667000 2.49741600
C -0.18495000 -4.56287300 2.88996200
H -1.32797200 -4.38668700 1.07391700
C 0.98763100 -2.57645000 3.62031600

H 0.77946100 -0.83668400 2.35369200
C 0.64321700 -3.91636200 3.81557500
H -0.46621500 -5.60850400 3.04183300
H 1.62325100 -2.05989400 4.34450200
H 1.01124200 -4.45628500 4.69228900
C -2.77009100 -2.03857000 0.24974700
C -3.43757600 -2.81733100 -0.70804100
C -3.48264500 -1.58497300 1.37541200
C -4.79177900 -3.13533800 -0.54225200
H -2.90908700 -3.18468900 -1.58970700
C -4.82942000 -1.91144300 1.54288400
H -2.98214200 -0.97012700 2.12934600
C -5.49023900 -2.68618000 0.58139000
H -5.29824900 -3.74331500 -1.29701600
H -5.36776200 -1.55416100 2.42498600
H -6.54654200 -2.93757100 0.70949900
C 2.57535000 2.01747200 -1.25988600
C 3.75030500 2.78532700 -1.18852500
C 1.66646100 2.26446300 -2.30484600
C 4.00836100 3.77550000 -2.14191700
H 4.47164500 2.62007200 -0.38588900
C 1.93101200 3.24806900 -3.26323900
H 0.74248400 1.68227700 -2.36604900
C 3.10193400 4.00832800 -3.18175500
H 4.92420600 4.36853200 -2.06972200
H 1.21517500 3.42446400 -4.07064000
H 3.30610100 4.78404200 -3.92478300
C 3.10485100 -0.77320300 -0.66285900
C 3.48575900 -0.88197700 -2.01121300
C 3.39445100 -1.84119500 0.20794600
C 4.14965900 -2.02386700 -2.47371600
H 3.27084900 -0.07305100 -2.71235000
C 4.06574300 -2.97592600 -0.25489700
H 3.10654700 -1.78739900 1.25983400
C 4.44644700 -3.07190300 -1.59806000
H 4.44074500 -2.08775600 -3.52577200
H 4.29124800 -3.78969900 0.43981900
H 4.97178400 -3.96002800 -1.95944700
C 3.05430500 1.17605200 1.49968500
C 4.42802700 0.94473300 1.69811700
C 2.32529600 1.82993300 2.50867100
C 5.05443200 1.36456600 2.87551700
H 5.01774200 0.43362100 0.93427700
C 2.95474100 2.25395800 3.68365500
H 1.25423800 2.00517800 2.37503700
C 4.32065200 2.02103000 3.86982100

H 6.12274400 1.17784500 3.01521000
H 2.37246500 2.76150400 4.45738400
H 4.81319400 2.34653900 4.79013800
Pd -0.32032800 0.67473300 0.13298800
C -1.96333200 1.90559400 0.11877200
C -1.16016400 2.88604400 0.42986700
C -3.39222300 4.19473500 1.01865500
C -2.06075100 4.66471700 0.40755800
O -1.36618400 5.50706400 1.02924800
H -2.08830800 4.70058400 -0.71200600
H -0.11906600 3.04228300 0.72659200
H -3.17852200 3.87246400 2.05445700
H -4.03569500 5.08884400 1.08915600
C -4.10254300 3.11834500 0.24075600
C -3.38775100 1.96700100 -0.19457800
C -4.04817700 0.98478800 -0.95167200
C -5.40279400 1.11353400 -1.26484900
C -6.11277700 2.23528300 -0.82574900
C -5.46044000 3.22828800 -0.08635600
H -3.48590500 0.11837200 -1.30112700
H -5.90191300 0.33973800 -1.85404400
H -7.17403500 2.34433600 -1.06579900
H -6.01665700 4.11110000 0.24232700

TS-exo-1d

P -2.24137700 -0.46323200 0.09058200
P 1.33179200 1.63424800 -0.18367500
C 0.48107300 3.21361400 -0.62513600
C -0.37068300 3.20016600 -1.74523800
C 0.63362400 4.40632300 0.09957300
C -1.04126900 4.35969400 -2.14120600
H -0.51193600 2.27495500 -2.31169800
C -0.04773200 5.56456100 -0.29327200
H 1.28585800 4.44104100 0.97463500
C -0.88283200 5.54552600 -1.41394500
H -1.69656900 4.33526300 -3.01601900
H 0.07911600 6.48632900 0.28115700
H -1.41348900 6.45147900 -1.71906900
C 2.11560100 1.96716800 1.45765600
C 3.36271000 2.60020200 1.59978600
C 1.42881600 1.55063500 2.61253000
C 3.90486700 2.81838800 2.87048200
H 3.91864600 2.92593000 0.71778800
C 1.96876600 1.77729000 3.88242600
H 0.46762200 1.03772200 2.51728100
C 3.20903100 2.41064600 4.01362200
H 4.87689700 3.30988200 2.96647100

H	1.42174800	1.44992800	4.77067400	Pd	0.04787500	-0.49624700	-0.31406200
H	3.63594900	2.58137800	5.00565300	C	1.09864000	-3.04418600	-0.48096800
C	2.76620800	1.59071900	-1.35542200	C	-0.01156100	-2.45298900	-0.81152600
C	3.21914200	2.71532000	-2.06570800	C	3.04336000	-4.49331100	-1.42178500
C	3.42042300	0.35953100	-1.54257400	C	1.52754500	-4.70013800	-1.58229900
C	4.30691000	2.60943700	-2.93974500	O	0.99472400	-4.74881400	-2.71832400
H	2.72566700	3.68153900	-1.94121000	H	1.10840400	-5.33679300	-0.75876200
C	4.51218900	0.25803300	-2.40903300	H	-0.81595000	-2.83206600	-1.45051900
H	3.07043400	-0.52875200	-1.00881100	H	3.55973700	-5.46271700	-1.53958700
C	4.95653300	1.38324600	-3.11230900	H	3.37686800	-3.84367500	-2.25214900
H	4.64701000	3.49243500	-3.48784600	C	4.48005200	-4.01650900	0.67758600
H	5.01066600	-0.70603000	-2.54139400	C	3.31771100	-3.86696800	-0.08453600
H	5.80500100	1.30310800	-3.79729700	C	2.25620900	-3.05863500	0.39276800
C	-3.24071200	-1.32101300	-1.20259200	C	2.37700800	-2.42345700	1.64612200
C	-4.36625600	-2.10600300	-0.90197400	C	3.54263600	-2.58084700	2.39794000
C	-2.84313800	-1.18356300	-2.54526300	C	4.59458700	-3.37284800	1.91537100
C	-5.08440300	-2.73220600	-1.92642200	H	5.29850600	-4.64076300	0.30717800
H	-4.69121400	-2.23265600	0.13268100	H	1.55643700	-1.80681300	2.02126800
C	-3.56826300	-1.80255800	-3.56715900	H	3.63440300	-2.08174100	3.36660400
H	-1.95632800	-0.59265100	-2.79181200	H	5.50468700	-3.49242100	2.50972000
C	-4.69010500	-2.58001800	-3.25935000	TS-L4-exo			
H	-5.95735200	-3.34210700	-1.67841000	P	-0.25593600	2.52692900	-0.24265900
H	-3.24939500	-1.68424500	-4.60618900	P	-2.80478900	-1.49976600	0.21559400
H	-5.25245900	-3.07185200	-4.05764300	Pd	-1.29821800	0.34932200	-0.13568700
C	-3.00373100	1.21587200	0.20895000	C	0.46618900	3.07937100	-1.91715500
C	-4.04166000	1.64079800	-0.63640000	C	1.95975100	2.74711200	-2.11855100
C	-2.50696800	2.10767700	1.17848900	C	-0.35335400	2.50564200	-3.09506600
C	-4.57451400	2.92921100	-0.51026300	H	0.36437400	4.17986900	-1.92699800
H	-4.44607100	0.96973800	-1.39621300	C	2.47373800	3.22904800	-3.48462800
C	-3.04911500	3.38754600	1.30940900	H	2.10613700	1.65535700	-2.04419800
H	-1.69253600	1.80121500	1.84001900	H	2.57349900	3.20610300	-1.33040600
C	-4.08373800	3.80375400	0.46262900	C	0.16088900	2.99716500	-4.45558500
H	-5.38247000	3.24507100	-1.17585900	H	-0.28427700	1.40683900	-3.06876900
H	-2.65679100	4.06592700	2.07157800	H	-1.42084500	2.74972900	-2.98895600
H	-4.50361100	4.80832100	0.56153200	C	1.64504500	2.66891500	-4.64367900
C	-2.74157300	-1.26685000	1.68055800	H	3.53482500	2.94605800	-3.59658400
C	-3.84871000	-0.82426500	2.42683300	H	2.44111600	4.33431900	-3.51331800
C	-2.00280200	-2.36780700	2.14858700	H	-0.44037400	2.54305200	-5.26226800
C	-4.20612900	-1.47110500	3.61418700	H	0.01407100	4.09078100	-4.53381300
H	-4.44091500	0.02685100	2.08491900	H	2.01113600	3.06595100	-5.60641400
C	-2.36674800	-3.01617100	3.33245700	H	1.77586300	1.57151500	-4.68350400
H	-1.13767300	-2.72156500	1.58290300	C	-1.37813900	3.99146800	0.18501800
C	-3.46721500	-2.56760300	4.06991000	C	-2.50336100	4.19497700	-0.85011500
H	-5.06862600	-1.11491900	4.18409100	C	-1.97178800	3.87870600	1.60277400
H	-1.78208100	-3.87134800	3.68194000	H	-0.72495800	4.88141000	0.15063600
H	-3.74716000	-3.07019400	4.99971900	C	-3.41381300	5.37932800	-0.49127100

