

# Electronic Supplementary Information

## Oxymetalation or Oxidative Cyclization? Mechanism of Pd-Catalyzed Annulation of Enynones

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## 1. Complete reference for Gaussian 09

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.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; 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, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J. Gaussian 09, revision D.01; Gaussian, Inc.: Wallingford, CT, 2013.

## 2. Computational methods.

All DFT calculations were carried out using Gaussian 09 program. In the gas phase, all geometry optimizations were performed with the B3LYP functional<sup>1</sup> using the def2-SVP basis set<sup>2</sup> for all atoms. The vibrational frequencies were computed at the same level of theory as for the geometry optimizations to confirm whether each optimized structure is an energy minimum or a transition state, and to evaluate the zero-point vibrational energy (ZPVE) and thermal corrections. The single-point energies and solvent effects were computed with the M06-2X<sup>3</sup> functional using the def2-TZVP basis set<sup>2</sup> for all atoms, based on the gas-phase optimized structures. The solvation energies were evaluated by a self-consistent reaction field (SCRF) using the SMD implicit solvent model.<sup>4</sup>

The global reactivity index (GRI) values were also calculated using B3LYP functional and the def2-SVP basis set for all atoms. The  $\omega$  (electrophilicity index)<sup>5</sup> values were calculated according to eq 1. In eq 1, the  $\mu$  (electronic chemical potential)

value could be obtained by  $\mu = (\epsilon_{\text{HOMO}} + \epsilon_{\text{LUMO}})/2$  and the  $\eta$  (chemical hardness) value could be obtained by  $\eta = \epsilon_{\text{HOMO}} - \epsilon_{\text{LUMO}}$ .<sup>6</sup>

$$\omega = (\mu)^2/2\eta \quad (1)$$

$$N = \epsilon_{\text{HOMO}}(\text{Nu}) - \epsilon_{\text{HOMO}}(\text{TCE}) \quad (2)$$

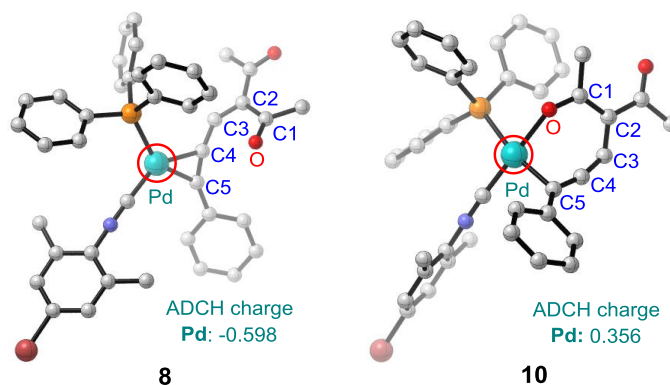
The  $\epsilon_{\text{HOMO}}$  values refer to the orbital energies of the highest occupied molecular orbital (HOMO), and the corresponding orbital and the  $\epsilon_{\text{LUMO}}$  values refer to the orbital energies of the lowest unoccupied molecular orbital (LUMO). The N (nucleophilicity index)<sup>7</sup> values were calculated with eq 2. In eq 2, tetracyanoethylene (TCE) with the lowest HOMO energy among the organic molecules serves as a reference.<sup>8</sup>

The  $\omega_k$  (local electrophilicity) values were calculated according to eq 3.<sup>9</sup> In eq 3, the  $f_k^+$  (Fukui function) value could be obtained by  $f_k^+ = q_k(N+1) - q_k(N)$ .<sup>10</sup>

$$\omega_k = \omega \cdot f_k^+ \quad (3)$$

### 3. The critical electronic and geometric information for intermediate 8, 10, and transition state 9-ts.

**Table S1.** Optimized geometries for intermediate 8 and 10. Bond lengths are given in angstroms.

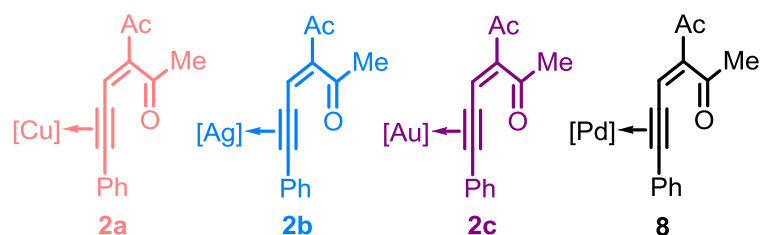


Complex	8	9-ts	10
Pd-O	4.07	2.34	2.19
O-C1	1.22	1.26	1.28
C1-C2	1.50	1.45	1.44
C2-C3	1.38	1.43	1.44
C3-C4	1.41	1.36	1.35

C4-C5	1.28	1.28	1.29
C5-Pd	2.08	2.12	2.12

#### 4. Detailed information of reactivity index calculation.

**Table S2.** Nucleophilicity ( $N$ , eV) and electrophilicity ( $\omega$ , eV) values of the complexes **2a**, **2b**, **2c**, and **8**, involved in the reaction pathway.



Complex	$E_{\text{HOMO}}$	$E_{\text{LUMO}}$	$E_{\text{TCE}}$	$\eta$	$\mu$	$\omega$	$f_k^+$	$\omega_k$	$N$
<b>2a</b>	-9.201	-5.659	-9.275	3.542	-7.430	7.79	0.027	0.21	0.07
<b>2b</b>	-9.201	-5.627	-9.275	3.574	-7.414	7.69	0.023	0.18	0.07
<b>2c</b>	-9.183	-5.688	-9.275	3.495	-7.435	7.91	0.018	0.15	0.09
<b>8</b>	-5.493	-2.036	-9.275	3.456	-3.765	2.05	0.000	0.00	3.78

#### 5. M06-2X/def2-TZVP//B3LYP/def2-SVP calculated absolute energies, enthalpies, and free energies of all structures.

**Table S3.** M06-2X/def2-TZVP//B3LYP/def2-SVP calculated absolute energies, enthalpies, and free energies of all structures.

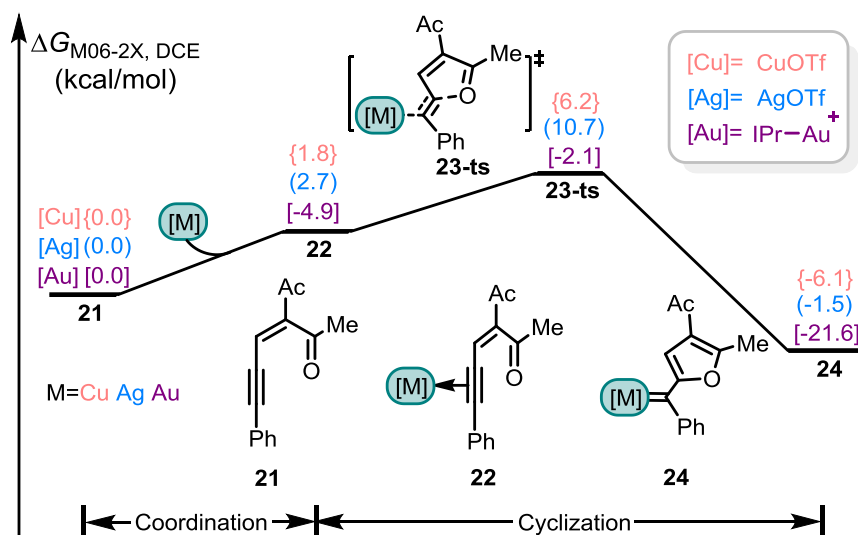
Geometry	$E_{(\text{elec-B3LYP})}^1$	$H_{(\text{corr-B3LYP})}^2$	$G_{(\text{corr-B3LYP})}^3$	$E_{(\text{solv-M06-2X})}^4$	$IF^5$
1	-690.591188	0.234804	0.170736	-691.073745	-
[Cu]	-2799.383354	0.603009	0.503834	-2800.365407	-
[Ag]	-1306.053747	0.602917	0.499930	-1306.788359	-
[Au]	-1294.821784	0.603349	0.502138	-1295.495220	-
2a	-3490.029630	0.839722	0.698307	-3491.466611	-
2b	-1996.685878	0.839519	0.695761	-1997.885245	-
2c	-1985.468288	0.839840	0.697773	-1986.603417	-
3a-ts	-3490.027050	0.838573	0.700712	-3491.452966	235.84 <i>i</i>
3b-ts	-1996.684407	0.838392	0.697143	-1997.874069	215.57 <i>i</i>
3c-ts	-1985.468279	0.838857	0.699842	-1986.601027	71.18 <i>i</i>
4a	-3490.059593	0.841075	0.703468	-3491.477720	-
4b	-1996.715089	0.840878	0.700305	-1997.898408	-
4c	-1985.510595	0.841397	0.702778	-1986.635148	-
5	-2199.428812	0.586342	0.470857	-2200.416511	-

6	-2890.035223	0.823101	0.675743	-2891.514953	-
7	-2976.072523	0.155113	0.105448	-2976.676045	-
8	-4830.407985	0.687446	0.546419	-4831.924189	-
9-ts	-4830.398898	0.686112	0.552443	-4831.922138	21.32 <i>i</i>
10	-4830.400923	0.687160	0.550824	-4831.924189	-
11-ts	-4830.382527	0.685717	0.548965	-4831.906562	304.19 <i>i</i>
12	-4830.418798	0.688234	0.555634	-4831.936693	-
13-ts	-4830.394553	0.686493	0.550735	-4831.908094	275.58 <i>i</i>
14	-4830.430623	0.688925	0.553080	-4831.958307	-
PPh <sub>3</sub>	-1035.715362	0.290555	0.227673	-1036.261684	-
15	-3666.741548	0.394513	0.306563	-3667.825416	-
16-ts	-4830.381252	0.686077	0.549200	-4831.899962	409.77 <i>i</i>
17	-4830.393037	0.687993	0.553384	-4831.920765	-
18-ts	-4830.381452	0.686862	0.550771	-4831.903155	291.78 <i>i</i>
19-ts	-5866.071327	0.978087	0.802112	-5868.158521	412.68 <i>i</i>
20	-5866.128385	0.981613	0.809200	-5868.225136	-
21	-690.591188	0.234804	0.170736	-691.075204	-
CuOTf	-2601.209583	0.038457	-0.008250	-2602.074733	-
AgOTf	-1107.886113	0.038325	-0.009469	-1108.503766	-
IPr-Au <sup>+</sup>	-1294.821784	0.603349	0.502138	-1295.501162	-
22a	-3291.866901	0.275413	0.185036	-3293.169579	-
22b	-1798.516498	0.275042	0.181482	-1799.594920	-
22c	-1985.468288	0.839840	0.697773	-1986.609071	-
23a-ts	-3291.860717	0.274064	0.186232	-3293.163846	271.56 <i>i</i>
23b-ts	-1798.510538	0.273887	0.184240	-1799.584959	304.49 <i>i</i>
23c-ts	-1985.468279	0.838857	0.699842	-1986.606656	71.18 <i>i</i>
24a	-3291.884481	0.276854	0.189229	-3293.186478	-
24b	-1798.538139	0.276625	0.187348	-1799.607502	-
24c	-1985.510595	0.841397	0.702778	-1986.640624	-
25-ts	-5866.113739	0.979354	0.802619	-5868.196615	96.02 <i>i</i>
26	-5866.158298	0.982693	0.807472	-5868.248050	-
27-ts	-2890.011555	0.821493	0.674187	-2891.483211	455.18 <i>i</i>
28	-2890.034945	0.823722	0.673963	-2891.500679	-
Cu <sup>+</sup> -PPh <sub>3</sub>	-2675.850995	0.294191	0.225067	-2676.637997	-
Ag <sup>+</sup> -PPh <sub>3</sub>	-1182.532506	0.294190	0.224688	-1183.065969	-
Pd-PPh <sub>3</sub>	-1163.662495	0.293665	0.224883	-1164.110809	-
29a	-3366.499900	0.530589	0.416754	-3367.732477	-
29b	-1873.163101	0.529593	0.417701	-1874.158227	-
29c	-1854.294713	0.529976	0.416266	-1855.214184	-
30a-ts	-3366.498167	0.529360	0.418545	-3367.721435	213.15 <i>i</i>
30b-ts	-1873.162338	0.529358	0.416884	-1874.147795	184.07 <i>i</i>
30c-ts	-1854.275347	0.528459	0.416699	-1855.184647	438.47 <i>i</i>
31a	-3366.531399	0.532080	0.421361	-3367.744290	-
31b	-1873.194207	0.531889	0.420464	-1874.171265	-

31c	-1854.297423	0.530832	0.419686	-1855.208882	-
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<sup>1</sup>The electronic energy calculated by B3LYP in gas phase. <sup>2</sup>The thermal correction to enthalpy calculated by B3LYP in gas phase. <sup>3</sup>The thermal correction to Gibbs free energy calculated by B3LYP in gas phase. <sup>4</sup>The electronic energy calculated by M06-2X in tetrahydrofuran or dichloromethane solvent. <sup>5</sup>The B3LYP calculated imaginary frequencies for the transition states.

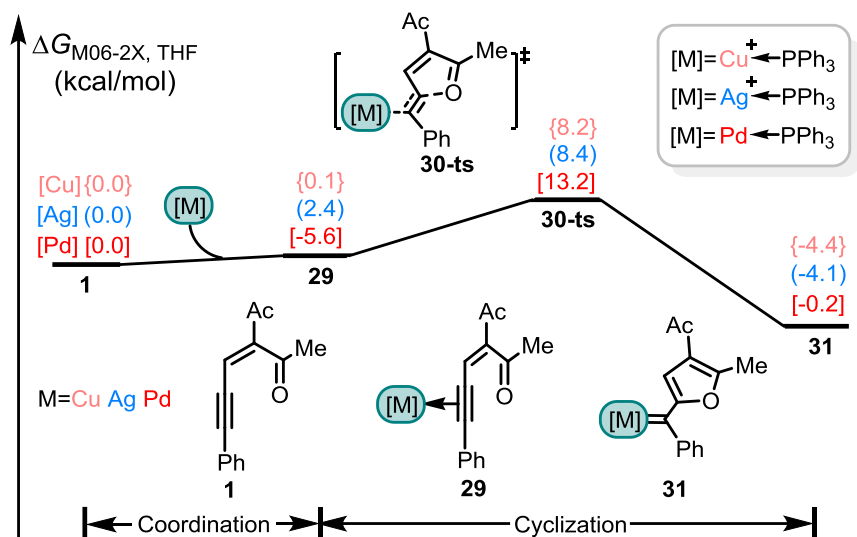
## 6. Free-energy profiles for coinage-metals-catalyzed cyclization of enynones.



**Figure S1.** Free-energy profiles for the CuOTf, AgOTf, or IPr-Au<sup>+</sup>(I)-catalyzed cyclization of enynone to afford metal carbene complexes. The energies are in kcal/mol and represent the relative free energies, which were calculated using the M06-2X/def2-TZVP//B3LYP/def2-SVP method in dichloromethane solvent.

CuOTf(I), AgOTf(I), or IPrAu<sup>+</sup>(I) were used as active catalysts,<sup>11</sup> enynone **21** can be activated by the coordination in corresponding complex **22**. An intramolecular nucleophilic attack via five membered ring type transition state **23-ts** leads to the formation of furanyl-carbene intermediates **24**. DFT calculations found that the activation free energy for this step is only 6.2, 10.7, or -2.1 kcal/mol, when Cu(I), Ag(I), or Au(I) was used respectively.

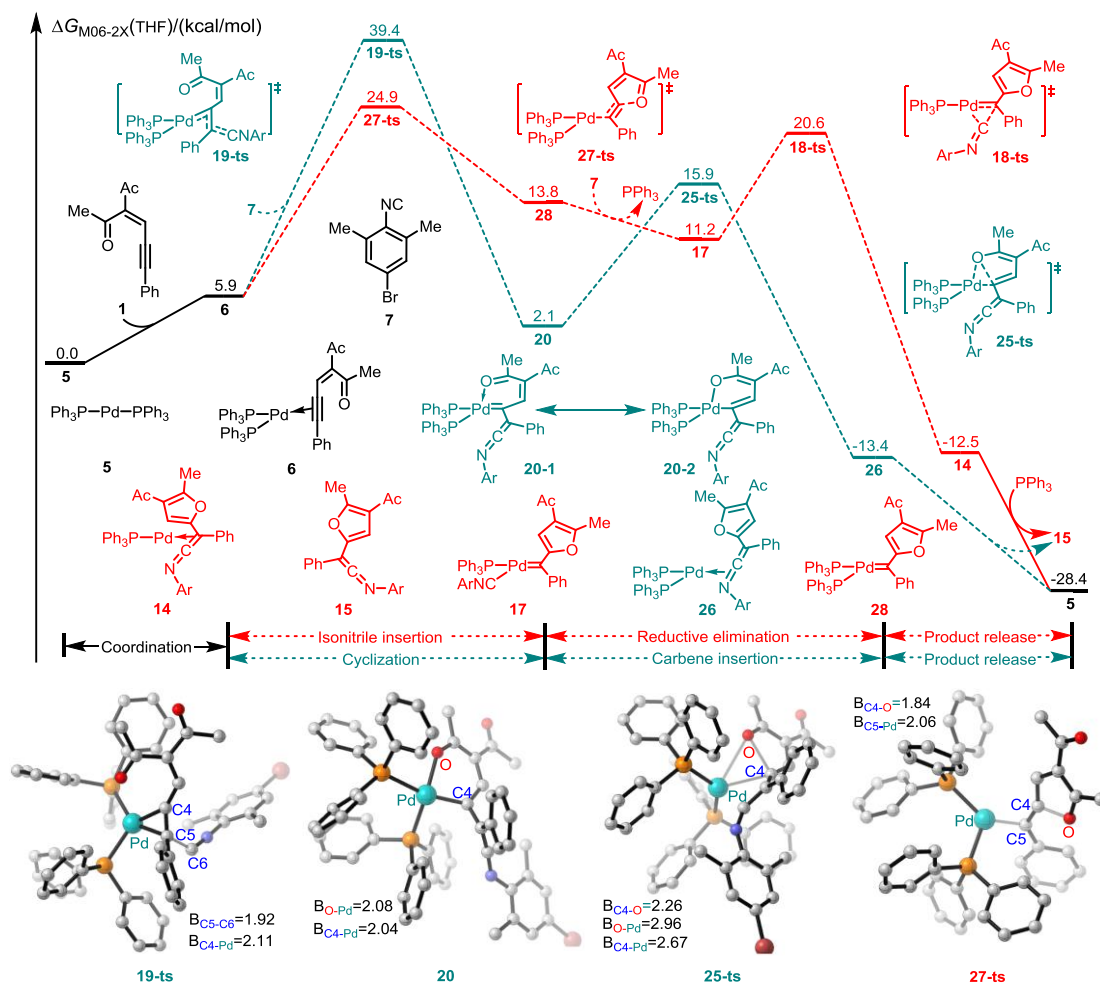
## 7. Free-energy profiles for transition-metals-mediated cyclization of enynones.



**Figure S2.** Free-energy profiles for the Cu, Ag, or Pd-mediated cyclization of enynones to afford metal carbene complexes. The energies are in kcal/mol and represent the relative free energies, which were calculated using the M06-2X/def2-TZVP//B3LYP/def2-SVP method in tetrahydrofuran solvent.

As shown in Figure S2, we calculated the free energy profiles for the cyclization process by using Cu, Ag or Pd with PPh<sub>3</sub> ligand. The coordination of enynone **1** onto Cu, Ag or Pd forms corresponding complex **29**. Subsequently, an intramolecular nucleophilic attack would take place via a five-membered ring-type transition state **30-ts** to afford the furan metal-carbene intermediate **31**. The calculated free energy barrier for this step is 8.2 or 8.4 kcal/mol, when Cu or Ag was used. However, the free energy barrier for this step with Pd was as high as 13.2 kcal/mol, which was evidently higher than that with coinage metals. This free-energy profiles reveals that the ligand cannot affect the reactivity in direct cyclization pathway.

## 8. Free-energy profiles for Pd-catalyzed enynones and isocyanide to ketenimine.



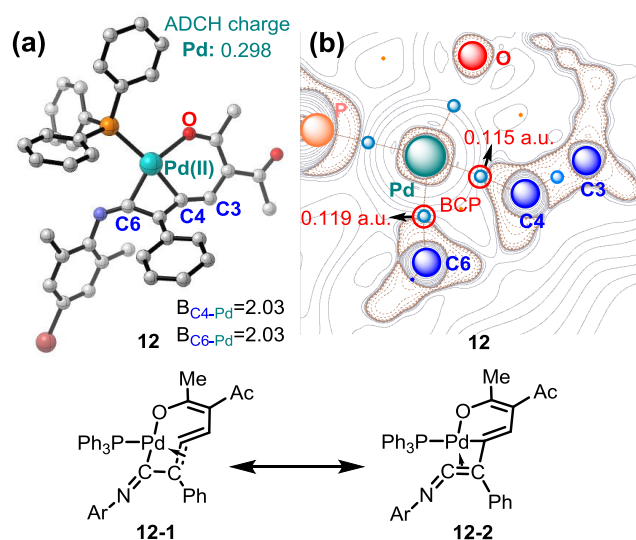
**Figure S3.** Gibbs energy profiles for Pd-catalyzed enynes and isocyanide. Values are given in kcal/mol and represent the relative free energies calculated by using the M06-2X/def2-TZVP//B3LYP/def2-SVP method in tetrahydrofuran solvent. Optimized geometries of transition states **19-ts**, **25-ts**, **27-ts** and intermediate **20**. Bond lengths are given in angstroms.

The coordination of enyne **1** onto Pd forms complex **6** with endergonic 5.9 kcal/mol. Subsequent an intramolecular nucleophilic attack would take place via transition state **19-ts** with an energy barrier of 33.5 kcal/mol to afford six-membered palladacycle **20**, with a free energy release of 3.8 kcal/mol. In geometry of that intermediate, the bond lengths of Pd-O and Pd-C4 are 2.08 and 2.04 Å, which can be considered as two resonance structures of Pd(0)-carbene **20-1** and Pd(II)-vinyl **20-2**. The following allylic reductive elimination can occur via transition states **25-ts** to irreversibly afford a ketenimine-coordinated Pd(0) complex **26**. After ligand dissociation, active species **5** can be regenerated with the release of furanyl ketenimine



product **15**. Alternatively, an intramolecular nucleophilic attack would take place via transition state **27-ts** to afford furan ring in Pd-carbene intermediate **28** with a free energy barrier of only 19.0 kcal/mol, which is much higher than the metal of copper, silver and gold in Figure 1. Then the Pd-carbene intermediate **28** can react with enynone through ligand exchange to afford complex **17** with exothermic 2.6 kcal/mol. The Subsequent migratory insertion could occur via a three-membered ring concerted transition state **18-ts** with an energy barrier of only 9.4 kcal/mol to form intermediate **14**, which undergoes the ligand exchange with phosphine to obtain furanyl ketenimine product **15** with the regeneration of active species **5**.

### 9. Details about the electronic properties of intermediate **12**.



**Figure S4.** (a) Optimized structure of intermediate **12**. (b) Laplacian plots of electron density for intermediate **12** on the C4-Pd-C6 plane.

We gave the critical atomic charge and geometric information for the intermediate **12** in Figure S4 (a). The bond lengths of Pd-C6 and Pd-C4 are 2.03 and 2.03 Å. Moreover, the ADCH charge and localized orbital bonding analysis (LOBA) determine that the oxidation state of Pd is +2. To further investigate the two resonance structures of intermediate **12**, the Laplacians of the electron density on the plane defined by Pd, C4 and C6 of intermediate **12** were plotted using Atoms-in-Molecules (AIM) analysis. As shown in Figure S4 (b), the electron densities at the BCPs (bond critical points) of

Pd-C6 and Pd-C4 bond were calculated to 0.119 a.u. and 0.115 a.u.. It indicates that the bond strengths of those two bonds are close, therefore, both of resonance structures **12-1** and **12-2** contribute to this intermediate.

**Reference:**

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- 11: (a) J. Ma, H. Jiang and S. Zhu, *Org. Lett.*, 2014, **16**, 4472; (b) Q. Yang, Y. Zhu and G. Deng, *Tetrahedron*, 2020, **76**, 13519.

## 10. B3LYP geometries for all the optimized compounds and transition states.

**1**

C	-3.82138900	-0.69406900	0.00699500	C	5.09272900	0.00025600	-0.47574400
O	-4.79289200	0.04158200	0.02471300	H	6.13199200	0.00021500	-0.81288400
C	-2.42483300	-0.15293100	0.00166100	C	4.43277300	1.20933100	-0.26146700
C	-1.37292800	-1.03605300	0.00033800	H	4.96405300	2.14696300	-0.43604300
H	-1.60854400	-2.10471500	-0.00067800	C	3.10070000	1.24188400	0.17541200
C	-2.13871800	1.33315600	-0.00024500	C	2.38753200	2.57939700	0.35612500
O	-0.98208200	1.71469900	0.02121600	H	1.44679500	2.39318500	0.89660200
C	-4.03965300	-2.20393200	-0.00833900	C	2.01584600	3.17840800	-1.01401000
H	-3.59707600	-2.67174800	-0.90194000	H	2.91346500	3.38889100	-1.61680600
H	-3.59767600	-2.68845700	0.87670400	H	1.45956300	4.12139400	-0.89411400
H	-5.12217500	-2.38241700	-0.00946300	H	1.38118300	2.48458200	-1.59207900
C	-3.26407500	2.34387300	-0.03293400	C	3.19649600	3.57853500	1.20007600
H	-3.90995400	2.19398700	-0.91020400	H	4.12505500	3.88888000	0.69615200
H	-3.92341300	2.23132600	0.83983900	H	3.47064100	3.15293700	2.17763600
H	-2.81245500	3.34471900	-0.05020800	H	2.60511000	4.48978300	1.38045900
C	0.00359100	-0.76543700	-0.00023600	C	2.38772500	-2.57873100	0.35732500
C	1.22397600	-0.66591200	-0.00112200	H	1.44688000	-2.39232300	0.89755300
C	2.61404100	-0.36538500	-0.00079200	C	3.19668600	-3.57719100	1.20209900
C	3.59320600	-1.38339700	-0.00726000	H	2.60547000	-4.48846700	1.38290700
C	3.02570300	0.98801200	0.00628100	H	3.47048300	-3.15090700	2.17945400
C	4.94731000	-1.05358400	-0.00667400	H	4.12545300	-3.88759600	0.69861000
H	3.27605200	-2.42832500	-0.01271700	C	2.01625400	-3.17871600	-1.01243100
C	4.38192300	1.30630400	0.00678600	H	1.38139900	-2.48543700	-1.59096900
H	2.26077600	1.76730000	0.01133700	H	1.46019100	-4.12176300	-0.89192600
C	5.34417800	0.28891900	0.00030400	H	2.91389700	-3.38937700	-1.61513300
H	5.69960300	-1.84615700	-0.01168900	C	-2.45837100	0.00002000	0.38281900
H	4.69344000	2.35375600	0.01230700	C	-3.10045300	-1.24163300	0.17538000
H	6.40722800	0.54311000	0.00070400	C	-4.43254200	-1.20932700	-0.26147200