H	-3.11039300	3.27276300	-0.91324500	C	-4.22435200	-1.04564200	1.38695000
H	-2.08124300	4.36436800	-1.85146000	C	-4.91269100	-2.20143400	2.14012000
C	-2.88029700	5.06686100	1.95081600	C	-3.81771300	0.06183100	2.38009100
H	-2.55464500	2.94324700	1.67530100	H	-4.96683200	-0.60367000	0.69740600
H	-1.17065700	3.80530600	2.35244200	C	-6.12152800	-1.69920900	2.94636100
C	-3.99568600	5.25376800	0.91904500	H	-4.19315000	-2.66531500	2.83661800
H	-4.22260200	5.46006200	-1.23805600	H	-5.23433300	-2.99225000	1.44659300
H	-2.83108600	6.31671300	-0.56096200	C	-5.01720600	0.56265600	3.19655300
H	-3.30572300	4.92226200	2.95899800	H	-3.04437800	-0.32668900	3.06734700
H	-2.27092600	5.98857800	1.99899800	H	-3.35220900	0.89894500	1.83414900
H	-4.60491300	6.14070000	1.16497300	C	-5.73280000	-0.58270100	3.92134100
H	-4.67803000	4.38406200	0.95707900	H	-6.57928000	-2.54274500	3.49175300
C	1.20034100	2.66004300	0.95351500	H	-6.89270100	-1.32339900	2.24840600
C	1.70684500	4.08505100	1.24764700	H	-4.68401700	1.32712900	3.91977000
C	0.98832900	1.87013700	2.26277500	H	-5.73076100	1.06514100	2.51702200
H	1.99599400	2.12617200	0.40603400	H	-6.62566800	-0.20534800	4.44932100
C	2.98249200	4.06106200	2.10441200	H	-5.06220800	-0.99673300	4.69741800
H	0.92853300	4.64875800	1.78969700	C	-3.64229700	-1.97476100	-1.40161600
H	1.89627400	4.63462300	0.31115000	C	-4.71587100	-3.07693000	-1.33732400
C	2.26356800	1.85686700	3.11877700	C	-4.18760600	-0.73394600	-2.13863400
H	0.16800000	2.31661600	2.84960600	H	-2.79771100	-2.35812200	-2.00283700
H	0.67550700	0.83890200	2.02771300	C	-5.22884800	-3.43997500	-2.73989300
C	2.77816300	3.27275100	3.40284400	H	-5.56739400	-2.72318100	-0.73073500
H	3.30043700	5.09425800	2.32791600	H	-4.32436800	-3.97802200	-0.83903300
H	3.80274100	3.60015900	1.52336800	C	-4.71376400	-1.09334300	-3.53611600
H	2.07161100	1.32086700	4.06441700	H	-5.00753300	-0.28386400	-1.54958000
H	3.04934200	1.28618900	2.59025600	H	-3.39967000	0.03445100	-2.21472900
H	3.71936400	3.23027900	3.97793000	C	-5.76176600	-2.21079200	-3.48426600
H	2.04690600	3.80505400	4.03960700	H	-6.01434100	-4.21150700	-2.66093000
C	-2.10762700	-3.11749700	0.88629600	H	-4.40449100	-3.89164400	-3.32243300
C	-1.31085300	-3.93476100	-0.15071000	H	-5.13447300	-0.19412900	-4.01856200
C	-1.24457500	-2.85511700	2.13770100	H	-3.86586300	-1.41867900	-4.16704700
H	-2.97562900	-3.72628700	1.18960000	H	-6.07806500	-2.48696600	-4.50504100
C	-0.77260900	-5.23896200	0.45888400	H	-6.66574000	-1.83784800	-2.96718100
H	-0.46631700	-3.33370100	-0.52758600	C	1.17094200	-1.10544400	-1.19399700
H	-1.93923100	-4.17671100	-1.02183200	C	-0.00040400	-0.69351100	-1.45805800
C	-0.69896600	-4.15709400	2.74229100	C	2.28879300	-1.26363100	-0.25729800
H	-0.40039900	-2.19980000	1.85624800	N	3.25390300	-2.23004700	-0.84655800
H	-1.82342800	-2.30592600	2.89776900	C	3.61040000	-1.92667500	-2.22707700
C	0.07401100	-4.98639300	1.71097000	C	2.38695900	-2.01641600	-3.12636200
H	-0.18376800	-5.78471000	-0.29867200	O	2.25197300	-1.31903400	-4.12822700
H	-1.62423300	-5.89380900	0.72233900	H	1.77029800	-2.92923700	-2.96472700
H	-0.05592600	-3.92314600	3.60840300	S	4.40387500	-2.91848700	0.15271800
H	-1.54253800	-4.75613200	3.13312200	O	3.69933400	-3.29342200	1.39156300
H	0.39449400	-5.94507700	2.15473800	O	5.07720900	-3.95939700	-0.64042200
H	0.99949400	-4.45212400	1.42789700	C	5.62281300	-1.67848200	0.57705900

C	5.45756300	-0.91562500	1.74047100	C	1.20214500	5.14316300	0.05427500
C	6.71637300	-1.47111900	-0.27040200	H	0.15557400	3.26275800	-0.20919800
C	6.39745300	0.06811900	2.04452400	H	1.06974300	3.37115500	1.29560600
H	4.61320100	-1.09999200	2.40682300	C	1.27601000	5.54402300	-1.42189300
C	7.64524200	-0.47908600	0.05120700	H	2.41703100	5.05149800	-3.21039200
H	6.85179700	-2.08376700	-1.16358000	H	3.38155300	5.14977600	-1.73072900
C	7.50352600	0.30659800	1.20728700	H	0.33767600	5.62587500	0.54217400
H	6.27360500	0.66011100	2.95572100	H	2.10268900	5.51264500	0.57934000
H	8.50173400	-0.31775100	-0.60880200	H	1.40646200	6.63568000	-1.52019800
H	-0.64517500	-0.73815700	-2.34120000	H	0.31653600	5.29764800	-1.91382800
H	4.31911300	-2.68981000	-2.58737800	C	3.19862400	0.84768600	1.48705800
H	4.07288400	-0.92917100	-2.34729900	C	4.61420600	1.45717600	1.48972500
H	2.78604800	-0.28843700	-0.07971700	C	2.42522600	1.31440800	2.73713100
H	1.95969200	-1.65743800	0.71619900	H	3.30045300	-0.24862100	1.57638700
C	8.50998700	1.36910200	1.56049900	C	5.37454800	1.09276700	2.77547900
H	9.27014200	1.48700700	0.77460100	H	4.54178500	2.55683300	1.42276700
H	8.01839000	2.34375500	1.71621800	H	5.19346400	1.12971200	0.61218600
H	9.02836300	1.12030600	2.50241100	C	3.17588700	0.94279600	4.02466000
TS-L4-endo-1d				H	2.29633300	2.41019200	2.70705400
P	2.20442100	1.01497300	-0.11270100	H	1.41297200	0.87799700	2.74486100
P	-2.46237900	0.12975300	0.03062600	C	4.60141700	1.50700700	4.03259300
Pd	-0.02299600	0.11158300	0.13160800	H	6.37162800	1.56645600	2.76547600
C	3.35571800	0.25544100	-1.41281300	H	5.54800800	0.00090800	2.79626000
C	4.04035000	-1.04988600	-0.95502300	H	2.61506900	1.30709500	4.90291600
C	2.60814900	-0.00315400	-2.73933100	H	3.21749700	-0.15855900	4.11467700
H	4.14685500	1.00458900	-1.59619600	H	5.13942700	1.17915800	4.93892700
C	4.97617900	-1.60700500	-2.03991400	H	4.55325000	2.61110500	4.08042900
H	3.26910900	-1.80248800	-0.71679100	C	-3.50982400	-1.22227600	0.82676500
H	4.62184800	-0.89312000	-0.03560200	C	-3.38137300	-2.58181600	0.11093000
C	3.54396200	-0.54564400	-3.82897400	C	-3.18912200	-1.38068600	2.32766300
H	1.80734800	-0.73859500	-2.55181000	H	-4.55972200	-0.89536500	0.73562900
H	2.10975600	0.90747700	-3.09942100	C	-4.26274500	-3.65306700	0.77153200
C	4.25796200	-1.82254600	-3.37536900	H	-2.32920100	-2.91286400	0.13851600
H	5.42520200	-2.55210600	-1.68827000	H	-3.65477800	-2.49220600	-0.95198900
H	5.81437400	-0.90052000	-2.18737000	C	-4.06994900	-2.45234200	2.98701900
H	2.96821400	-0.73421800	-4.75176600	H	-2.12775400	-1.66109000	2.44270200
H	4.29543100	0.22541000	-4.08259900	H	-3.31831700	-0.42366500	2.85586000
H	4.97308200	-2.16028000	-4.14554400	C	-3.96241000	-3.80016300	2.26672200
H	3.51422100	-2.63262400	-3.26172600	H	-4.12247900	-4.61819100	0.25448100
C	2.26951600	2.88352300	-0.47146400	H	-5.32625100	-3.37989800	0.63876000
C	2.31041400	3.28024400	-1.96006300	H	-3.79035500	-2.56048900	4.04937200
C	1.10679700	3.62010900	0.22490700	H	-5.12326900	-2.11510000	2.97453200
H	3.21556100	3.22742900	-0.01941100	H	-4.64427100	-4.53739000	2.72501400
C	2.41175200	4.80415400	-2.13458900	H	-2.93883000	-4.19902700	2.39391600
H	1.39505300	2.92206200	-2.46453400	C	-3.12144100	1.75005700	0.76614500
H	3.16303800	2.80711000	-2.46920000	C	-4.60976000	1.79408600	1.16976000