**[Cu]**

N	1.08237200	0.00035100	0.83849100	H	-4.96366400	-2.14704700	-0.43604300
N	-1.08236700	0.00018400	0.83849200	C	-5.09272700	-0.00037100	-0.47573000
C	0.00000300	0.00028600	0.02294700	H	-6.13199300	-0.00052600	-0.81286400
C	0.68172400	0.00027300	2.16665400	C	-4.43306600	1.20877900	-0.26095800
H	1.39653100	0.00040700	2.98495800	H	-4.96457900	2.14635100	-0.43514200
C	-0.68171700	0.00016200	2.16665500	C	-3.10099800	1.24148000	0.17591800
H	-1.39652400	0.00018100	2.98495900	C	-2.38812600	2.57908700	0.35711200
C	2.45837700	0.00035300	0.38281700	H	-1.44739100	2.39290100	0.89760000
C	3.10076000	-1.24122900	0.17587700	C	-2.01646200	3.17859900	-1.01281200
C	4.43284000	-1.20877500	-0.26098400	H	-2.91408900	3.38908500	-1.61559400
H	4.96419400	-2.14643600	-0.43516900	H	-1.38161300	2.48509600	-1.59105300
				H	-1.46039400	4.12167000	-0.89257300
				C	-3.19735500	3.57779800	1.20131200

H	-2.60615100	4.48909400	1.38204800	C	3.09707300	-3.34736300	1.67543800
H	-3.47152200	3.15183900	2.17870800	H	2.55530600	-4.28378500	1.88226200
H	-4.12591800	3.88814600	0.69739600	H	3.11972800	-2.75615200	2.60415600
C	-2.38711900	-2.57904100	0.35633700	H	4.13613200	-3.61369300	1.42526000
H	-1.44626700	-2.39260700	0.89654500	C	2.34528100	-3.42771800	-0.75042100
C	-3.19580600	-3.57793200	1.20086700	H	1.82949100	-2.89330100	-1.56563700
H	-3.46956900	-3.15201500	2.17839200	H	1.79634000	-4.36322900	-0.55947700
H	-2.60440600	-4.48916100	1.38131000	H	3.34701200	-3.70177600	-1.11701900
H	-4.12457400	-3.88833200	0.69737800	C	-2.46164900	0.00970300	0.46535700
C	-2.01563900	-3.17852200	-1.01363500	C	-3.10476900	-1.23433300	0.27641500
H	-1.45935500	-4.12148200	-0.89348100	C	-4.43940400	-1.20541800	-0.15360100
H	-1.38097900	-2.48491600	-1.59200700	H	-4.97280300	-2.14533400	-0.31075700
H	-2.91327900	-3.38918300	-1.61634200	C	-5.10036700	0.00131600	-0.37759800
Cu	-0.00001700	-0.00092500	-1.88263100	H	-6.14134400	-0.00194500	-0.70938900
<b>[Ag]</b>				C	-4.44070000	1.21233400	-0.17340700
N	1.08248600	0.01457800	0.91055500	H	-4.97525000	2.14889600	-0.34580800
N	-1.08243100	0.01457900	0.91058300	C	-3.10579200	1.24990300	0.25488900
C	0.00004300	0.00132300	0.09696100	C	-2.42181600	2.59491400	0.48827600
C	0.68159400	0.03568200	2.23791600	H	-1.37571200	2.40180900	0.77092800
H	1.39655500	0.04782900	3.05588200	C	-2.39162000	3.45319000	-0.78894800
C	-0.68147500	0.03567500	2.23796500	H	-3.40475500	3.72938800	-1.12088400
H	-1.39642100	0.04781100	3.05596800	H	-1.90241000	2.92383100	-1.62325300
C	2.46167300	0.00970700	0.46530800	H	-1.83779400	4.38830400	-0.61065200
C	3.10477000	-1.23431000	0.27632700	C	-3.07211400	3.35837000	1.65717000
C	4.43940000	-1.20540700	-0.15370600	H	-2.53478000	4.30053800	1.84900600
H	4.97279900	-2.14532200	-0.31089100	H	-3.05991600	2.76589000	2.58531600
C	5.10037600	0.00133000	-0.37768800	H	-4.12144400	3.61251500	1.43905200
H	6.14135600	-0.00192700	-0.70949600	C	-2.41883400	-2.57490400	0.52887800
C	4.44070300	1.21234500	-0.17345800	H	-1.38331100	-2.37496700	0.84372300
H	4.97525700	2.14891000	-0.34585200	C	-3.09719100	-3.34755500	1.67529600
C	3.10580300	1.24989000	0.25486300	H	-3.12006700	-2.75644200	2.60407600
C	2.42185600	2.59490800	0.48826500	H	-2.55537900	-4.28395300	1.88211700
H	1.37576300	2.40183300	0.77094400	H	-4.13617900	-3.61395100	1.42489400
C	2.39163200	3.45318500	-0.78895700	C	-2.34496200	-3.42755500	-0.75044900
H	3.40475900	3.72937500	-1.12092300	H	-1.79604700	-4.36308500	-0.55952400
H	1.83782300	4.38830600	-0.61064800	H	-1.82900500	-2.89301200	-1.56548200
H	1.90239600	2.92383500	-1.62324900	H	-3.34661700	-3.70156300	-1.11729300
C	3.07218700	3.35836800	1.65713600	Ag	-0.00010600	-0.04446300	-2.00838700
H	4.12150800	3.61252100	1.43898700	<b>[Au]</b>			
H	3.06002500	2.76589400	2.58528000	Au	0.00008900	0.03955800	-1.71165500
H	2.53485700	4.30053300	1.84898900	N	-1.08949000	-0.01991400	1.07906600
C	2.41887400	-2.57489300	0.52880600	N	1.08942900	-0.02010000	1.07910800
H	1.38328700	-2.37499900	0.84343400	C	-0.00001700	-0.00467700	0.27940500

C	-0.68169800	-0.04448900	2.40345900	C	2.44585100	-3.47244000	-0.60835100
H	-1.39756700	-0.05865000	3.22056100	H	3.47043500	-3.75396300	-0.89772500
C	0.68158300	-0.04464500	2.40348900	H	1.98865200	-2.95218700	-1.46536100
H	1.39743000	-0.05895000	3.22061500	H	1.88524400	-4.40505800	-0.43861100
C	-2.47450100	-0.01427400	0.64241700	C	3.04014700	-3.34904000	1.85967600
C	-3.11686500	1.23136900	0.46681200	H	2.50095200	-4.29208400	2.04146200
C	-4.45816100	1.20201500	0.05884600	H	2.99300000	-2.74798300	2.78129800
H	-4.99412000	2.14184500	-0.08896000	H	4.09771700	-3.59950700	1.68083300
C	-5.12176300	-0.00481000	-0.15648200	C	2.42793300	2.57093300	0.71426700
H	-6.16780000	-0.00112000	-0.47189100	H	1.38053200	2.37240500	0.98991300
C	-4.45913300	-1.21650200	0.03361700	C	3.06971400	3.32241300	1.89550900
H	-4.99604500	-2.15250400	-0.13347900	H	3.05772700	2.71841400	2.81629800
C	-3.11765100	-1.25559100	0.43974900	H	2.52662200	4.25925500	2.09671600
C	-2.42964800	-2.60043200	0.66135100	H	4.11823700	3.58538700	1.68442200
H	-1.37291400	-2.40927400	0.90488900	C	2.40130500	3.44248000	-0.55412200
C	-2.44605900	-3.47258400	-0.60661100	H	1.84628300	4.37518200	-0.36716600
H	-3.47058500	-3.75355000	-0.89670700	H	1.91571100	2.92061100	-1.39463600
H	-1.88618100	-4.40550200	-0.43611900	H	3.41595700	3.72255600	-0.87802200
H	-1.98784400	-2.95291700	-1.46342900				
C	-3.04141900	-3.34815300	1.86113800	<b>2a</b>			
H	-4.09890200	-3.59869400	1.68185900	C	5.18568200	1.26845700	-0.97090400
H	-2.99475200	-2.74663500	2.78247900	O	6.21086400	1.54915600	-0.38432000
H	-2.50233600	-4.29111800	2.04367900	C	3.90582200	2.00180100	-0.65747600
C	-2.42738800	2.57123600	0.71272700	C	2.71127600	1.40215300	-0.94699600
H	-1.37972400	2.37270600	0.98734500	H	2.73003500	0.41826500	-1.42342000
C	-3.06808400	3.32251000	1.89470800	C	3.90710900	3.36429400	0.00821700
H	-2.52497200	4.25944200	2.09544400	O	2.83606100	3.92582500	0.15976600
H	-3.05503500	2.71842300	2.81542800	C	5.17113200	0.17417000	-2.02331400
H	-4.11688000	3.58526800	1.68469600	H	4.63305700	-0.71388100	-1.65287900
C	-2.40197900	3.44301100	-0.55551600	H	4.68396100	0.50317400	-2.95394900
H	-1.91748700	2.92118900	-1.39668600	H	6.20986900	-0.11376200	-2.22874800
H	-1.84648500	4.37551600	-0.36898200	C	5.18921800	4.01362800	0.45684900
H	-3.41691000	3.72348200	-0.87820900	H	5.69287000	3.39897800	1.21676000
C	2.47445900	-0.01456000	0.64255300	H	5.90401800	4.09726500	-0.37569200
C	3.11716400	1.23103400	0.46775600	H	4.94829500	5.00700100	0.85614800
C	4.45845900	1.20158700	0.05980500	C	1.41834000	1.92012900	-0.68894800
H	4.99463500	2.14137400	-0.08739500	C	0.27491900	2.40748000	-0.58862500
C	5.12176100	-0.00524500	-0.15628900	C	-0.75606100	3.39046600	-0.41602000
H	6.16777900	-0.00160600	-0.47169300	C	-2.10923300	3.12628600	-0.71875700
C	4.45884100	-1.21689000	0.03303600	C	-0.37581000	4.66938800	0.05694500
H	4.99549800	-2.15292800	-0.13465700	C	-3.06413600	4.12738400	-0.55534700
C	3.11734400	-1.25591400	0.43914300	H	-2.40671400	2.14284500	-1.08839300
C	2.42902300	-2.60073200	0.65994200	C	-1.34308000	5.65824100	0.21560700
H	1.37220700	-2.40949500	0.90309600	H	0.67430600	4.85866200	0.28443800

C	-2.68410800	5.39144700	-0.08918400	C	-5.39549400	0.74156400	-0.73603200
H	-4.10923300	3.92168100	-0.79549400	H	-6.25232100	1.37427000	-0.98081600
H	-1.05016600	6.64660300	0.57699300	C	-4.99488800	0.59744200	0.59134700
H	-3.43640400	6.17416600	0.03524400	H	-5.54273300	1.12259600	1.37666000
N	-0.11920100	-2.46438000	0.57801800	C	-3.90420700	-0.21409900	0.93723000
N	-2.11517400	-1.73615500	0.21350400	C	-3.49409200	-0.34839500	2.40178100
C	-0.80972500	-1.35713100	0.19582800	H	-2.64067500	-1.04083900	2.45439400
C	-0.98018200	-3.52187100	0.83249100	C	-3.01648400	0.99564500	2.98110400
H	-0.62091000	-4.49647900	1.15085400	H	-3.82244000	1.74646100	2.98780700
C	-2.24078300	-3.06183500	0.60122700	H	-2.17898300	1.41084900	2.39867800
H	-3.20688000	-3.55278300	0.67696600	H	-2.67685100	0.86630900	4.02098800
C	1.32055300	-2.53937100	0.69622400	C	-4.62201600	-0.95775800	3.25418600
C	2.06266600	-3.01826000	-0.40740500	H	-4.28190200	-1.10518600	4.29135700
C	3.45664000	-3.08421600	-0.26328300	H	-4.94585800	-1.93434000	2.86138700
H	4.06548100	-3.45723100	-1.08957300	H	-5.50679100	-0.30237800	3.28735200
C	4.07953500	-2.69470300	0.92282200	C	-2.89969200	-1.48338700	-2.60300700
H	5.16669400	-2.75763500	1.01335200	H	-2.18861200	-2.19273600	-2.15352400
C	3.31936200	-2.23673600	1.99758400	C	-3.86247000	-2.30629500	-3.47651100
H	3.82155100	-1.94413800	2.92195500	H	-4.44685200	-3.01884100	-2.87400000
C	1.92101100	-2.15583300	1.91628200	H	-3.29891700	-2.88059800	-4.22856600
C	1.11601800	-1.65141800	3.11149000	H	-4.57360100	-1.66572900	-4.02105200
H	0.04996100	-1.81884000	2.89556000	C	-2.07878300	-0.49523000	-3.45217400
C	1.30677600	-0.13559800	3.30478200	H	-1.52847200	-1.02520700	-4.24574200
H	2.35660000	0.11323600	3.52806900	H	-1.34317700	0.04590700	-2.83430600
H	0.69001200	0.23111600	4.14047400	H	-2.72519100	0.25431400	-3.93614600
H	1.01618200	0.42190400	2.39938400	Cu	-0.08307200	0.39358100	-0.24400500
C	1.43870000	-2.42571100	4.40121600				
H	2.47543200	-2.25954400	4.73352000	<b>2b</b>			
H	1.29866200	-3.50975600	4.26887100	C	5.66045100	0.38049600	-0.57922800
H	0.77802100	-2.09550400	5.21812300	O	6.80227200	0.63790500	-0.25532000
C	1.40844300	-3.42963300	-1.72529700	C	4.56037700	1.38479800	-0.35912600
H	0.32324900	-3.49839900	-1.55771100	C	3.25504800	0.99838000	-0.50305900
C	1.87397200	-4.81299400	-2.21006000	H	3.05238000	-0.03725300	-0.78606300
H	1.30797400	-5.11164100	-3.10623200	C	4.83952900	2.81778300	0.03761300
H	1.72120000	-5.58446200	-1.43964300	O	3.88406400	3.57197600	0.12503800
H	2.94099900	-4.81851100	-2.48286500	C	5.32672300	-0.95876300	-1.21464700
C	1.62748900	-2.35631100	-2.80834000	H	4.67196500	-1.56126500	-0.56437900
H	1.21934400	-1.38170700	-2.49386700	H	4.81699400	-0.83414300	-2.18291800
H	1.12579400	-2.64054700	-3.74692900	H	6.26739900	-1.50280200	-1.36595000
H	2.69864200	-2.22410100	-3.03140200	C	6.23486800	3.30742800	0.31276100
C	-3.23220100	-0.87696000	-0.11417800	H	6.69623200	2.73517200	1.13066000
C	-3.62204300	-0.76070700	-1.46804600	H	6.88647200	3.14892700	-0.55944700
C	-4.71400200	0.07263600	-1.75263200	H	6.18081800	4.37412300	0.56507800
H	-5.04525100	0.19027500	-2.78651100	C	2.11056500	1.80703800	-0.32331300

C	1.05739300	2.47250200	-0.24045800	C	-2.87302100	1.28000300	3.20848000
C	0.25162200	3.65482400	-0.11162700	H	-1.98229600	1.67648200	2.69558500
C	-1.15203100	3.64089000	-0.26573300	H	-2.56203200	0.92150500	4.20240900
C	0.91233900	4.87546000	0.16852800	H	-3.56796800	2.11951600	3.36772500
C	-1.87872000	4.82293200	-0.14365500	C	0.53508700	-3.02989200	0.40506300
H	-1.67122700	2.70559300	-0.48826900	C	1.13969900	-3.04336200	1.68214100
C	0.17190400	6.04844900	0.28919600	C	2.45712300	-3.51888300	1.76345200
H	1.99700900	4.87587500	0.28262000	H	2.95809900	-3.54872800	2.73338500
C	-1.21985700	6.02636000	0.13417500	C	3.13446800	-3.96750200	0.63037700
H	-2.96350300	4.80517000	-0.26697400	H	4.15601300	-4.34499000	0.72114700
H	0.68371500	6.98916400	0.50441400	C	2.50798600	-3.94958000	-0.61572400
H	-1.79332400	6.95165100	0.22902800	H	3.04686800	-4.31690500	-1.49191700
N	-2.55541300	-1.29155600	0.03932700	C	1.19304400	-3.48245400	-0.76108100
N	-0.82847200	-2.55958100	0.28967700	C	0.52920500	-3.50039900	-2.13607300
C	-1.19806300	-1.26866100	0.08423800	H	-0.48103800	-3.07725200	-2.03147800
C	-3.03204500	-2.58264800	0.21491300	C	1.28207900	-2.61840000	-3.14804600
H	-4.09372100	-2.81233600	0.21080700	H	2.30000300	-2.99367500	-3.34008800
C	-1.94213200	-3.38298900	0.37348200	H	1.36674400	-1.57824600	-2.79323600
H	-1.85771400	-4.45363000	0.53661200	H	0.75165400	-2.60123700	-4.11319600
C	-3.40271700	-0.13427400	-0.15646000	C	0.36531100	-4.93820800	-2.66267200
C	-3.87091800	0.55836100	0.98329200	H	-0.16883700	-4.93672700	-3.62594600
C	-4.70752300	1.66256600	0.76372700	H	-0.20539900	-5.56465300	-1.95950900
H	-5.09536600	2.22016000	1.61883200	H	1.34054600	-5.42416200	-2.82485900
C	-5.06034000	2.05608600	-0.52669800	C	0.42119400	-2.58264800	2.94785200
H	-5.72035600	2.91483800	-0.67267100	H	-0.59284400	-2.26167700	2.66600300
C	-4.58354600	1.35162500	-1.63152100	C	0.26450000	-3.73305900	3.95946900
H	-4.87515900	1.66806500	-2.63524900	H	-0.26247600	-4.59287600	3.51714900
C	-3.74699000	0.23617800	-1.47613800	H	-0.31119600	-3.39653300	4.83611900
C	-3.26731900	-0.52813200	-2.70802700	H	1.24068700	-4.09120500	4.32313800
H	-2.61344400	-1.34491000	-2.36769600	C	1.11717700	-1.36747600	3.58678300
C	-2.42826700	0.36148800	-3.64256100	H	0.55001200	-1.01685500	4.46339800
H	-3.02171400	1.19150000	-4.05731100	H	1.19696200	-0.52779600	2.87725100
H	-2.04662500	-0.22647400	-4.49220900	H	2.13481100	-1.61367400	3.92932200
H	-1.56385500	0.79907800	-3.11734800	Ag	0.04717000	0.42642500	-0.10389700
C	-4.44482400	-1.17493600	-3.46095700				
H	-5.13724300	-0.41613400	-3.85860400	<b>2c</b>			
H	-5.02502900	-1.84463000	-2.80711900	C	-5.65774000	0.56852500	-0.33173200
H	-4.07712500	-1.76749500	-4.31353300	O	-6.79657600	0.96892800	-0.19473500
C	-3.52545000	0.13813100	2.40975800	C	-4.49855000	1.51662500	-0.20204100
H	-2.78658700	-0.67532500	2.35380500	C	-3.21290300	1.04721700	-0.25201600
C	-4.76110400	-0.42036400	3.14045200	H	-3.05357000	-0.02481100	-0.38726300
H	-4.48824800	-0.76721300	4.14970900	C	-4.67760000	3.00009000	-0.00747800
H	-5.20421800	-1.27041900	2.59830200	O	-3.65981600	3.67493400	0.04587700
H	-5.54427900	0.34646700	3.25216600	C	-5.38874800	-0.89363000	-0.64133000

H	-4.83801000	-1.01052700	-1.58818000	H	5.41286700	0.08305900	3.43557000
H	-4.79467200	-1.37481200	0.15177300	H	5.08296300	-1.50014900	2.69909000
H	-6.35604400	-1.40494400	-0.72168800	H	4.30741800	-1.05295100	4.23901800
C	-6.03257800	3.63711000	0.11706900	C	3.28279800	-0.46462800	-2.65043800
H	-6.64550100	3.42678400	-0.77199900	H	2.58059400	-1.26428400	-2.37057200
H	-6.58913200	3.20835100	0.96336500	C	4.44960900	-1.12963000	-3.40415900
H	-5.89677000	4.71828300	0.24758300	H	4.07867300	-1.66098200	-4.29479400
C	-2.03306200	1.81402500	-0.14763700	H	4.98017700	-1.85774200	-2.77083100
C	-0.91196400	2.39017300	-0.10329500	H	5.18703300	-0.38577000	-3.74508500
C	-0.09454700	3.57645500	-0.04939300	C	2.51271700	0.50970800	-3.55974000
C	1.31425400	3.52148200	-0.13445800	H	1.65815200	0.96477000	-3.03422000
C	-0.73525900	4.83209300	0.08469000	H	2.12520300	-0.01857800	-4.44517400
C	2.06370100	4.69434600	-0.08834100	H	3.15698900	1.32679200	-3.92121200
H	1.81808900	2.55928500	-0.24180900	C	-0.64136500	-3.07077500	0.23244100
C	0.02763000	5.99570700	0.13196300	C	-1.27308000	-3.44418300	-0.97566300
H	-1.82233000	4.87026500	0.14790100	C	-2.58185700	-3.94037800	-0.88650200
C	1.42392200	5.93195900	0.04555700	H	-3.10119100	-4.25095200	-1.79567400
H	3.15212300	4.64216400	-0.15739700	C	-3.22726000	-4.05874800	0.34434300
H	-0.47080500	6.96213900	0.23597700	H	-4.24348700	-4.45804100	0.38936900
H	2.01509900	6.85027200	0.08208700	C	-2.57695800	-3.68103700	1.51834100
Au	-0.03495300	0.36644400	-0.04352800	H	-3.09296000	-3.78644300	2.47504000
N	2.48692000	-1.35005500	0.03648200	C	-1.26560400	-3.18220700	1.49455700
N	0.72797400	-2.60264100	0.17618500	C	-0.57532300	-2.80428000	2.80281700
C	1.12995900	-1.31125500	0.05665600	H	0.43311000	-2.43563600	2.56215900
C	2.93382600	-2.65841000	0.14459700	C	-1.31139900	-1.66038400	3.52281400
H	3.99146500	-2.90558000	0.14888200	H	-2.32649800	-1.95831700	3.83008300
C	1.82782100	-3.44636500	0.23228000	H	-1.40127100	-0.77186600	2.87765300
H	1.72081000	-4.52284800	0.32915600	H	-0.76550300	-1.36463400	4.43255400
C	3.36968700	-0.20680800	-0.07871600	C	-0.40096200	-4.02703500	3.72234700
C	3.76240300	0.21372800	-1.36940200	H	0.15069900	-3.74647300	4.63342300
C	4.64877700	1.29811900	-1.44645300	H	0.15743800	-4.83422600	3.22291100
H	4.97943700	1.65169800	-2.42528400	H	-1.37217200	-4.44001900	4.03787600
C	5.12495000	1.92494300	-0.29555700	C	-0.58244400	-3.35978000	-2.33467500
H	5.82438700	2.76025200	-0.38114700	H	0.38951400	-2.86425900	-2.19093700
C	4.71993500	1.48486400	0.96404100	C	-0.29775600	-4.76302600	-2.90301600
H	5.10572100	1.98364200	1.85563000	H	0.30863200	-5.36729000	-2.21024600
C	3.83343100	0.40722600	1.10661100	H	0.24955600	-4.68909900	-3.85602700
C	3.42884900	-0.06361900	2.50129400	H	-1.23050600	-5.31639100	-3.09677700
H	2.68169500	-0.86333600	2.38686800	C	-1.37685900	-2.50432200	-3.33692100
C	2.76089000	1.05867200	3.31514100	H	-0.82108100	-2.40888100	-4.28295300
H	3.45837600	1.88601400	3.52000200	H	-1.55779900	-1.48930900	-2.94890000
H	2.41650500	0.67257200	4.28749400	H	-2.35338500	-2.95408200	-3.57694400
H	1.88994300	1.47752500	2.78684800				
C	4.62668400	-0.66785000	3.25768800				

**3a-ts**



C	5.54100600	1.03756100	-0.45697500	C	0.71509000	-2.27630100	2.92916300
O	6.62160900	1.58873200	-0.37203900	H	-0.34286400	-2.23395100	2.62985300
C	4.28181800	1.82081000	-0.27401900	C	1.12557100	-0.85172100	3.34643900
C	3.02769100	1.26610000	-0.27420600	H	2.17737000	-0.81648600	3.67343000
H	2.89021600	0.18999000	-0.40407700	H	0.50241000	-0.49384700	4.18129300
C	4.24822300	3.29282800	-0.07241000	H	1.01035700	-0.14393700	2.50903600
O	3.12070800	3.78216400	0.03601300	C	0.80712500	-3.25603000	4.11125800
C	5.43839500	-0.44413300	-0.75646100	H	1.82514900	-3.30672700	4.52833800
H	4.92754900	-0.98413400	0.05624700	H	0.51407300	-4.27546600	3.81609600
H	4.86820600	-0.62382900	-1.68208900	H	0.13868600	-2.93303100	4.92469200
H	6.45336500	-0.84416300	-0.87323100	C	1.14034200	-3.32822500	-2.10906300
C	5.47017100	4.15356000	-0.00052600	H	0.08960200	-3.00666700	-2.05948600
H	6.12537100	3.81666700	0.81679700	C	1.14761900	-4.77766700	-2.62819400
H	6.06972400	4.04166300	-0.91647700	H	0.66305000	-4.83469300	-3.61562600
H	5.16931200	5.19870100	0.14424300	H	0.60901200	-5.45504700	-1.94732500
C	1.86368900	2.04141400	-0.11186300	H	2.17294700	-5.16480300	-2.73955500
C	0.61622800	2.32502100	-0.04736000	C	1.85114500	-2.37958700	-3.09117900
C	-0.30101900	3.43826900	0.07172100	H	1.80216100	-1.33352900	-2.74783200
C	-1.69730900	3.23208000	-0.01206400	H	1.37781800	-2.42847900	-4.08454100
C	0.18556900	4.75441300	0.26755400	H	2.91274100	-2.64483600	-3.22047200
C	-2.57974300	4.30435300	0.09503000	C	-3.30926200	-0.50465000	-0.31001300
H	-2.08867400	2.22493200	-0.17133300	C	-3.58398300	-0.10109100	-1.63657000
C	-0.70498500	5.81823800	0.37790500	C	-4.58054700	0.86867800	-1.82002100
H	1.25998000	4.92070100	0.32848200	H	-4.81792000	1.20992400	-2.82960700
C	-2.08598000	5.59869500	0.29182800	C	-5.28260500	1.39668000	-0.73712800
H	-3.65493900	4.12865100	0.02465500	H	-6.06458900	2.14102400	-0.90682900
H	-0.32105200	6.82950300	0.53048000	C	-4.99636500	0.97209500	0.55971300
H	-2.77834900	6.43983400	0.37744700	H	-5.55790600	1.39063500	1.39758000
N	-0.42710000	-2.52681600	0.23754200	C	-4.00352700	0.01235800	0.80740500
N	-2.30487500	-1.52193600	-0.08820700	C	-3.72986300	-0.44424600	2.23837600
C	-0.96817800	-1.29434900	0.03446600	H	-2.85449300	-1.11067400	2.21905000
C	-1.40919200	-3.50720100	0.24290500	C	-3.37683500	0.73314400	3.16444600
H	-1.17647600	-4.55764200	0.39229800	H	-4.22422400	1.42585800	3.28781600
C	-2.59472100	-2.87219900	0.03600600	H	-2.52426700	1.31305500	2.77753200
H	-3.60888600	-3.25469000	-0.03475900	H	-3.11030800	0.36290400	4.16700300
C	0.97799100	-2.81575300	0.41903100	C	-4.91098100	-1.25851400	2.79948600
C	1.73021700	-3.22980400	-0.70395600	H	-4.68004800	-1.62557300	3.81206300
C	3.07360800	-3.57145100	-0.48803300	H	-5.14205800	-2.13072700	2.16804700
H	3.68415200	-3.90710000	-1.32908600	H	-5.82494000	-0.64694100	2.86729500
C	3.64048300	-3.50305200	0.78428900	C	-2.83203800	-0.65674000	-2.84321400
H	4.68575600	-3.78629700	0.93071900	H	-2.22142000	-1.50536800	-2.49940300
C	2.87588600	-3.08322200	1.87222100	C	-3.78065000	-1.19838700	-3.92649400
H	3.33360900	-3.03689100	2.86249900	H	-4.46494000	-1.95998800	-3.52148000
C	1.52480400	-2.73746900	1.72019100	H	-3.20201600	-1.66077400	-4.74162000