C -2.24795800 2.25502300 1.93424900
H -2.97952700 2.45922600 -0.07022200
C -5.02609300 3.20723800 1.61005300
H -4.78463000 1.09897100 2.00851300
H -5.25664000 1.46019700 0.34619100
C -2.66143900 3.66347700 2.38367500
H -2.33842500 1.56150100 2.78899600
H -1.18675600 2.24494600 1.63895200
C -4.14795000 3.73219500 2.75084200
H -6.08737800 3.20290600 1.91394100
H -4.95174600 3.89351400 0.74595300
H -2.03936800 3.98070300 3.23866100
H -2.45550200 4.37836900 1.56511000
H -4.43281200 4.76652900 3.01064600
H -4.32688000 3.12207400 3.65592300
C -3.04129700 0.13596300 -1.76888800
C -4.55412400 0.23742800 -2.04060000
C -2.27842300 1.17896900 -2.61026800
H -2.70765500 -0.85829900 -2.11739300
C -4.86261400 0.07589200 -3.53789300
H -4.92124300 1.22451600 -1.71199900
H -5.11141900 -0.51737600 -1.46356800
C -2.59200800 1.03729600 -4.10716500
H -2.55468300 2.19653500 -2.27838200
H -1.19366600 1.07838600 -2.43832600
C -4.09787000 1.09724100 -4.38680500
H -5.94916300 0.17312400 -3.70686200
H -4.58707700 -0.94631800 -3.85776900
H -2.06453700 1.82358000 -4.67461400
H -2.19320600 0.07102900 -4.46810900
H -4.29567600 0.93091100 -5.45993800
H -4.47049000 2.11242800 -4.15410200
C 0.49010000 -1.93211600 0.70736300
C 0.64975500 -2.03792100 1.96837600
C 2.08410500 -4.33292900 1.11521700
C 1.23976900 -4.26106300 2.37849800
O 1.75384000 -4.27870800 3.50028200
H 0.16301000 -4.52286300 2.24629800
H 0.63334600 -1.53551000 2.92841300
H 2.93179500 -3.63738600 1.24722400
H 2.51559400 -5.35056500 1.09907900
C 1.36085000 -4.08248300 -0.18429800
C 0.60941500 -2.89204600 -0.39941800
C -0.00915100 -2.69083700 -1.64686200
C 0.08830800 -3.63883100 -2.66738900
C 0.81722500 -4.81202600 -2.45570500

C 1.44402600 -5.02155500 -1.22302100
H -0.57386600 -1.77054200 -1.80513700
H -0.40619800 -3.45911700 -3.62584000
H 0.90040200 -5.56356600 -3.24551400
H 2.01867000 -5.93792400 -1.05987000

TS-L4-exo-1d

P -2.64127200 0.16988000 -0.26146300
P 1.90372700 -1.35340700 0.07474400
Pd -0.28246200 -0.29732500 -0.03427500
C -3.09684000 1.61370500 -1.40803900
C -3.20639700 2.98687400 -0.71293400
C -2.10100700 1.71470600 -2.58423200
H -4.09344400 1.36183700 -1.81400800
C -3.59457000 4.09372100 -1.70647900
H -2.23884400 3.23977800 -0.24387000
H -3.95266400 2.96186900 0.09385200
C -2.49495100 2.81238200 -3.58216500
H -1.10198600 1.93824300 -2.17405800
H -2.00664300 0.75287200 -3.10901700
C -2.63288300 4.17427700 -2.89541200
H -3.63606400 5.06212300 -1.17846200
H -4.61745500 3.89834600 -2.07907800
H -1.74593800 2.86292600 -4.39140800
H -3.45466300 2.54336300 -4.06172600
H -2.97549600 4.93774100 -3.61524200
H -1.63903500 4.50267900 -2.53895600
C -3.70229000 -1.23296100 -0.96152600
C -3.34520400 -1.57257100 -2.42340800
C -3.65355000 -2.50089000 -0.08631300
H -4.73584300 -0.84334600 -0.95022400
C -4.20612000 -2.71643000 -2.98062900
H -2.27815700 -1.85639200 -2.48315200
H -3.47340300 -0.68955200 -3.06601500
C -4.51414900 -3.63750500 -0.65796600
H -2.60722100 -2.84356400 -0.00290400
H -3.99134200 -2.27570600 0.93504000
C -4.13805300 -3.96926100 -2.10409400
H -3.88681500 -2.94645300 -4.01182200
H -5.25671300 -2.37769100 -3.04802100
H -4.41555900 -4.53055000 -0.01689300
H -5.57902300 -3.34155500 -0.61842500
H -4.80014200 -4.75631300 -2.50457600
H -3.11118500 -4.37943100 -2.13029400
C -3.43498200 0.61748200 1.38967100
C -4.97502800 0.66692600 1.40393400
C -2.91224800 -0.20872900 2.58441400

H	-3.06207200	1.64456800	1.54610900
C	-5.50043700	1.22747200	2.73525800
H	-5.37565200	-0.35187700	1.26315400
H	-5.35872300	1.27248300	0.56707900
C	-3.43151000	0.36039800	3.91314300
H	-3.24010900	-1.25734700	2.49458900
H	-1.81110400	-0.22822100	2.58307900
C	-4.96243500	0.44207300	3.93682100
H	-6.60428100	1.21794600	2.73371600
H	-5.19714600	2.28686000	2.82651100
H	-3.06788900	-0.25886100	4.75133500
H	-3.00834900	1.37084800	4.06427500
H	-5.30767300	0.90099000	4.87940200
H	-5.37993800	-0.58206400	3.91687100
C	2.87032800	-1.15039200	1.67935800
C	3.56566500	0.22039600	1.80300900
C	1.94605200	-1.40538400	2.88905900
H	3.65657600	-1.92321300	1.67492100
C	4.29849300	0.36481300	3.14526000
H	2.81403100	1.02101900	1.71782500
H	4.28220400	0.36611600	0.98002800
C	2.67744400	-1.23415000	4.22819100
H	1.10180100	-0.69543000	2.84755400
H	1.50644000	-2.41448000	2.82909900
C	3.35662800	0.13546100	4.33123800
H	4.75867200	1.36628300	3.20708500
H	5.12977800	-0.36361400	3.19059800
H	1.96402900	-1.37629700	5.05838600
H	3.44110500	-2.02732100	4.33326700
H	3.90739000	0.22054700	5.28409800
H	2.58917900	0.93156900	4.33623500
C	1.75229900	-3.22601000	-0.19473500
C	2.80095800	-4.11717200	0.49964000
C	0.33156900	-3.73909100	0.11227200
H	1.89971000	-3.32352200	-1.28555600
C	2.63424900	-5.59158800	0.09852400
H	2.68653500	-4.03444400	1.59409200
H	3.82257000	-3.78418000	0.26347200
C	0.16226400	-5.21480900	-0.27520200
H	0.11983200	-3.61614200	1.18996800
H	-0.40915000	-3.11970000	-0.42003600
C	1.21955800	-6.10462500	0.38747700
H	3.38172900	-6.20605900	0.62972700
H	2.84963600	-5.70128700	-0.98063700
H	-0.85228100	-5.55707500	-0.00714400
H	0.24418600	-5.31010100	-1.37409500

H	1.11196000	-7.14867700	0.04591500
H	1.05339900	-6.11431600	1.48093500
C	3.07250700	-0.78320100	-1.28426600
C	4.43848200	-1.49136900	-1.35791800
C	2.37803500	-0.80247900	-2.66164700
H	3.24919800	0.27639400	-1.02783200
C	5.33083500	-0.87358600	-2.44600000
H	4.28597500	-2.55925500	-1.59170400
H	4.95390900	-1.44997700	-0.38519900
C	3.27313600	-0.20085900	-3.75522800
H	2.12643600	-1.84322300	-2.93604000
H	1.42271600	-0.25376800	-2.60751200
C	4.64337300	-0.88519200	-3.81553800
H	6.29039400	-1.41719300	-2.49293700
H	5.57464900	0.16846300	-2.16781500
H	2.76481400	-0.27129200	-4.73246500
H	3.41426900	0.87655300	-3.55236500
H	5.28261900	-0.39596900	-4.57071100
H	4.51343700	-1.93247200	-4.14719900
C	0.82165500	2.51701500	0.64169200
C	0.11019300	1.49344400	0.95452900
C	2.50569900	4.20850500	1.86392200
C	1.12202400	3.84582100	2.39901800
O	0.96262500	3.26670100	3.49109800
H	0.30791700	4.49583400	1.99685000
H	-0.45049100	1.32213800	1.88211300
H	2.77628700	5.20759700	2.25274600
H	3.22912000	3.49285800	2.29446700
C	3.37810600	4.98663700	-0.42483200
C	2.54290400	4.18553300	0.35851300
C	1.66622900	3.25434700	-0.26064800
C	1.65624900	3.15745000	-1.66916300
C	2.49652200	3.96587800	-2.43948800
C	3.35848300	4.88033400	-1.82123700
H	4.04809800	5.70429400	0.05812000
H	0.98525300	2.44651600	-2.15478300
H	2.47707700	3.88315400	-3.52992300
H	4.01127300	5.51501500	-2.42683300
TS-L4-endo-1e			
P	0.82828400	2.53106000	-0.24652700
P	1.92540900	-2.07701500	0.01195000
Pd	0.99746000	0.16170900	0.16455000
C	0.40906200	3.70175800	1.19420100
C	-1.09153200	4.01765400	1.36463200
C	0.97124500	3.15759600	2.52572200
H	0.92380900	4.65134500	0.95949800

C	-1.33777700	4.98022300	2.53795700	H	-0.84460700	3.70048600	-4.86912700
H	-1.65402800	3.08287300	1.53563600	C	0.86873500	-3.62440200	0.21705500
H	-1.50524700	4.46891600	0.45148500	C	0.36996900	-3.83546300	1.66106000
C	0.74099800	4.13137300	3.68968100	C	-0.31825900	-3.62028400	-0.76763400
H	0.46788100	2.20382000	2.74967400	H	1.51885100	-4.47830600	-0.03818200
H	2.04298400	2.92650700	2.43926400	C	-0.48523900	-5.10652700	1.78179500
C	-0.74478300	4.46537300	3.85250300	H	-0.22867800	-2.96414900	1.97649500
H	-2.42216500	5.15535600	2.64696100	H	1.21847000	-3.90326100	2.35953300
H	-0.88691500	5.96101500	2.29681800	C	-1.17262900	-4.88983700	-0.64081100
H	1.14244400	3.69684700	4.62173600	H	-0.94903700	-2.73653600	-0.56745500
H	1.30983800	5.06274200	3.50903900	H	0.03856800	-3.51672800	-1.80414300
H	-0.89001900	5.20808700	4.65614000	C	-1.65808200	-5.10628600	0.79600700
H	-1.28860400	3.55452200	4.16517500	H	-0.85416300	-5.20578300	2.81731800
C	2.44883800	3.28153300	-0.88375700	H	0.15010800	-5.99141500	1.59031800
C	3.54888600	3.37342200	0.19274600	H	-2.03057600	-4.83049300	-1.33279100
C	2.98167200	2.53230500	-2.12084600	H	-0.57453700	-5.76382200	-0.95950300
H	2.19352300	4.31282700	-1.18345900	H	-2.22461200	-6.05048000	0.87274600
C	4.84282900	3.99201000	-0.35899600	H	-2.36107500	-4.29686900	1.06779200
H	3.76587900	2.36240800	0.58328200	C	2.82803100	-2.32166500	-1.64080400
H	3.20665500	3.97660200	1.04611400	C	3.10350900	-3.77268000	-2.08579000
C	4.27335200	3.15703700	-2.66798100	C	2.16664200	-1.53858000	-2.79391500
H	3.17598400	1.48058000	-1.84259600	H	3.80347600	-1.83962500	-1.44442700
H	2.22320300	2.50793500	-2.91720600	C	3.96980100	-3.81127200	-3.35536200
C	5.35985400	3.24806300	-1.59318800	H	2.14685100	-4.28006200	-2.29749600
H	5.61060600	4.00561400	0.43393700	H	3.59396100	-4.34820600	-1.28792600
H	4.65208800	5.04826600	-0.62560000	C	3.02060500	-1.57812400	-4.06912300
H	4.63112000	2.56914700	-3.53100000	H	1.17225400	-1.96946900	-3.00916800
H	4.05340300	4.17090000	-3.05123800	H	1.99136700	-0.49564200	-2.48505400
H	6.25976400	3.74582700	-1.99409000	C	3.33833200	-3.01388500	-4.50132000
H	5.66992200	2.22730300	-1.30107600	H	4.13231500	-4.85944600	-3.66125600
C	-0.45208400	2.98242300	-1.56346800	H	4.96834900	-3.39462100	-3.12636400
C	-0.32384200	4.39180800	-2.17257700	H	2.50427200	-1.03769400	-4.88149700
C	-0.61229600	1.92549700	-2.67581900	H	3.96688600	-1.03554000	-3.88557800
H	-1.39036000	2.95340800	-0.98476000	H	4.00436100	-3.01221200	-5.38158400
C	-1.51917400	4.71914100	-3.08161200	H	2.40347200	-3.51325700	-4.81776000
H	0.60195200	4.45200200	-2.77061200	C	3.26928500	-2.27055400	1.32505000
H	-0.23673500	5.15486900	-1.38193700	C	4.08057500	-3.57941600	1.32780800
C	-1.81112300	2.25457500	-3.57882600	C	4.21665800	-1.05387000	1.34993000
H	0.30042300	1.88087000	-3.29373500	H	2.68227900	-2.23593000	2.26059100
H	-0.73515900	0.92481300	-2.22980800	C	5.03492800	-3.64096700	2.53127600
C	-1.70616900	3.66263600	-4.17632900	H	4.67791900	-3.64268800	0.40233300
H	-1.38284200	5.71814800	-3.53116000	H	3.41443600	-4.45669300	1.33688200
H	-2.43734600	4.77473500	-2.46818300	C	5.18507000	-1.11500000	2.54055400
H	-1.89171600	1.50178600	-4.38221000	H	4.79997200	-1.01831800	0.41160800
H	-2.74012000	2.18197000	-2.98431700	H	3.62694800	-0.12226900	1.38727000
H	-2.60174000	3.89093600	-4.77983200	C	5.97267700	-2.42951100	2.57295200

H	5.61863500	-4.57723800	2.49613200	H	-0.93330300	4.22789900	1.60254400
H	4.44184700	-3.67724500	3.46396100	C	-3.37606400	3.35376900	2.63117100
H	5.87528000	-0.25439400	2.50416500	H	-2.66685600	1.70198500	1.41849800
H	4.60867800	-1.01339100	3.47878200	H	-2.92975300	3.20781300	0.52854800
H	6.61401100	-2.47007000	3.47040800	C	-1.37960500	3.22110700	4.16228500
H	6.65254200	-2.46756600	1.70118200	H	-0.65462300	1.53401100	3.03833500
C	-0.76459000	-0.11934600	1.46410500	H	0.51226600	2.84973000	3.16254200
C	-0.57426700	-0.31482700	2.70569600	C	-2.86621100	2.89167200	3.99919100
C	-1.96382000	-0.05052600	0.56877500	H	-4.43080200	3.05895700	2.49222600
N	-3.18298500	0.17936400	1.36819500	H	-3.35459700	4.45893700	2.59128000
C	-3.44731600	-0.79034200	2.42518300	H	-1.00236200	2.83363300	5.12456500
C	-2.61837500	-0.54814100	3.67884400	H	-1.24396200	4.31862800	4.19150700
O	-2.48627700	-1.44140200	4.52614200	H	-3.45919500	3.35633000	4.80609400
H	-2.51925500	0.52929200	3.94882700	H	-3.00406100	1.79876100	4.09396200
S	-4.50046100	0.87325800	0.59634100	C	1.30871000	3.92174900	0.04977400
O	-5.44978900	1.26017500	1.65161400	C	2.08636300	4.22150800	1.34698500
O	-3.95810300	1.91095600	-0.29875900	C	2.29142200	3.69458800	-1.11504400
C	-5.29077000	-0.37058700	-0.42063000	H	0.69170000	4.80780500	-0.18058700
C	-6.41765100	-1.04095100	0.06457700	C	3.07427200	5.38537900	1.17108600
C	-4.76188000	-0.67162100	-1.68391800	H	2.63968800	3.31643800	1.65876600
C	-7.01334700	-2.02840800	-0.72401900	H	1.39435900	4.46759100	2.16551500
H	-6.83518500	-0.78659600	1.04014100	C	3.27237300	4.86352600	-1.28671700
C	-5.36995100	-1.66135800	-2.45354700	H	2.86178800	2.76796900	-0.92196700
H	-3.89324300	-0.13525800	-2.06996400	H	1.74593500	3.53411600	-2.05675100
C	-6.50267400	-2.35750100	-1.98991300	C	4.03991300	5.15434500	0.00571200
H	-7.89778200	-2.54889000	-0.34693300	H	3.63229700	5.53882500	2.11102600
H	-4.96102800	-1.89490100	-3.44061300	H	2.50549800	6.31668800	0.99135800
H	-3.29661400	-1.82985500	2.08248200	H	3.97241400	4.64014600	-2.11040400
H	-4.49733700	-0.69220500	2.74578500	H	2.71255500	5.76783600	-1.59008600
H	-1.87014300	0.76705100	-0.15261200	H	4.70143800	6.02814700	-0.12537400
H	-2.05175700	-0.99161500	-0.00671200	H	4.69674400	4.29593300	0.24038800
C	-7.14389800	-3.41955600	-2.84272000	C	-1.02294400	2.60642300	-1.29870400
H	-8.01341200	-3.87172900	-2.34400500	C	-1.39122400	4.03015700	-1.75631900
H	-7.47912900	-3.00126900	-3.80687500	C	-0.53402700	1.75974700	-2.49157800
H	-6.42543800	-4.22298500	-3.07758400	H	-1.94680400	2.11761300	-0.94561200
C	0.34855400	-0.47973400	3.83728200	C	-2.43078800	4.00402300	-2.88829300
H	0.03815200	-1.32846500	4.47083300	H	-0.48545400	4.54507000	-2.12032400
H	1.38640900	-0.65433900	3.50417600	H	-1.77342300	4.62741200	-0.91237500
H	0.35003300	0.41364900	4.48653700	C	-1.57521100	1.73728200	-3.62070100
TS-L4-exo-1e				H	0.41274300	2.16631100	-2.88548100
P	0.08657200	2.48424300	0.23115800	H	-0.31602700	0.73309400	-2.15272600
P	2.77561600	-1.42830900	-0.19826600	C	-1.96038700	3.15094600	-4.07166600
Pd	1.15970400	0.28595500	0.30558500	H	-2.64702900	5.03461500	-3.21952600
C	-1.03757300	3.12789100	1.63220300	H	-3.38173200	3.59509700	-2.49922200
C	-2.53580500	2.79763500	1.46934100	H	-1.18780400	1.15415600	-4.47410500
C	-0.55458800	2.62954300	3.01124700	H	-2.48070400	1.20972300	-3.26723700