H	-4.39393800	-0.40070900	-4.37443800	C	0.99528100	-3.42163900	-1.12313900
C	-1.86564500	0.39550800	-3.41827900	C	2.27748800	-3.98749900	-1.06335200
H	-1.28214300	-0.02494800	-4.25271100	H	2.78237900	-4.27222400	-1.98903700
H	-1.15805300	0.74734200	-2.64949900	C	2.91335700	-4.20847000	0.15811500
H	-2.40856800	1.27586700	-3.79796300	H	3.90761500	-4.66147600	0.18005100
Cu	-0.07964500	0.43547300	-0.03755600	C	2.27998500	-3.86476300	1.35172400
<b>3b-ts</b>							
C	5.82586100	0.18338500	-0.11617300	C	0.99611300	-3.29831400	1.35630100
O	6.98749900	0.54262700	-0.11334600	C	0.32316200	-2.96016800	2.68442700
C	4.72572700	1.19347400	-0.07639700	H	-0.65727900	-2.51289500	2.46396600
C	3.39427300	0.86894000	-0.06898800	C	1.12472400	-1.91503500	3.48079300
H	3.07221400	-0.17420400	-0.09141000	H	2.11636600	-2.29623600	3.77234000
C	4.94933500	2.66235300	-0.04049900	H	0.59165500	-1.64512100	4.40607100
O	3.92453900	3.34939300	-0.01586300	H	1.27694800	-0.99208700	2.89796700
C	5.46040000	-1.28754200	-0.16034500	C	0.06558900	-4.22573200	3.52302900
H	4.87443700	-1.58125900	0.72515800	H	1.00673500	-4.71985200	3.81213600
H	4.85435800	-1.52296400	-1.04978100	H	-0.54010000	-4.96107700	2.97078400
H	6.38788800	-1.87290000	-0.18996500	H	-0.47273600	-3.97033800	4.44941200
C	6.30320600	3.29956000	-0.03261000	C	0.31351900	-3.22609600	-2.47533100
H	6.88796000	2.94037800	0.82761500	H	-0.62916500	-2.68543500	-2.30386000
H	6.87488900	2.98945200	-0.92035200	C	-0.04673000	-4.57895200	-3.11794400
H	6.19081400	4.39052100	-0.00148500	H	-0.58259700	-4.42430400	-4.06779000
C	2.38056400	1.84569700	-0.03361100	H	-0.69129900	-5.18255400	-2.46001500
C	1.20047000	2.33851200	-0.01299100	H	0.85463800	-5.17352900	-3.33639500
C	0.47665200	3.59074700	0.01198900	C	1.15646300	-2.36341500	-3.43073200
C	-0.93742100	3.61958700	0.00973800	H	1.39832800	-1.38455700	-2.98649200
C	1.18282100	4.81943400	0.03760300	H	0.60635600	-2.18142600	-4.36738500
C	-1.62336200	4.83129800	0.03178700	H	2.10464500	-2.85499700	-3.70060500
H	-1.50123600	2.68368400	-0.01130000	C	-3.42801100	0.02992300	-0.06468000
C	0.48806900	6.02516400	0.06044200	C	-3.76962100	0.55139600	-1.33322700
H	2.27173600	4.80625700	0.03882200	C	-4.55593800	1.71278600	-1.35891800
C	-0.91269700	6.03640900	0.05751200	H	-4.84401400	2.14498100	-2.31961000
H	-2.71521200	4.83441600	0.02859100	C	-4.98641700	2.32035400	-0.17996400
H	1.04202800	6.96646600	0.08042700	H	-5.60686000	3.21887700	-0.22604200
H	-1.45084400	6.98734600	0.07515900	C	-4.63792700	1.77918600	1.05690600
N	-0.96014400	-2.53772100	0.07371600	H	-4.98807100	2.26174800	1.97193800
N	-2.63007600	-1.17617200	-0.00402900	C	-3.85341500	0.61977300	1.14711900
C	-1.27167900	-1.21589800	0.01961200	C	-3.51092500	0.04221000	2.51824900
C	-2.10950100	-3.31599100	0.08459400	H	-2.86412700	-0.83464200	2.36593900
H	-2.07245900	-4.40076600	0.12597900	C	-2.71792200	1.04153800	3.37902700
C	-3.16345800	-2.45608000	0.03540900	H	-3.31112400	1.93947200	3.61399200
H	-4.23460700	-2.63595300	0.02506500	H	-1.79836500	1.37285200	2.87049000
C	0.37842200	-3.08463700	0.10347900	H	-2.42901600	0.57906400	4.33607600
				C	-4.77300500	-0.44986100	3.25090300

H	-4.50278500	-0.91733200	4.21103300	Au	-0.02383100	0.37324400	-0.03778000
H	-5.32408100	-1.19401700	2.65473700	N	2.50876400	-1.32493100	0.03935400
H	-5.46468100	0.37948300	3.46901600	N	0.76065000	-2.59443000	0.15886400
C	-3.33534100	-0.09847000	-2.64465800	C	1.15117300	-1.29811400	0.05270700
H	-2.71992900	-0.97741000	-2.40122400	C	2.96709200	-2.63001900	0.13822700
C	-4.54559700	-0.60565700	-3.45045800	H	4.02688900	-2.86766200	0.14568600
H	-5.15682800	-1.30956600	-2.86423700	C	1.86788100	-3.42872000	0.21320600
H	-4.20946400	-1.12546700	-4.36159800	H	1.77042200	-4.50698100	0.29979400
H	-5.20077600	0.22232600	-3.76478600	C	3.38105500	-0.17254800	-0.06382700
C	-2.45751100	0.84463500	-3.48648400	C	3.77416800	0.26187200	-1.34981700
H	-2.10754500	0.33285300	-4.39693200	C	4.64810100	1.35710700	-1.41542900
H	-1.57173500	1.18114900	-2.92396700	H	4.97834800	1.72189800	-2.39033300
H	-3.01074800	1.74203100	-3.80579400	C	5.11239300	1.98117400	-0.25816200
Ag	0.02455300	0.45215000	-0.00249900	H	5.80210700	2.82543900	-0.33491500
<b>3c-ts</b>				C	4.70791500	1.52693800	0.99657600
C	-5.69886000	0.50458600	-0.28890700	H	5.08417000	2.02360900	1.89344500
O	-6.84049200	0.90811200	-0.18570900	C	3.83352500	0.43798900	1.12765800
C	-4.54619200	1.45808300	-0.17541300	C	3.42975100	-0.04816300	2.51732700
C	-3.25061500	1.01579300	-0.21582800	H	2.68966200	-0.85311800	2.39427100
H	-3.05605300	-0.05249600	-0.33268200	C	2.75087000	1.06141700	3.33947700
C	-4.72018300	2.93958700	-0.00816600	H	3.44105100	1.89283700	3.55242800
O	-3.69211500	3.60400700	0.03813100	H	2.40824700	0.66420700	4.30798200
C	-5.41768100	-0.96574100	-0.53926100	H	1.87724600	1.47720000	2.81320000
H	-4.86171000	-1.11370000	-1.47874700	C	4.63117400	-0.64873900	3.27100700
H	-4.82094200	-1.40910800	0.27355400	H	5.41068200	0.10725100	3.45671800
H	-6.37956000	-1.48933400	-0.60402000	H	5.09555800	-1.47241600	2.70630800
C	-6.06727900	3.59192600	0.10004500	H	4.31331100	-1.04486800	4.24841600
H	-6.67551800	3.37276800	-0.79023200	C	3.30677000	-0.41179800	-2.63783300
H	-6.63208600	3.17680900	0.94782300	H	2.61782100	-1.22569700	-2.36643700
H	-5.92565900	4.67376000	0.21737600	C	4.48440200	-1.05044600	-3.39745000
C	-2.10363100	1.82840600	-0.12325900	H	4.12206100	-1.57975900	-4.29284300
C	-0.95246300	2.35853900	-0.08984700	H	5.02681900	-1.77551500	-2.77065800
C	-0.15658600	3.56318300	-0.04551500	H	5.20966500	-0.29184200	-3.73188200
C	1.25339700	3.52595600	-0.12919300	C	2.52051900	0.55857400	-3.53740400
C	-0.80985400	4.81368700	0.07769000	H	1.65596800	0.98992000	-3.00820700
C	1.99006800	4.70718000	-0.09242400	H	2.14541100	0.03391800	-4.43034400
H	1.76856500	2.56886900	-0.22865800	H	3.14983300	1.39243900	-3.88674000
C	-0.06077400	5.98638200	0.11620700	C	-0.60437300	-3.07581000	0.20132600
H	-1.89691000	4.84243900	0.13997600	C	-1.22662400	-3.43713400	-1.01536900
C	1.33633300	5.93841400	0.03118300	C	-2.53067900	-3.94792700	-0.94038100
H	3.07905900	4.66641500	-0.16056400	H	-3.04237900	-4.24990200	-1.85676000
H	-0.57042600	6.94777600	0.21220600	C	-3.18073900	-4.09196000	0.28527400
H	1.91677800	6.86382700	0.06075200	H	-4.19293200	-4.50246900	0.31914500
				C	-2.53996700	-3.72563200	1.46811200