H -2.74404900 3.10623700 -4.84772300
H -1.08309400 3.63399700 -4.54135100
C 2.14671200 -3.17238900 -0.53871500
C 1.64010500 -3.89078300 0.72842400
C 1.04632000 -3.14975200 -1.61946100
H 3.00274900 -3.74733000 -0.93025900
C 1.11070400 -5.29747200 0.40855800
H 0.83093500 -3.29752500 1.18757500
H 2.44287600 -3.96810000 1.47830200
C 0.50790200 -4.55391700 -1.93007100
H 0.21757900 -2.51052000 -1.26799900
H 1.42284200 -2.68532700 -2.54437600
C 0.02010900 -5.27155900 -0.66723600
H 0.72877700 -5.76664100 1.33186600
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H -0.30950300 -4.48063500 -2.66813800
H 1.30694200 -5.15286800 -2.40552500
H -0.30111100 -6.29915200 -0.91122000
H -0.87364200 -4.75123800 -0.27753200
C 3.81146800 -0.97312700 -1.72275300
C 4.46834000 -2.13220500 -2.50011500
C 3.04659400 -0.05759100 -2.69999900
H 4.62099500 -0.36414600 -1.27985600
C 5.39206100 -1.60520700 -3.61052800
H 3.68384100 -2.75569200 -2.96192200
H 5.03824600 -2.79081100 -1.82947600
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H 2.20920300 -0.61911900 -3.15127900
H 2.59523000 0.78291800 -2.14973700
C 4.65229600 -0.66976800 -4.57273300
H 5.82987100 -2.45515200 -4.16239300
H 6.23880400 -1.06211200 -3.15094900
H 3.37509700 1.09403400 -4.51343100
H 4.72690700 1.13071000 -3.37196700
H 5.34925400 -0.26356300 -5.32618800
H 3.89292300 -1.24986100 -5.12974800
C 4.04305200 -1.65193900 1.18072400
C 5.19058200 -2.64875400 0.93318700
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C 6.06052700 -2.81913700 2.18895800
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H 5.20067200 0.16276700 0.85117700
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H 5.45557200 -3.28263900 2.99030000
H 5.90692300 0.51881800 3.19541000
H 4.85881100 -0.79364700 3.75148500
H 7.19248100 -1.61724200 3.61017500
H 7.31891800 -1.07803600 1.92946800
C -1.12063400 -1.15084100 1.48816200
C 0.01911800 -0.72776000 1.85729400
C -2.12563200 -1.37206300 0.43981800
N -3.14825700 -2.29791200 0.99226100
C -3.61405300 -1.89651100 2.31438900
C -2.44187100 -1.85197200 3.28606300
O -2.40464300 -1.04914300 4.22472900
H -1.82629800 -2.77890700 3.29626600
S -4.22352500 -3.01906000 -0.06478000
O -3.42214500 -3.48413900 -1.21074400
O -4.99260000 -3.99487000 0.72368200
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C -7.11798400 0.21717900 -1.57010300
H -5.72071200 0.44797100 -3.21022900
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H -4.31874100 -2.65400500 2.69254700
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H -8.89472800 1.44382300 -1.37537400
H -7.52874100 2.24397100 -2.20027200
H -8.47233700 1.01238600 -3.05332100
C 0.83314900 -0.70917400 3.10941600
H 0.16009800 -0.80518600 3.97978000
H 1.54186900 -1.55270100 3.13394100
H 1.41513900 0.21601500 3.22673300
TS-L4-endo-1f
P -0.83770600 -2.53958900 -0.51104100
P -1.54710300 2.18436200 -0.39251100
Pd -0.93922100 -0.17765000 -0.02274200
C -0.66700000 -3.81571100 0.89335700
C 0.78221000 -4.21953600 1.23852100

C	-1.37779500	-3.33370500	2.17532700	H	3.08154800	-2.33503500	-2.74349000
H	-1.18604600	-4.71962600	0.52549900	H	3.07072300	-3.95518500	-4.62580800
C	0.82544600	-5.27011200	2.36051800	H	1.35749600	-3.63427300	-4.93212400
H	1.35523200	-3.32786500	1.54981500	C	-0.69446200	3.62989000	0.47408400
H	1.29786100	-4.63159600	0.35970700	C	-1.00514700	3.70926700	1.98208600
C	-1.35355700	-4.39570600	3.28328200	C	0.83064500	3.60766300	0.24849400
H	-0.86370300	-2.42914400	2.53582900	H	-1.09590700	4.54365900	0.00493500
H	-2.41559900	-3.03694600	1.96663300	C	-0.31468900	4.91614900	2.63603800
C	0.07969100	-4.81772900	3.61891800	H	-0.65841700	2.78688700	2.47643300
H	1.87670900	-5.50685100	2.59965600	H	-2.09008500	3.77474500	2.15544300
H	0.37230100	-6.20808900	1.98873600	C	1.52622300	4.80649200	0.91084000
H	-1.86071600	-4.00469900	4.18243000	H	1.24043100	2.67841900	0.67577800
H	-1.93200800	-5.28077500	2.95831200	H	1.06544400	3.58852500	-0.82757200
H	0.08109600	-5.62143400	4.37558200	C	1.19971300	4.89932800	2.40550500
H	0.61299900	-3.96066400	4.07060100	H	-0.53839400	4.92803700	3.71687200
C	-2.39648900	-3.15366000	-1.39731800	H	-0.73938700	5.84839700	2.21873200
C	-3.63831300	-3.21622500	-0.48571000	H	2.61709200	4.73113900	0.75882700
C	-2.70264000	-2.32385400	-2.66013400	H	1.20499700	5.73818400	0.40874900
H	-2.16458500	-4.18682800	-1.70896100	H	1.66587300	5.79844300	2.84477900
C	-4.87833800	-3.72314200	-1.23866400	H	1.63212300	4.03022600	2.93428000
H	-3.84501900	-2.21099600	-0.07553400	C	-1.48456700	2.62490900	-2.23999000
H	-3.45402500	-3.87768500	0.37320300	C	-1.40038100	4.12096600	-2.60601100
C	-3.94338200	-2.83704800	-3.40560200	C	-0.39163800	1.83855800	-2.99153500
H	-2.86220300	-1.27017400	-2.36706600	H	-2.45792700	2.24567900	-2.60202700
H	-1.84149700	-2.32882400	-3.34421800	C	-1.50119900	4.33136800	-4.12560400
C	-5.17206000	-2.89779600	-2.49427300	H	-0.43685700	4.53128400	-2.25891500
H	-5.74850900	-3.71693700	-0.55960100	H	-2.18728200	4.69973900	-2.10186700
H	-4.71711500	-4.77828200	-1.52819200	C	-0.47550300	2.05354700	-4.50956100
H	-4.14156800	-2.19297400	-4.27984300	H	0.60413700	2.15626900	-2.63213100
H	-3.73523200	-3.84756000	-3.80398700	H	-0.47757500	0.76652300	-2.75591200
H	-6.03564200	-3.31846000	-3.03792900	C	-0.43030600	3.53914000	-4.88251600
H	-5.45806700	-1.87124300	-2.19869800	H	-1.41746600	5.40768100	-4.35618200
C	0.57758100	-3.01755800	-1.67587200	H	-2.50308700	4.01518100	-4.47124600
C	0.43918500	-4.39062700	-2.36221700	H	0.34204700	1.50594000	-5.00996000
C	0.95428200	-1.93448400	-2.70581300	H	-1.41943100	1.61412000	-4.88291200
H	1.43196800	-3.07820800	-0.98136000	H	-0.55513000	3.66651000	-5.97183600
C	1.72010800	-4.76785200	-3.12353600	H	0.56687200	3.94706500	-4.63210700
H	-0.40095700	-4.36131000	-3.07733000	C	-3.36304300	2.40547500	0.07682300
H	0.19839500	-5.17606800	-1.62757500	C	-4.01123500	3.77157200	-0.21514900
C	2.23872300	-2.31476600	-3.45850100	C	-4.23452500	1.26552500	-0.48634300
H	0.13832000	-1.79828900	-3.43520800	H	-3.33770400	2.27230800	1.17281500
H	1.08408000	-0.96493600	-2.20040000	C	-5.44435400	3.83841600	0.33646500
C	2.12042400	-3.68632700	-4.13287200	H	-4.04754100	3.93573300	-1.30574200
H	1.57762600	-5.73629800	-3.63389200	H	-3.41148400	4.59200900	0.20975400
H	2.54323400	-4.91382900	-2.39993700	C	-5.67408300	1.33594600	0.04494600
H	2.47776800	-1.53811000	-4.20558900	H	-4.25383900	1.32228700	-1.59012500

H	-3.78303100	0.29199800	-0.22990100
C	-6.31544000	2.70381000	-0.21325000
H	-5.89133900	4.81806600	0.09346800
H	-5.41299400	3.77450800	1.44006200
H	-6.28045200	0.53536200	-0.41296400
H	-5.66582600	1.13764000	1.13258000
H	-7.32508800	2.74375200	0.23101300
H	-6.44762300	2.84409800	-1.30250100
C	0.64227400	-0.05778200	1.46506500
C	0.36225300	0.09404900	2.70188400
C	1.92387400	-0.16165600	0.68928600
N	3.06416600	-0.31331200	1.61185300
C	3.21300800	0.75565700	2.59132600
C	2.24837000	0.62630900	3.76137800
O	1.98082500	1.62337300	4.45746400
H	2.21173200	-0.40040200	4.19376600
S	4.45111400	-1.05318100	1.03424300
O	5.29143400	-1.33850700	2.20822700
O	4.00316100	-2.16834500	0.18080700
C	5.34157700	0.10799200	0.00123400
C	6.37263500	0.87504300	0.55953300
C	4.98727200	0.25196200	-1.34464800
C	7.04203400	1.79807400	-0.24233200
H	6.65838200	0.74077700	1.60411000
C	5.67002800	1.18309800	-2.13039200
H	4.19832000	-0.36027900	-1.78463300
C	6.70354100	1.97120000	-1.59718100
H	7.85052800	2.39316000	0.19169500
H	5.39694200	1.29279800	-3.18328300
H	3.09808500	1.75094500	2.12651500
H	4.22129800	0.70452600	3.03293000
H	1.90231200	-1.03651500	0.03241000
H	2.05919700	0.72961800	0.04849700
C	7.44131700	2.97308800	-2.44476000
H	8.52205500	2.75325500	-2.46452400
H	7.07273200	2.97856000	-3.48078700
H	7.33184900	3.99161600	-2.03526800
C	-0.61645500	0.11193400	3.81075100
H	-0.34082400	0.93132300	4.49909700
H	-0.46820500	-0.81288900	4.40261200
C	-2.10864500	0.23507100	3.45576800
C	-3.00763400	0.12932400	4.69193800
H	-2.38352000	-0.54491100	2.72626800
H	-2.28430300	1.20025600	2.95445000
C	-4.49581400	0.29132800	4.38376400
H	-2.83769800	-0.84746700	5.18134100

H	-2.70001800	0.89263500	5.43038800
H	-5.10936800	0.19585700	5.29521600
H	-4.71072200	1.27998400	3.94335900
H	-4.84517300	-0.47307300	3.66845300

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P	2.39717700	-1.56617500	-0.85547900
P	0.30388100	2.55373000	0.25564600
Pd	1.10425200	0.26595500	0.03153100
C	1.59790200	-3.26351700	-1.17224500
C	1.68967000	-4.26135700	0.00112900
C	0.11809600	-3.11229200	-1.58566000
H	2.15905500	-3.69364200	-2.02190800
C	1.05198500	-5.61357600	-0.36062200
H	1.17186000	-3.84266100	0.88237600
H	2.73476700	-4.43478600	0.29554000
C	-0.51761300	-4.45704600	-1.96604300
H	-0.43565000	-2.69254800	-0.73283800
H	0.00288000	-2.39760800	-2.41298500
C	-0.40130400	-5.46975700	-0.82295500
H	1.11313400	-6.29105300	0.50888600
H	1.64660900	-6.08564700	-1.16523600
H	-1.57697100	-4.29649400	-2.22792500
H	-0.02400400	-4.85780000	-2.87146800
H	-0.80429200	-6.45043800	-1.13099200
H	-1.01923000	-5.12426900	0.02451900
C	3.11521900	-1.14915900	-2.56084000
C	2.08022600	-1.20674300	-3.70233200
C	3.82463400	0.21990800	-2.55843400
H	3.86788400	-1.93157900	-2.75985900
C	2.70680500	-0.86315400	-5.06296100
H	1.25846800	-0.49859400	-3.49098300
H	1.62877200	-2.20728300	-3.76605200
C	4.44762000	0.55670700	-3.92091700
H	3.08873700	1.00043000	-2.29193400
H	4.60461600	0.25173000	-1.78365800
C	3.41440900	0.49434600	-5.04886600
H	1.92543800	-0.88383000	-5.84230400
H	3.43630300	-1.64947100	-5.33265700
H	4.91289700	1.55671800	-3.87686100
H	5.26434400	-0.15788200	-4.13434700
H	3.89399700	0.68892500	-6.02379300
H	2.66563100	1.29515100	-4.90234400
C	3.90886100	-1.98588800	0.20217200
C	4.99778600	-2.83664600	-0.47929100
C	4.54237900	-0.77007800	0.90893300
H	3.45805800	-2.59923600	1.00106000

C	6.07132300	-3.27904800	0.52820800	H	4.12375400	5.66263700	1.38900700
H	5.48218100	-2.24501200	-1.27540900	C	-0.97999100	2.86364900	-1.09471800
H	4.55927000	-3.72132100	-0.96895700	C	-1.54737400	4.28899200	-1.22954900
C	5.61063400	-1.21357300	1.91967800	C	-0.49540400	2.34977900	-2.46567200
H	5.01108400	-0.10260200	0.16647400	H	-1.80675900	2.20062000	-0.78150100
H	3.76297000	-0.17735700	1.41353900	C	-2.67334700	4.34319200	-2.27463400
C	6.68863000	-2.08426900	1.26387200	H	-0.74294400	4.97586100	-1.54351300
H	6.85555200	-3.85582100	0.00771100	H	-1.92145800	4.65914500	-0.26190400
H	5.61590400	-3.96599600	1.26535300	C	-1.60883900	2.41551600	-3.52131200
H	6.06879700	-0.32716300	2.39179300	H	0.36174300	2.95754200	-2.80857400
H	5.12492600	-1.78469900	2.73282700	H	-0.12616900	1.31491500	-2.36763400
H	7.41333900	-2.43295700	2.01989900	C	-2.20686500	3.82186600	-3.63819600
H	7.26066000	-1.47073400	0.54278300	H	-3.04671900	5.37792800	-2.36635700
C	-0.51491200	3.22576100	1.81530400	H	-3.52602900	3.73357900	-1.92165800
C	-1.91157100	2.62833000	2.07941200	H	-1.21663700	2.08213300	-4.49763800
C	0.38566300	3.04037000	3.05341200	H	-2.40711600	1.70131700	-3.24655600
H	-0.64394300	4.30847200	1.64836200	H	-3.04380200	3.82420400	-4.35782700
C	-2.54949700	3.23103400	3.34088800	H	-1.44226700	4.50931200	-4.04606100
H	-1.82430300	1.53553000	2.20429800	C	-1.16363900	-1.06353000	1.39360900
H	-2.57863700	2.79802100	1.22010100	C	0.05607100	-0.79004500	1.65724600
C	-0.25240000	3.64073000	4.31485200	C	-2.19194600	-0.88579400	0.34312500
H	0.56124900	1.96268400	3.21355200	N	-3.01523300	-2.11365500	0.29651100
H	1.37456400	3.49517700	2.88704800	C	-3.45790600	-2.53252200	1.62567800
C	-1.65090900	3.06994100	4.57148600	C	-2.24028800	-2.82096000	2.50611700
H	-3.53248000	2.76152800	3.51906200	O	-1.54403700	-3.83026400	2.34459100
H	-2.74402800	4.30630200	3.17019200	H	-2.23178900	-2.27502500	3.47237000
H	0.40266700	3.45983500	5.18463400	S	-4.03806900	-2.34390200	-1.00504300
H	-0.32159000	4.73840500	4.19927900	O	-3.27772400	-1.94657100	-2.20362600
H	-2.11026900	3.55731900	5.44888700	O	-4.54412900	-3.72246900	-0.89809900
H	-1.56477600	1.99574200	4.81988000	C	-5.43108800	-1.23246800	-0.84559900
C	1.70908700	3.77413700	-0.12038200	C	-5.35598300	0.05086600	-1.39692200
C	1.52528300	5.23127500	0.35139900	C	-6.56979400	-1.64958000	-0.14312300
C	3.08177700	3.24161600	0.34139000	C	-6.43320100	0.92455800	-1.23217300
H	1.72267000	3.77922600	-1.22572400	H	-4.47483400	0.36184200	-1.96072100
C	2.67130400	6.12736900	-0.14607900	C	-7.63359600	-0.76223400	0.00984600
H	1.50886700	5.26225000	1.45416500	H	-6.62934300	-2.65983000	0.26574600
H	0.56346000	5.64149600	0.01171500	C	-7.58505400	0.53810300	-0.52715700
C	4.23091100	4.13695400	-0.14295300	H	-6.37747900	1.92606600	-1.66711100
H	3.10324700	3.18678800	1.44469000	H	-8.52530400	-1.08756900	0.55314600
H	3.22289700	2.21097500	-0.02174500	H	-4.03594800	-3.46411500	1.54086800
C	4.04114200	5.59532500	0.28804700	H	-4.08295100	-1.75755600	2.10814200
H	2.52410200	7.15656900	0.22498800	H	-2.82547200	-0.00789300	0.58384300
H	2.63451500	6.18513600	-1.24990300	H	-1.74840400	-0.72387900	-0.64988500
H	5.19249200	3.74666300	0.23333100	C	-8.74722300	1.47855800	-0.34940600
H	4.28471100	4.08814500	-1.24670600	H	-9.66978300	1.04994600	-0.77595500
H	4.84720500	6.22658100	-0.12449500	H	-8.94647100	1.66023500	0.72032000