H	-3.05923300	-3.85101500	2.42070100	C	-2.12287600	4.44302900	-0.04011400
C	-1.23379600	-3.21286900	1.45837000	H	-1.73824900	2.36989900	-0.46611100
C	-0.55380700	-2.84852600	2.77584200	C	-0.23565300	5.72449600	0.78478800
H	0.44974900	-2.46072400	2.54562100	H	1.63083200	4.68858100	0.95876200
C	-1.30870000	-1.72861100	3.51374500	C	-1.58716400	5.65103500	0.42073100
H	-2.32120500	-2.04576800	3.81016100	H	-3.17707500	4.37552300	-0.31615900
H	-1.40681200	-0.82916900	2.88522600	H	0.17592700	6.66267500	1.16410700
H	-0.77125100	-1.44313900	4.43176400	H	-2.22436100	6.53464700	0.50855900
C	-0.36494900	-4.08532500	3.67345600	N	-2.42429400	-1.40146800	-0.11653900
H	0.17850800	-3.81360800	4.59211600	N	-0.60648300	-2.51433900	0.18747900
H	0.20769800	-4.87458900	3.16165900	C	-1.07777400	-1.24754900	0.02078100
H	-1.33118900	-4.51878900	3.97654700	C	-2.78763200	-2.73740400	-0.03563200
C	-0.53035000	-3.32489900	-2.36951200	H	-3.81992000	-3.06389600	-0.12395200
H	0.43613300	-2.82272200	-2.21307300	C	-1.63869600	-3.44133800	0.15755600
C	-0.22994600	-4.71615500	-2.95880700	H	-1.46371100	-4.50686500	0.27576800
H	0.37887900	-5.32576800	-2.27288500	C	-3.36197800	-0.32091400	-0.32648600
H	0.32111100	-4.62179600	-3.90784400	C	-4.01418200	0.23715700	0.79616900
H	-1.15655900	-5.27491300	-3.16594600	C	-4.93585500	1.26759500	0.55885300
C	-1.32790500	-2.46066100	-3.36167500	H	-5.46439900	1.71859000	1.40134600
H	-0.76909000	-2.34597000	-4.30378400	C	-5.19414000	1.72152900	-0.73391800
H	-1.51877600	-1.45335500	-2.95864900	H	-5.92150900	2.52110000	-0.89550000
H	-2.29961800	-2.91481300	-3.61272600	C	-4.53599900	1.15099600	-1.82291000
				H	-4.75318200	1.51296300	-2.83003300
				C	-3.61104700	0.11081300	-1.64899800
				C	-2.91084400	-0.49464700	-2.86330500
				H	-2.33914200	-1.37037900	-2.52132700
				C	-1.90135200	0.49610700	-3.47178800
				H	-2.40270500	1.40283300	-3.84704600
				H	-1.36613300	0.03575000	-4.31762500
				H	-1.15316100	0.81007700	-2.72615700
				C	-3.91112600	-0.99712800	-3.91917700
				H	-4.49207400	-0.17247800	-4.36149400
				H	-4.62543000	-1.71669500	-3.48967500
				H	-3.37743500	-1.49862100	-4.74187800
				C	-3.77078400	-0.25144900	2.22179000
				H	-2.93869900	-0.97078500	2.19421900
				C	-5.00123300	-0.99713600	2.77220600
				H	-4.79504300	-1.39151800	3.77994000
				H	-5.28585700	-1.84464500	2.12902700
				H	-5.87502800	-0.33019500	2.84764900
				C	-3.34411800	0.88916600	3.16211500
				H	-2.45485500	1.41554600	2.78169000
				H	-3.10288700	0.49011500	4.16008600
				H	-4.14437900	1.63460700	3.29427600
<b>4a</b>							
C	5.74419700	0.84315800	-0.33150200				
O	6.77293800	1.48356500	-0.42423700				
C	4.43770200	1.55403400	-0.22699400				
C	3.13270600	1.04755600	-0.11298400				
H	2.82966200	0.00275800	-0.07203600				
C	4.29974100	2.95573300	-0.24720500				
O	3.02286100	3.29204700	-0.13783900				
C	5.72554400	-0.66724700	-0.32045400				
H	5.24654800	-1.04723200	0.59636600				
H	5.14156000	-1.05262600	-1.17241400				
H	6.75541400	-1.04057100	-0.38270600				
C	5.30227600	4.03672200	-0.37381500				
H	6.00747600	3.99806300	0.47205700				
H	5.91699400	3.87961700	-1.27340700				
H	4.81067100	5.01734400	-0.41147000				
C	2.23903900	2.12980700	-0.04821800				
C	0.84484300	2.14370800	0.05443600				
C	0.07212400	3.36828300	0.19559600				
C	-1.31152600	3.31652300	-0.12680000				
C	0.58680400	4.60992100	0.66405600				

C	0.78308700	-2.87093200	0.36331400	H	6.75546500	2.99416600	0.47748100
C	1.31999300	-2.88353200	1.67077400	H	6.64706000	2.94704500	-1.27016600
C	2.66148600	-3.26877800	1.81272300	H	5.77430700	4.24756200	-0.37063900
H	3.11036400	-3.29410000	2.80791300	C	2.70458100	1.88085300	-0.07121200
C	3.42785900	-3.63568900	0.70698300	C	1.33897100	2.14996500	0.03334400
H	4.46587200	-3.94898300	0.84383800	C	0.79597900	3.48943100	0.18256300
C	2.87060900	-3.61635700	-0.57116500	C	-0.57307900	3.69702600	-0.14162200
H	3.48089200	-3.91512700	-1.42631200	C	1.52972900	4.61279600	0.66010700
C	1.53563900	-3.23593300	-0.77594600	C	-1.16216600	4.95334200	-0.04765100
C	0.95503900	-3.24111100	-2.18827700	H	-1.16620800	2.84869300	-0.49056900
H	-0.09060000	-2.90574400	-2.12620900	C	0.92700800	5.85898300	0.78867000
C	1.68858900	-2.24833300	-3.10788200	H	2.56963000	4.49557600	0.95626500
H	2.74559800	-2.52638000	-3.24847400	C	-0.41405400	6.03863700	0.42288200
H	1.65769000	-1.22487900	-2.70109700	H	-2.20995100	5.08482400	-0.32575900
H	1.21979900	-2.22883800	-4.10450100	H	1.50393300	6.70216500	1.17538700
C	0.94210700	-4.65785500	-2.79056900	H	-0.87767900	7.02392400	0.51646900
H	0.46286000	-4.64941800	-3.78228800	N	-2.69392700	-1.09006900	-0.11437900
H	0.38828400	-5.36424400	-2.15271500	N	-1.07253400	-2.47552600	0.18692200
H	1.96161200	-5.05501200	-2.91894700	C	-1.34158300	-1.15211200	0.02020700
C	0.50990300	-2.47534300	2.89833800	C	-3.26229700	-2.35329500	-0.03354300
H	-0.54259600	-2.38210600	2.59163200	H	-4.33354300	-2.51193000	-0.11778100
C	0.55882600	-3.53119100	4.01573500	C	-2.23822600	-3.22904000	0.15767500
H	0.23624000	-4.51974800	3.65368400	H	-2.23278700	-4.30884100	0.27554100
H	-0.10677400	-3.23931000	4.84323300	C	-3.45289700	0.12570500	-0.31249800
H	1.57082900	-3.64175500	4.43633200	C	-3.95076400	0.80442700	0.82254300
C	0.95680600	-1.09321200	3.41012200	C	-4.69126300	1.97456800	0.59894200
H	0.33232500	-0.77048500	4.25835100	H	-5.09556100	2.52438000	1.45168800
H	0.87520900	-0.33188400	2.61739800	C	-4.92771100	2.44424700	-0.69234900
H	2.00411100	-1.11227300	3.75307200	H	-5.51389300	3.35438100	-0.84226800
Cu	-0.08855600	0.43262500	0.01457500	C	-4.42882300	1.74971300	-1.79365000
				H	-4.62886000	2.12447100	-2.79986000
<b>4b</b>				C	-3.68326300	0.57229900	-1.63307700
C	5.90489900	-0.03268800	-0.41865200	C	-3.17749400	-0.17666400	-2.86377600
O	7.03696600	0.40164700	-0.49773300	H	-2.58683500	-1.03762700	-2.51756600
C	4.75818000	0.91114600	-0.28390800	C	-2.24184900	0.69502000	-3.71983100
C	3.38393000	0.65385500	-0.17210900	H	-2.76612900	1.56936100	-4.13719000
H	2.89218200	-0.31707000	-0.16041000	H	-1.84476200	0.11442100	-4.56757500
C	4.88375100	2.31487600	-0.26407300	H	-1.38743000	1.06535800	-3.13102300
O	3.69296000	2.88024100	-0.13782800	C	-4.34479500	-0.73447900	-3.69903900
C	5.59562400	-1.51131500	-0.45362500	H	-4.97633300	0.07309100	-4.10223300
H	5.06881300	-1.82319000	0.46304900	H	-4.99170200	-1.39509300	-3.10075100
H	4.93464500	-1.74907700	-1.30336900	H	-3.96353800	-1.31592800	-4.55349900
H	6.53318200	-2.07311600	-0.54944600	C	-3.73087900	0.30872000	2.24967800
C	6.07159700	3.19107600	-0.36391900	H	-3.09615000	-0.58861000	2.20301800

C	-5.05869600	-0.10932500	2.90849300	H	2.89839500	-0.31775700	-0.14919000
H	-4.87739600	-0.51782100	3.91535600	C	4.75162500	2.41305800	-0.30044800
H	-5.57924200	-0.87990000	2.31845200	O	3.53209100	2.91592800	-0.16986300
H	-5.74398800	0.74655400	3.01584700	C	5.66244300	-1.37214300	-0.44476500
C	-2.98235500	1.34415500	3.10744000	H	5.15123900	-1.69736000	0.47605900
H	-2.01684200	1.62028000	2.65472200	H	5.01599100	-1.65651000	-1.29138700
H	-2.78358100	0.93827800	4.11208700	H	6.62820900	-1.88541400	-0.53205900
H	-3.56840600	2.26793000	3.23664500	C	5.88811400	3.35202900	-0.42133200
C	0.24460700	-3.04232900	0.37215400	H	6.56551900	3.23484700	0.44054100
C	0.75824900	-3.14982200	1.68393400	H	6.49421000	3.10203200	-1.30514900
C	2.02616100	-3.73200400	1.83331700	H	5.52963800	4.38787800	-0.47804500
H	2.45315900	-3.83760500	2.83303800	C	2.60458500	1.86954100	-0.08264200
C	2.74382300	-4.19363700	0.73069400	C	1.22573700	2.08728000	0.02864800
H	3.72249900	-4.65871500	0.87363600	C	0.65266200	3.41799800	0.18381800
C	2.20991100	-4.07719500	-0.55266800	C	-0.69273000	3.63073800	-0.22144800
H	2.77843500	-4.45317700	-1.40625100	C	1.34840900	4.52013900	0.75369700
C	0.94907300	-3.49971800	-0.76484400	C	-1.29080800	4.88201700	-0.11689000
C	0.38222800	-3.41256500	-2.17968400	H	-1.25594600	2.79558600	-0.64178500
H	-0.56124500	-2.84918900	-2.13108300	C	0.73177000	5.75869900	0.89362900
C	1.31402900	-2.64054500	-3.13013200	H	2.36520300	4.39200600	1.11851600
H	2.27546300	-3.15909800	-3.27334600	C	-0.58195800	5.94980100	0.44590200
H	1.52742200	-1.62814700	-2.75153100	H	-2.31819600	5.02265100	-0.45930600
H	0.84838400	-2.53749500	-4.12298400	H	1.27688500	6.58549900	1.35462100
C	0.05135100	-4.80995800	-2.73640300	H	-1.05632400	6.92908100	0.54771600
H	-0.40722400	-4.72900000	-3.73469500	N	-2.63955700	-1.18064100	-0.10373100
H	-0.65183200	-5.35075300	-2.08392600	N	-0.97261400	-2.51953700	0.19825900
H	0.95663400	-5.43029100	-2.83495300	C	-1.28583600	-1.20646000	0.02867900
C	-0.00644200	-2.67648400	2.91748900	C	-3.16667700	-2.46017600	-0.01753500
H	-0.97256800	-2.27117900	2.58282200	H	-4.23276200	-2.65108000	-0.09934300
C	-0.31339500	-3.84162400	3.87596700	C	-2.11626100	-3.30457200	0.17396800
H	-0.87364900	-4.64423500	3.37138700	H	-2.07795500	-4.38329400	0.29487800
H	-0.91807600	-3.48888000	4.72639500	C	-3.43889000	0.00917500	-0.30897500
H	0.60726400	-4.28557200	4.28709300	C	-3.95278800	0.68050900	0.82279700
C	0.73268400	-1.53564200	3.63971900	C	-4.73835500	1.81927600	0.59185200
H	0.13807200	-1.17251400	4.49292700	H	-5.15732200	2.36277500	1.44145100
H	0.91251500	-0.68313900	2.96484800	C	-5.00082000	2.26553100	-0.70261600
H	1.70698400	-1.86639400	4.03394000	H	-5.62164100	3.15144700	-0.85796200
Ag	0.01274800	0.47580400	0.00536500	C	-4.48308600	1.57890600	-1.80015600
<b>4c</b>				H	-4.70372400	1.93522000	-2.80875100
C	5.89352000	0.12082700	-0.43186900	C	-3.69304800	0.43183900	-1.63275300
O	7.00036400	0.61335000	-0.52444400	C	-3.16599600	-0.30888500	-2.85953800
C	4.69920000	1.00514300	-0.30137300	H	-2.54810600	-1.14921500	-2.51003300
C	3.34089800	0.67611600	-0.17550500	C	-2.25781100	0.58631500	-3.72095400
				H	-2.80928900	1.44191400	-4.14214300