H	-8.56334300	2.44859000	-0.83380900	H	5.46329200	3.06500500	-0.49412100
C	1.07850700	-0.97775500	2.73782600	H	4.62122200	4.60581300	-0.27796900
H	1.85785300	-1.66715300	2.37253400	H	3.27496500	4.65091900	-3.87432800
H	1.59645900	-0.01987800	2.91411300	H	3.26065200	5.58468800	-2.37231900
C	0.53507400	-1.50631900	4.07709800	H	5.45722900	4.46490600	-2.60838200
C	1.62376300	-1.60210500	5.15053000	H	4.67384500	2.89402000	-2.83124300
H	0.08711100	-2.50100800	3.92104500	C	-1.04373800	3.34817100	-0.98821600
H	-0.27569400	-0.84561700	4.43124900	C	-1.21621200	4.87147900	-1.16328800
C	1.11164900	-2.14716500	6.48362600	C	-1.29107600	2.60628600	-2.31820700
H	2.44334100	-2.24568500	4.78120900	H	-1.84070600	3.01716300	-0.29992500
H	2.07146200	-0.60365700	5.30807200	C	-2.59286600	5.20880900	-1.75889500
H	1.91824400	-2.20482800	7.23342200	H	-0.43273100	5.26821100	-1.83024200
H	0.31562000	-1.50680400	6.90131400	H	-1.10207400	5.39377700	-0.20091900
H	0.69192900	-3.16133200	6.36865100	C	-2.66728700	2.95673700	-2.90399000
TS-L4-endo-1g				H	-0.51113600	2.87062400	-3.05107200
P	0.49370500	2.74747600	-0.06500900	H	-1.21311800	1.51780000	-2.15855900
P	1.63756300	-1.75959500	-1.23587300	C	-2.84422900	4.46921300	-3.07714600
Pd	0.81813000	0.32654200	-0.28795300	H	-2.67401300	6.29954500	-1.90765600
C	0.25442200	3.63656200	1.59227400	H	-3.37888100	4.93232100	-1.03208000
C	-0.91895200	3.04161600	2.39649900	H	-2.80365700	2.43984800	-3.86972100
C	1.51479400	3.72767900	2.47344500	H	-3.45479900	2.57638900	-2.22803800
H	-0.01289000	4.66983200	1.31006300	H	-3.85556300	4.69617000	-3.45661800
C	-1.18835700	3.83213800	3.68514500	H	-2.13360900	4.83487300	-3.84193800
H	-0.68035400	1.99752800	2.65843600	C	0.51649000	-3.24150400	-1.53121500
H	-1.83907000	3.00632600	1.79397800	C	0.10046100	-3.96302900	-0.23434000
C	1.24165600	4.50639300	3.77087900	C	-0.72825700	-2.85380700	-2.35511000
H	1.86879300	2.71251500	2.72367600	H	1.11174300	-3.95167900	-2.12949600
H	2.33256100	4.22462200	1.93140300	C	-0.78958900	-5.17972100	-0.53087900
C	0.06387200	3.92892500	4.56118800	H	-0.44533800	-3.26116900	0.41838800
H	-2.01420200	3.35676500	4.24207900	H	0.98716600	-4.29055000	0.32966400
H	-1.53236500	4.85044100	3.42443500	C	-1.61882400	-4.07049900	-2.64624100
H	2.15459000	4.51721900	4.39120800	H	-1.31072800	-2.10178800	-1.79514200
H	1.02546700	5.56100600	3.51733600	H	-0.43470900	-2.37560100	-3.30221900
H	-0.13641900	4.54447200	5.45525700	C	-2.02052800	-4.80306600	-1.36189500
H	0.32928000	2.92040500	4.92866900	H	-1.09649100	-5.65265600	0.41787800
C	2.01527900	3.62415300	-0.78021400	H	-0.19785400	-5.93601800	-1.07954600
C	3.30434700	2.88693100	-0.35189700	H	-2.51604700	-3.74846400	-3.20259900
C	2.02866800	3.80469600	-2.31138000	H	-1.07399400	-4.76805600	-3.30920200
H	2.01456100	4.63086600	-0.32437500	H	-2.61149700	-5.70372700	-1.60231800
C	4.56811000	3.63293400	-0.80127400	H	-2.67891600	-4.14871200	-0.76090100
H	3.29323200	1.87942000	-0.80682700	C	2.40775700	-1.38378800	-2.92915700
H	3.33205800	2.72781800	0.73557100	C	2.56745600	-2.56615200	-3.90713700
C	3.28792200	4.55498100	-2.77479200	C	1.71144600	-0.20518800	-3.63952800
H	1.99642100	2.81502800	-2.79880600	H	3.42054200	-1.03801400	-2.65332300
H	1.14114200	4.35336800	-2.65306500	C	3.33419600	-2.14239200	-5.17033100
C	4.57695200	3.86719100	-2.31495100	H	1.57157500	-2.93305500	-4.20795100

H	3.08254600	-3.41173600	-3.42972000	C	-6.91071800	-2.16537600	-1.47387400
C	2.46417200	0.21761300	-4.90878700	H	-7.90062600	-2.82171300	0.33489200
H	0.67871800	-0.49164300	-3.90672200	H	-5.73946200	-1.27868100	-3.06690700
H	1.62462400	0.64843000	-2.94757200	H	-2.93316400	-2.37860500	1.75994900
C	2.66422400	-0.95688800	-5.87296300	H	-3.95704300	-1.52881500	2.94551000
H	3.41463500	-3.00118000	-5.85911700	H	-2.00572800	0.78239500	0.07237900
H	4.36853300	-1.86665300	-4.89267400	H	-2.13538400	-0.96173900	-0.21054400
H	1.92118300	1.03815600	-5.40899100	C	-7.71019900	-3.04501100	-2.39774900
H	3.45181600	0.62507000	-4.62288000	H	-7.04933800	-3.70814700	-2.98093800
H	3.26059600	-0.63999500	-6.74597300	H	-8.42534000	-3.67145800	-1.84512100
H	1.68084200	-1.27675600	-6.26536300	H	-8.27547300	-2.43927300	-3.12627400
C	3.05792800	-2.43856600	-0.19891600	C	0.94349600	-1.26257100	3.09121700
C	3.79231200	-3.67833500	-0.74337300	C	1.27575000	-2.60615200	3.38023100
C	4.06735800	-1.33073600	0.16660400	C	1.70481300	-0.25812000	3.73634400
H	2.54871000	-2.72877100	0.73683800	C	2.32425100	-2.92080100	4.24907300
C	4.84504000	-4.18626900	0.25451000	H	0.69803400	-3.40929400	2.91983400
H	4.30183400	-3.41946800	-1.68699100	C	2.74580600	-0.58329600	4.60478700
H	3.08082000	-4.48615200	-0.97695600	H	1.46399100	0.79033100	3.55260900
C	5.13825700	-1.83782100	1.14430400	C	3.08090400	-1.92185600	4.88261800
H	4.56377600	-0.96290500	-0.74980200	H	2.55522300	-3.97265500	4.44483300
H	3.53570600	-0.46974300	0.60467000	H	3.31230200	0.22264600	5.08274000
C	5.85056600	-3.08944800	0.62040200	C	4.21036900	-2.25781900	5.82414200
H	5.36735700	-5.06105300	-0.17024500	H	5.17712000	-1.88510400	5.44264800
H	4.33776100	-4.53868100	1.17152000	H	4.06165900	-1.79364000	6.81425600
H	5.86852800	-1.03431900	1.34293100	H	4.30495000	-3.34441300	5.97146000
H	4.65875200	-2.07096500	2.11183400				
H	6.57052700	-3.46191900	1.36955500	TS-L4-exo-1g			
H	6.44139700	-2.82544900	-0.27679200	P	0.34702100	2.70833300	-0.15467800
C	-0.56231000	-0.41001800	1.13832800	P	2.14184300	-1.64333800	-0.86948100
C	-0.19067800	-0.93771800	2.25864500	Pd	0.93310200	0.34060900	-0.13262600
C	-1.93835300	-0.19389000	0.56160500	C	1.91010800	3.76583600	-0.33285100
N	-2.96882900	-0.25066700	1.61282300	C	2.66036400	3.94361700	1.00492600
C	-3.00211600	-1.47907500	2.39814100	C	2.88785300	3.19103800	-1.37998300
C	-1.91545200	-1.53520600	3.46423100	H	1.57671800	4.76132000	-0.67477300
O	-1.66178000	-2.62512800	4.01372100	C	3.90244800	4.83416000	0.84526400
H	-1.79746700	-0.57428900	4.01808600	H	2.97339800	2.95161400	1.37563500
S	-4.43089800	0.51592300	1.31974200	H	2.00783700	4.37496900	1.77751800
O	-5.13187300	0.59302100	2.61083500	C	4.12854000	4.07961400	-1.55327700
O	-4.11580900	1.76341600	0.59879200	H	3.20256800	2.18527600	-1.04873500
C	-5.41096800	-0.51159300	0.22827800	H	2.39618800	3.05522800	-2.35232400
C	-6.39089100	-1.34992800	0.76816500	C	4.85895100	4.30172900	-0.22573600
C	-5.17265600	-0.47933600	-1.15315700	H	4.42110500	4.92019200	1.81584100
C	-7.13138000	-2.16955000	-0.08725800	H	3.58068800	5.85644300	0.57237800
H	-6.58464000	-1.35417300	1.84200700	H	4.80798100	3.62503300	-2.29501000
C	-5.92141200	-1.30579400	-1.98884000	H	3.82089500	5.05662700	-1.97057400
H	-4.42074100	0.18930000	-1.57580900	H	5.70782300	4.99394100	-0.36230400
				H	5.28902600	3.34203400	0.11646700

C	-0.78610300	3.19428500	-1.60719100	H	1.00102700	-6.04194900	-0.28648800
C	-0.09855700	3.68101100	-2.89681500	H	-1.63894000	-4.44619100	-2.57159300
C	-1.76842200	2.05228000	-1.93991200	H	-0.06389600	-5.25523000	-2.62035400
H	-1.37658000	4.04294800	-1.22261300	H	-1.41518700	-6.23757300	-0.79805000
C	-1.13212500	4.11782300	-3.94708900	H	-1.72795900	-4.64040100	-0.10757300
H	0.51538900	2.86785000	-3.32137100	C	2.86358000	-1.29652400	-2.58978300
H	0.58045100	4.52143100	-2.68724600	C	3.23931200	-2.51497500	-3.45761100
C	-2.79967900	2.47481100	-2.99631900	C	1.98284500	-0.32457200	-3.40218900
H	-1.19351900	1.18507900	-2.31200100	H	3.79711400	-0.75671400	-2.34733400
H	-2.28673100	1.70984500	-1.03192200	C	3.93567700	-2.07964600	-4.75731800
C	-2.12890900	3.00012600	-4.26947800	H	2.32623000	-3.07628000	-3.71913600
H	-0.61094900	4.44429000	-4.86373400	H	3.88893100	-3.21066100	-2.90726400
H	-1.68175000	5.00008900	-3.56950600	C	2.66681800	0.10747900	-4.70687900
H	-3.45932600	1.62219100	-3.23369100	H	1.01938100	-0.81026000	-3.63898000
H	-3.44954400	3.26379700	-2.57384800	H	1.74044100	0.55950100	-2.78931800
H	-2.88851600	3.35702700	-4.98637200	C	3.07911600	-1.09607900	-5.56159300
H	-1.59432600	2.16980500	-4.76740200	H	4.17230000	-2.96936500	-5.36639400
C	-0.53043000	3.52576500	1.31115400	H	4.90319700	-1.60449400	-4.50974600
C	-0.68071300	5.05942100	1.23448200	H	1.99620400	0.77276700	-5.27802400
C	-1.89316000	2.87705700	1.62565700	H	3.56507700	0.70471500	-4.46208300
H	0.13742500	3.29506900	2.15909500	H	3.62207200	-0.76026300	-6.46205700
C	-1.29159300	5.62829800	2.52567200	H	2.17070000	-1.61557000	-5.91968800
H	-1.33513200	5.32617900	0.38600500	C	3.64157800	-1.98789600	0.22241000
H	0.28770200	5.54678000	1.04565800	C	4.56338800	-3.15171200	-0.18840900
C	-2.50191400	3.44392000	2.91723400	C	4.47049900	-0.71086700	0.46728500
H	-2.59296800	3.06445600	0.79238100	H	3.17139500	-2.25276600	1.18647100
H	-1.78383000	1.78607100	1.71296500	C	5.66077800	-3.39153900	0.86064700
C	-2.63258800	4.96945300	2.86426600	H	5.04574900	-2.91536600	-1.15213700
H	-1.41398800	6.72091400	2.42693500	H	3.98664700	-4.07749800	-0.34075300
H	-0.58491000	5.46812100	3.36106600	C	5.58245900	-0.94572500	1.50074500
H	-3.48697600	2.97981500	3.09815000	H	4.92829600	-0.37794400	-0.48193600
H	-1.86154000	3.16082200	3.77320200	H	3.81044000	0.10578900	0.80212500
H	-3.01949100	5.35648600	3.82285000	C	6.48370700	-2.12459200	1.11754300
H	-3.37673900	5.24360600	2.09311800	H	6.31699000	-4.21567000	0.53086000
C	1.29421500	-3.32099300	-1.02528400	H	5.19352600	-3.72290900	1.80653400
C	0.99127600	-3.96549800	0.34114000	H	6.18152500	-0.02593700	1.61754300
C	0.00578200	-3.22284200	-1.86649600	H	5.12179200	-1.14557700	2.48532300
H	2.00338100	-3.97629400	-1.55904600	H	7.23356700	-2.30601200	1.90697000
C	0.30013100	-5.32901800	0.18725500	H	7.04936200	-1.86834500	0.20210400
H	0.33451100	-3.29825800	0.92100800	C	-1.20971600	-0.86790600	1.49293600
H	1.91461000	-4.09181400	0.92728400	C	-0.00687300	-0.45736100	1.66678100
C	-0.69689200	-4.58117700	-2.01326500	C	-2.29830700	-0.91597200	0.49356500
H	-0.68606500	-2.51416800	-1.38268300	N	-3.16681600	-2.07342000	0.80296400
H	0.22449800	-2.81104900	-2.86431100	C	-3.45170000	-2.19802600	2.23094500
C	-0.97568700	-5.23481400	-0.65534100	C	-2.14085100	-2.45195000	2.97247000
H	0.06757200	-5.73506300	1.18676200	O	-1.51765300	-3.50705100	2.81798800

H	-1.95766000	-1.80084500	3.85451000	H	-9.03611200	1.83556800	0.96989300
S	-4.31599100	-2.55013700	-0.30778300	H	-8.82118000	2.24334500	-0.75422100
O	-3.68403000	-2.43209400	-1.63387000	H	-9.90661300	0.91431200	-0.26624200
O	-4.81150500	-3.86139900	0.14244000	C	0.97164800	-0.45918800	2.77003800
C	-5.68725100	-1.40157400	-0.25387100	C	1.69116700	0.69297400	3.14271600
C	-5.69113900	-0.29237500	-1.10562600	C	1.18514800	-1.63193500	3.52752200
C	-6.72944000	-1.61268200	0.65929500	C	2.57336700	0.67716600	4.22512600
C	-6.74953700	0.61637200	-1.03257300	H	1.54745100	1.61697300	2.58343700
H	-4.88690200	-0.14722000	-1.82899200	C	2.07061200	-1.63877200	4.60724800
C	-7.77519100	-0.69344400	0.71708700	H	0.63314600	-2.53978900	3.28056800
H	-6.73117900	-2.49203400	1.30589000	C	2.78698700	-0.48844900	4.97963800
C	-7.80444100	0.43586300	-0.12302700	H	3.10527200	1.59567800	4.49147300
H	-6.75638800	1.48058600	-1.70217600	H	2.20583800	-2.56382100	5.17658600
H	-8.59178300	-0.85885500	1.42564400	C	3.76427800	-0.51332400	6.12726400
H	-4.10144400	-3.06986600	2.39738700	H	3.43157900	-1.19266800	6.92800700
H	-3.94497000	-1.29295000	2.63136300	H	4.75667400	-0.86841000	5.79525700
H	-2.88124200	0.02637100	0.54402200	H	3.90635700	0.48903300	6.56018300
H	-1.92364700	-1.02373100	-0.53447300				
C	-8.94751500	1.41255500	-0.04498000				