H	-1.84453800	0.01339300	-4.56622300	H	1.80584600	-1.87564100	4.05038900
H	-1.41447000	0.98350900	-3.13410700	Au	-0.01061400	0.42335600	0.00645100
C	-4.31621700	-0.90742100	-3.69029200				
H	-4.97293700	-0.12222100	-4.09737100	<b>5</b>			
H	-4.94207300	-1.58447000	-3.08791700	Pd	0.00019500	-0.02443600	0.03382600
H	-3.91772800	-1.48134100	-4.54196800	P	-2.31592300	-0.00955100	0.01311900
C	-3.70390800	0.20924000	2.25329800	P	2.31666800	-0.00998000	0.01160100
H	-3.02912000	-0.65872100	2.21244600	C	-3.09511100	1.61694300	0.44389100
C	-5.00878700	-0.26166900	2.92225700	C	-2.47251300	2.39054800	1.43999800
H	-4.80583500	-0.64779800	3.93380600	C	-4.25366200	2.11488000	-0.17464700
H	-5.49489600	-1.06345800	2.34441700	C	-3.00755900	3.62251600	1.82282600
H	-5.73294800	0.56281600	3.02034300	H	-1.55353900	2.02296000	1.90572500
C	-2.99812100	1.28547300	3.09680100	C	-4.78208600	3.35446300	0.20239400
H	-2.05254400	1.60471500	2.63116700	H	-4.74620600	1.53818600	-0.96052200
H	-2.76934600	0.89532500	4.10132700	C	-4.16394400	4.10874400	1.20331400
H	-3.62807900	2.17961000	3.22799900	H	-2.51279400	4.21070600	2.60022300
C	0.36067700	-3.05178100	0.37756700	H	-5.68153400	3.73154100	-0.29179700
C	0.87886500	-3.15322000	1.68761800	H	-4.57770400	5.07763100	1.49523800
C	2.15966000	-3.70805400	1.83072200	C	-3.08859200	-0.42590400	-1.61995600
H	2.59141400	-3.80929600	2.82882400	C	-4.26651800	-1.17835600	-1.75574000
C	2.88457000	-4.14767900	0.72385400	C	-2.44252800	0.03822000	-2.77993100
H	3.87382100	-4.59131100	0.86204500	C	-4.79081200	-1.45228300	-3.02385200
C	2.34510100	-4.03689700	-0.55772400	H	-4.77787100	-1.55842600	-0.86881400
H	2.91956400	-4.39594400	-1.41455100	C	-2.97351700	-0.22616400	-4.04429900
C	1.07084600	-3.48747500	-0.76399300	H	-1.50917700	0.60040400	-2.68260700
C	0.49711400	-3.40848500	-2.17652800	C	-4.14916100	-0.97433200	-4.16959100
H	-0.45760400	-2.86451300	-2.12358100	H	-5.70589500	-2.04369900	-3.11439200
C	1.40904000	-2.61553400	-3.12891200	H	-2.46082700	0.14396000	-4.93608300
H	2.38016500	-3.11430400	-3.27717900	H	-4.55990000	-1.19048500	-5.15936200
H	1.60197600	-1.59982200	-2.74899400	C	-3.13680400	-1.19339600	1.18047200
H	0.93708600	-2.52060900	-4.11959400	C	-4.30365500	-0.89440700	1.90218400
C	0.19293000	-4.81147100	-2.73458400	C	-2.53739400	-2.45417600	1.35264800
H	-0.27047500	-4.73813600	-3.73122700	C	-4.86295000	-1.83930100	2.76966800
H	-0.49671400	-5.36820100	-2.08095100	H	-4.77903500	0.08272500	1.79383800
H	1.11051900	-5.41276400	-2.83733500	C	-3.10348500	-3.40036500	2.20975400
C	0.10675800	-2.70289600	2.92504000	H	-1.61227900	-2.68428900	0.81614600
H	-0.86571200	-2.30965500	2.59402200	C	-4.26792400	-3.09431400	2.92259400
C	-0.18151500	-3.88191100	3.87241800	H	-5.76878000	-1.59015900	3.32895100
H	-0.72784300	-4.68944600	3.36036300	H	-2.62669000	-4.37666900	2.33056200
H	-0.79233300	-3.54731000	4.72576200	H	-4.70595700	-3.83059200	3.60165100
H	0.74648100	-4.31396800	4.27972800	C	3.07520900	1.35042500	-0.99414800
C	0.82729700	-1.55658500	3.65701000	C	4.22636800	1.18957900	-1.78214100
H	0.22573300	-1.20976300	4.51218500	C	2.44305100	2.60668600	-0.96518500
H	0.99335400	-0.69709200	2.98816700	C	4.73823200	2.26439800	-2.51770300

H	4.72633700	0.21986200	-1.82829100	H	-3.67028800	3.91184400	2.87848700
C	2.96179400	3.68125700	-1.69073700	H	-2.05566000	4.55850600	3.37256800
H	1.52898900	2.73135100	-0.37733100	C	-0.71778300	2.27797600	-0.87991200
C	4.11080200	3.51213100	-2.47107200	C	0.55150300	2.25673800	-1.04374900
H	5.63227300	2.12280200	-3.13086200	C	1.71268100	3.11564000	-1.21656300
H	2.45969800	4.65170500	-1.65626000	C	2.67996600	2.87163300	-2.21062700
H	4.51141000	4.35002500	-3.04769300	C	1.86815000	4.24530000	-0.38313700
C	3.11389500	-1.53804400	-0.67254900	C	3.76163200	3.73822600	-2.37638500
C	4.32044800	-2.06995900	-0.18914700	H	2.57091200	1.99859500	-2.85591600
C	2.45809300	-2.19454300	-1.72928700	C	2.95759000	5.10108100	-0.54678000
C	4.86337600	-3.22733800	-0.75768400	H	1.12241700	4.43205000	0.39222500
H	4.83977500	-1.58303700	0.63905800	C	3.90669300	4.85376300	-1.54511800
C	3.00698000	-3.34374600	-2.30300500	H	4.49884100	3.53758500	-3.15807600
H	1.50255400	-1.80272100	-2.09001500	H	3.06502200	5.97081000	0.10711700
C	4.21123900	-3.86409900	-1.81715100	H	4.75703300	5.52860400	-1.67436900
H	5.80090000	-3.63292300	-0.36797100	Pd	0.04073600	0.27093900	-0.60438500
H	2.48583900	-3.84152500	-3.12501300	P	2.12271800	-0.59881900	0.17758000
H	4.63645500	-4.76918900	-2.25882100	P	-1.73619900	-1.33718400	-0.33367200
C	3.13213800	0.18316400	1.66520200	C	3.53019600	-0.39771200	-1.00716200
C	4.28751400	0.95200000	1.88055800	C	3.31196600	-0.81020100	-2.33504500
C	2.54110700	-0.47404900	2.75937500	C	4.77537300	0.15250100	-0.66806100
C	4.84408100	1.05270200	3.16050700	C	4.32428000	-0.70556700	-3.29129700
H	4.75590300	1.48197700	1.04840200	H	2.33366200	-1.20537500	-2.62411000
C	3.10416300	-0.38133400	4.03399900	C	5.78393800	0.27119900	-1.63073100
H	1.62468100	-1.05122300	2.60528500	H	4.96228100	0.50335700	0.34790600
C	4.25734200	0.38433200	4.23824000	C	5.56565600	-0.16287100	-2.94044600
H	5.74094600	1.65890400	3.31375700	H	4.13922800	-1.03694200	-4.31644000
H	2.63374700	-0.89964900	4.87374600	H	6.74553200	0.70970900	-1.35164500
H	4.69284400	0.46562200	5.23765800	H	6.35668900	-0.07145900	-3.68930600
<b>6</b>				C	2.62268200	0.27460000	1.73361700
C	-4.13351100	3.83624600	-0.12220900	C	3.67644000	-0.19511000	2.54144900
O	-4.85090200	4.28691900	0.75926700	C	1.89985700	1.40418300	2.14939200
C	-2.73071300	3.40606800	0.13400400	C	4.01130100	0.46695500	3.72439800
C	-2.03860200	2.74408400	-0.86940600	H	4.23157200	-1.09089400	2.25317700
H	-2.59224200	2.51744800	-1.78663300	C	2.23276900	2.06001300	3.33979200
C	-2.06415300	3.65735300	1.44742800	H	1.05851000	1.77402000	1.56078700
O	-0.93150100	3.23241300	1.65869800	C	3.28982700	1.59769300	4.12587600
C	-4.69369500	3.73757700	-1.53874700	H	4.83303400	0.09249100	4.34068600
H	-4.06166000	4.26793500	-2.26800500	H	1.64564600	2.92982700	3.64379800
H	-4.77869500	2.68992400	-1.86624200	H	3.54865400	2.10910800	5.05695700
H	-5.69553300	4.18569600	-1.52999700	C	2.30240600	-2.36998600	0.71305200
C	-2.76469600	4.43655300	2.54231800	C	3.19664400	-3.27783400	0.12369700
H	-3.11366500	5.41504300	2.18153000	C	1.46313700	-2.82482400	1.74765100
				C	3.24807800	-4.60834700	0.55755500



H	3.86451000	-2.95146800	-0.67529100	C	-1.15176000	-1.23760300	0.00001900
C	1.52072400	-4.14945800	2.18224600	C	-1.83254300	-0.00001200	0.00014400
H	0.75990100	-2.13619400	2.22221600	C	-1.15172500	1.23760800	0.00023200
C	2.41251200	-5.04839800	1.58619100	C	0.24753200	1.21672600	0.00022500
H	3.95326500	-5.30034300	0.08921600	H	0.80252100	-2.15630500	-0.00025000
H	0.86077000	-4.48086600	2.98785300	H	0.80258400	2.15623200	0.00033700
H	2.45528800	-6.08701200	1.92407000	Br	2.83694300	0.00000600	-0.00004300
C	-3.38055000	-0.77136900	-0.98519600	C	-1.91630900	2.53433200	-0.00015000
C	-4.51239400	-0.57884900	-0.17927600	H	-2.57359700	2.60941900	0.88152900
C	-3.48288300	-0.51958900	-2.36661000	H	-1.23485400	3.39601200	0.00202900
C	-5.72406100	-0.15994300	-0.74387600	H	-2.56959900	2.61098400	-0.88473200
H	-4.45823500	-0.76098500	0.89557000	C	-1.91633600	-2.53433600	-0.00005300
C	-4.69390800	-0.11523100	-2.92979400	H	-1.23488300	-3.39601500	-0.00164100
H	-2.60763800	-0.64973600	-3.00957700	H	-2.57031800	-2.61096200	0.88402500
C	-5.82166800	0.06459800	-2.11839400	H	-2.57295600	-2.60943700	-0.88222800
H	-6.59553700	-0.01311700	-0.10073400	N	-3.21689200	0.00001700	0.00000000
H	-4.75842700	0.06307400	-4.00647200	C	-4.39563900	0.00004100	-0.00008800
H	-6.77004000	0.38397700	-2.55775500				
C	-2.08858300	-1.68433400	1.45153000	<b>PPh<sub>3</sub></b>			
C	-2.52383800	-2.92779100	1.93802800	P	-0.00134000	-0.00029700	1.20994900
C	-1.88398500	-0.63145200	2.36335500	C	-1.63411900	-0.35259100	0.40274500
C	-2.75639200	-3.11240200	3.30506700	C	-2.44324600	-1.33264300	1.00727000
H	-2.67581200	-3.76315300	1.25243000	C	-2.12261800	0.31356000	-0.73385300
C	-2.12706600	-0.81626000	3.72724400	C	-3.69430800	-1.65583500	0.47718300
H	-1.51922500	0.33601200	2.00641900	H	-2.08765000	-1.84593100	1.90571100
C	-2.56205400	-2.05781400	4.20197600	C	-3.38109400	-0.00153300	-1.25761300
H	-3.09074700	-4.08761700	3.66901800	H	-1.51728000	1.08498700	-1.21483700
H	-1.96400400	0.01270700	4.42038400	C	-4.16815000	-0.98815100	-0.65714700
H	-2.74401800	-2.20455600	5.26981700	H	-4.30622900	-2.42385900	0.95769800
C	-1.62778700	-3.01017400	-1.13109800	H	-3.74658000	0.52773100	-2.14185100
C	-2.76742200	-3.78646600	-1.41344400	H	-5.15120400	-1.23270900	-1.06788300
C	-0.36635500	-3.51434600	-1.48426200	C	0.50974500	1.59012000	0.40232400
C	-2.64263400	-5.03921100	-2.01926300	C	1.35144700	1.68182500	-0.71872000
H	-3.76193900	-3.40772700	-1.16805800	C	0.04579400	2.78001500	0.99396600
C	-0.24172300	-4.76877800	-2.08975300	C	1.71090200	2.92996100	-1.23871800
H	0.52554900	-2.92071700	-1.28196700	H	1.73093900	0.77279600	-1.19024600
C	-1.37891700	-5.53425600	-2.35810300	C	0.39443300	4.02564500	0.46725500
H	-3.53813800	-5.62901000	-2.23219600	H	-0.59374600	2.72752400	1.88026800
H	0.75015500	-5.14445800	-2.35296000	C	1.23144100	4.10380900	-0.65097600
H	-1.28316100	-6.51293400	-2.83565300	H	2.36839400	2.98328000	-2.11068700
				H	0.02039800	4.93885200	0.93778100
<b>7</b>				H	1.51335100	5.07789700	-1.05909700
C	0.93196900	-0.00003800	0.00011300	C	1.12108500	-1.23775700	0.40297600
C	0.24753800	-1.21675900	-0.00003900	C	2.37819800	-1.43971700	1.00315100

C	0.78681500	-2.00248400	-0.72725700	C	-4.99941500	-3.15752500	-1.75219300
C	3.28471000	-2.36209800	0.47593100	H	-4.16945300	-3.15571700	0.23799700
H	2.64675200	-0.86848500	1.89686700	C	-3.66443300	-2.10366600	-3.47140000
C	1.69006300	-2.93561600	-1.24785100	H	-1.79525600	-1.23761900	-2.81980100
H	-0.18618000	-1.87119300	-1.20558900	C	-4.82460400	-2.78559100	-3.08817300
C	2.94111400	-3.11571400	-0.65139400	H	-5.90713600	-3.68264800	-1.44378300
H	4.25823800	-2.50152800	0.95347500	H	-3.52307900	-1.80226400	-4.51257900
H	1.41264200	-3.52415300	-2.12657800	H	-5.59367100	-3.02026400	-3.82853400
H	3.64499100	-3.84553200	-1.05989800	C	-2.24643200	-1.90815600	1.68507500
				C	-2.42243100	-3.15876500	2.30541800
<b>8</b>				C	-2.64241900	-0.74490000	2.36718000
C	-5.96917100	1.63164900	-0.36473200	C	-2.99726100	-3.24247300	3.57622800
O	-6.93883400	1.84573100	0.34675700	H	-2.10166000	-4.07225100	1.79912000
C	-4.58648400	1.99282400	0.05931200	C	-3.21925600	-0.83408700	3.63811200
C	-3.52506100	1.70311300	-0.77119100	H	-2.49595400	0.24033500	1.91667100
H	-3.76207100	1.20830300	-1.71923000	C	-3.39865000	-2.08023200	4.24409500
C	-4.32581200	2.65488000	1.37961200	H	-3.12772000	-4.21974200	4.04861600
O	-3.20255800	2.62459300	1.86389400	H	-3.51838800	0.08243700	4.15238100
C	-6.18621000	0.96591500	-1.72080600	H	-3.84421700	-2.14789600	5.24010100
H	-5.82583400	1.59772400	-2.54795700	C	-0.34774100	-3.17226900	-0.08504900
H	-5.66483800	-0.00177100	-1.78836600	C	-0.51033100	-4.23533500	-0.98662100
H	-7.26458500	0.80023400	-1.83901400	C	0.76951600	-3.17687100	0.77113700
C	-5.43286900	3.38600900	2.11003900	C	0.42021000	-5.28072300	-1.02887400
H	-5.99940500	4.04715400	1.43779700	H	-1.36817100	-4.25495600	-1.66121300
H	-6.16555400	2.66690500	2.50388700	C	1.68923600	-4.22644700	0.73680500
H	-4.97740700	3.95747100	2.93039000	H	0.91704800	-2.35338200	1.47491500
C	-2.14191300	1.91908600	-0.60055600	C	1.51896800	-5.28215700	-0.16729600
C	-0.99595600	2.48926800	-0.67094900	H	0.27789800	-6.10077500	-1.73765000
C	-0.27207600	3.74242900	-0.76918900	H	2.54472600	-4.21954500	1.41744400
C	0.93663000	3.84626900	-1.48648500	H	2.24117400	-6.10202300	-0.19726200
C	-0.77802300	4.89475900	-0.12923600	C	1.39226700	0.27254600	-0.24188300
C	1.60660900	5.06690700	-1.57923000	N	2.56770300	0.19221600	-0.17016800
H	1.33889800	2.95516900	-1.97337500	C	3.94175700	0.13518500	-0.06234900
C	-0.09976300	6.11082700	-0.21910800	C	4.65091200	-0.81193200	-0.83659800
H	-1.69915800	4.81280000	0.45115500	C	4.59285100	1.02978800	0.81884800
C	1.09187200	6.20427300	-0.94643300	C	6.04350400	-0.85424600	-0.70811600
H	2.53790900	5.13236000	-2.14836700	C	3.92181400	-1.74232500	-1.76883700
H	-0.50323600	6.99290800	0.28539200	C	5.98639700	0.95296300	0.92002300
H	1.62009900	7.15868600	-1.01650800	C	3.80320200	2.03278000	1.61665600
Pd	-0.56365000	0.48198200	-0.36625400	C	6.69665200	0.01924700	0.16331600
P	-1.49790500	-1.72174000	0.00636700	H	6.61838400	-1.57414600	-1.29274300
C	-2.84766200	-2.17833900	-1.17643800	H	4.62512300	-2.38936000	-2.31085300
C	-4.01685700	-2.85970300	-0.80153100	H	3.21391600	-2.38478400	-1.21985600
C	-2.68860500	-1.79369000	-2.52062500	H	3.32871400	-1.18067400	-2.50909700

H	6.51659200	1.62873500	1.59299400	C	-6.29912400	-2.03173600	-0.71054700
H	3.06448000	1.53552500	2.26655100	H	-6.32219700	-3.30545000	1.03852900
H	4.46305600	2.64249000	2.24871300	H	-5.97188100	-0.70239900	-2.38470700
H	3.23431800	2.70868500	0.95721500	H	-7.37116700	-2.13074900	-0.89758700
Br	8.59372500	-0.06425700	0.32100800	C	-1.39461400	-2.23694500	1.69605200
<b>9-ts</b>				C	-0.75596700	-3.46592300	1.92256500
C	-5.44856900	2.65477900	-1.16780500	C	-1.76072900	-1.43838000	2.79802600
O	-6.49641100	2.24256500	-0.68052400	C	-0.49660300	-3.89618500	3.22939400
C	-4.11873100	2.41135900	-0.57507900	H	-0.45669100	-4.09463000	1.08194800
C	-2.95593900	2.80637300	-1.30134300	C	-1.50899600	-1.87904500	4.09884200
H	-3.06802300	3.04623900	-2.36495100	H	-2.23871500	-0.46923700	2.62467800
C	-3.95991300	1.65498400	0.65213900	C	-0.87512700	-3.10752000	4.31842700
O	-2.82598800	1.29422600	1.07053200	H	0.00172700	-4.85538800	3.39316800
C	-5.53076300	3.47462200	-2.45836300	H	-1.80259400	-1.25394200	4.94608200
H	-5.04521500	4.45769800	-2.35601900	H	-0.67371900	-3.44697800	5.33781100
H	-5.04380400	2.95486300	-3.30065200	C	-1.03814600	-2.77014400	-1.17526800
H	-6.59262400	3.61279400	-2.69936000	C	-1.63937100	-4.02819000	-1.36638500
C	-5.15386500	1.23020900	1.48060800	C	0.09384200	-2.44190300	-1.93840700
H	-5.80636500	2.08631600	1.70304400	C	-1.10640400	-4.93935100	-2.28100200
H	-5.78569500	0.51542600	0.93444600	H	-2.53672900	-4.29605200	-0.80420600
H	-4.78640200	0.77757100	2.41186900	C	0.62640400	-3.35466800	-2.85569200
C	-1.69996900	2.91919700	-0.78915000	H	0.55317400	-1.45898400	-1.82491300
C	-0.58186600	2.84543500	-0.17337300	C	0.02982200	-4.60601100	-3.02627700
C	0.42477700	3.73071400	0.40130900	H	-1.58587000	-5.91212400	-2.41757500
C	1.15565800	3.38334400	1.55461900	H	1.50525500	-3.08008000	-3.44472200
C	0.67417100	4.98725900	-0.19248500	H	0.44230300	-5.31794400	-3.74584800
C	2.09382900	4.26258400	2.09891300	C	1.07631400	0.40461100	-0.04327900
H	0.96875500	2.41707100	2.02732800	N	2.23695800	0.21207100	-0.12143400
C	1.61556100	5.86140900	0.35159100	C	3.60011600	0.00838200	-0.19388700
H	0.11695400	5.26573100	-1.08974100	C	4.40675500	0.99923000	-0.80109200
C	2.33160600	5.50414700	1.49966600	C	4.14056200	-1.18259200	0.34456300
H	2.64199000	3.97662600	3.00065200	C	5.78569600	0.77040300	-0.86494700
H	1.79249600	6.82949400	-0.12487100	C	3.79619600	2.25966600	-1.35220800
H	3.06935300	6.18936600	1.92492900	C	5.52421100	-1.37074700	0.26151900
Pd	-0.81874900	0.74978600	-0.00401300	C	3.24891300	-2.21073200	0.98823300
P	-1.72904100	-1.53680200	0.02137500	C	6.33101800	-0.40206000	-0.33865800
C	-3.54513900	-1.75673000	-0.21682400	H	6.43473400	1.51534400	-1.32792900
C	-4.34295700	-2.54852700	0.62576500	H	4.55973000	2.89466400	-1.82157900
C	-4.14601900	-1.09409200	-1.30172600	H	3.02318700	2.03453800	-2.10496700
C	-5.71176800	-2.68655700	0.37572600	H	3.30127300	2.84332500	-0.55894500
H	-3.89818000	-3.05904600	1.48231600	H	5.97137100	-2.27887000	0.66878700
C	-5.51309800	-1.23542900	-1.54906300	H	2.50726800	-2.60199100	0.27253200
H	-3.54265200	-0.45423900	-1.95134400	H	3.83527400	-3.05731300	1.37068900
				H	2.67885200	-1.77956300	1.82719500

Br	8.21179200	-0.68544200	-0.43950600	C	-2.13580700	-2.07144600	2.08118100
				C	-1.90992700	-3.34896100	2.62212900
<b>10</b>				C	-2.78412800	-1.09763900	2.86353300
C	-5.02803200	2.51087600	-2.27787400	C	-2.32620200	-3.64767400	3.92318400
O	-6.14469500	2.04750800	-2.06762800	H	-1.40416800	-4.11592700	2.03188300
C	-3.86498800	2.29939000	-1.39208200	C	-3.20045700	-1.40483100	4.16194500
C	-2.56797800	2.73998400	-1.84035700	H	-2.96814100	-0.10531100	2.44246600
H	-2.42234900	2.91411900	-2.91252900	C	-2.97179000	-2.67714000	4.69492700
C	-3.98427700	1.56778800	-0.16392900	H	-2.14458300	-4.64450300	4.33350900
O	-2.98686300	1.27337800	0.57755100	H	-3.70408000	-0.64156700	4.76059500
C	-4.83076400	3.36678600	-3.53209400	H	-3.29500900	-2.91242500	5.71232800
H	-4.39110400	4.34889500	-3.29869500	C	-0.36134100	-2.84462700	-0.09636600
H	-4.15977100	2.87309200	-4.25541100	C	-0.48132400	-3.65592700	-1.23624800
H	-5.81270600	3.50254400	-4.00359300	C	0.81231400	-2.93406300	0.67643100
C	-5.32454900	1.06636600	0.33446100	C	0.54598000	-4.53773300	-1.59171200
H	-6.06973800	1.87330200	0.36213500	H	-1.38134700	-3.60426900	-1.85165200
H	-5.74255600	0.30839600	-0.34421300	C	1.83066700	-3.82262600	0.32636600
H	-5.18806200	0.63901100	1.33721300	H	0.92686600	-2.31047400	1.56672500
C	-1.50107300	2.92624700	-1.03501400	C	1.70175600	-4.62652100	-0.81227800
C	-0.61892400	2.81904100	-0.10479800	H	0.43498200	-5.16272500	-2.48159700
C	0.15211000	3.74266400	0.72469600	H	2.73050800	-3.88604600	0.94357600
C	0.47840900	5.02541300	0.23229100	H	2.50000100	-5.32012100	-1.08827200
C	0.57210100	3.40732300	2.02709900	C	1.00743500	0.48750600	0.16708100
C	1.18863000	5.93442200	1.01607700	N	2.16148400	0.31731800	0.01261700
H	0.16494100	5.29557100	-0.77860800	C	3.51044900	0.11644400	-0.20500000
C	1.27953600	4.32152000	2.81121700	C	3.92068000	-0.46853500	-1.42509700
H	0.32157700	2.42141600	2.42518900	C	4.42915100	0.50809000	0.79521900
C	1.59447800	5.58868900	2.31015500	C	5.29152400	-0.65879500	-1.63047300
H	1.42960100	6.92181000	0.61282500	C	2.90894200	-0.87098900	-2.46421500
H	1.58242500	4.04315100	3.82443700	C	5.79078800	0.29860000	0.55059400
H	2.15168200	6.30198300	2.92284900	C	3.95112100	1.13163700	2.07894300
Pd	-0.89241100	0.74597200	0.21441000	C	6.20957900	-0.27799200	-0.64992000
P	-1.63923100	-1.59410600	0.36923600	H	5.64101000	-1.10579300	-2.56241700
C	-3.08994400	-2.01421000	-0.68376200	H	3.40249700	-1.27115700	-3.36033000
C	-4.00371800	-3.02590600	-0.34043900	H	2.22446100	-1.64231200	-2.07434100
C	-3.28993300	-1.28351200	-1.86719700	H	2.28577900	-0.01366500	-2.76708900
C	-5.08793800	-3.30789100	-1.17437200	H	6.52544000	0.59098200	1.30239700
H	-3.87390800	-3.59242400	0.58409100	H	3.27159100	0.45429200	2.62247100
C	-4.37521800	-1.57023400	-2.70061800	H	4.79563500	1.37125400	2.73930800
H	-2.60576800	-0.47217800	-2.12853200	H	3.38564600	2.05863400	1.88941700
C	-5.27548000	-2.58140500	-2.35538200	Br	8.06955100	-0.54901000	-0.95653000
H	-5.79448600	-4.09412900	-0.89628100				
H	-4.52952500	-0.98482700	-3.60979800	<b>11-ts</b>			
H	-6.13132900	-2.79546000	-3.00039800	C	-3.56808100	3.61455100	-2.68385900

O	-4.76196000	3.43621000	-2.90546800	H	-2.13287300	-4.08243200	1.91193700
C	-2.84130800	2.99451800	-1.55819300	C	-4.30788500	-1.32278700	3.57998100
C	-1.40153300	3.16114200	-1.51176800	H	-3.65938100	-0.03320600	1.96506900
H	-0.92133000	3.58457300	-2.40056600	C	-4.23101800	-2.59716400	4.15240400
C	-3.53097300	2.22360300	-0.56998400	H	-3.38268800	-4.58147600	3.99300100
O	-2.93825600	1.59098700	0.37008900	H	-4.91566100	-0.54567200	4.05025500
C	-2.79919400	4.53421000	-3.63961200	H	-4.77921700	-2.81917000	5.07166400
H	-2.28185500	5.34898900	-3.10907000	C	-0.73860400	-2.94310600	-0.04580100
H	-2.03892500	3.98023400	-4.21564900	C	-0.91474500	-3.90427800	-1.05370100
H	-3.52571600	4.95975100	-4.34365800	C	0.40969100	-3.00761300	0.76454900
C	-5.04121400	2.10236800	-0.56033500	C	0.03635300	-4.91338200	-1.24171600
H	-5.53353900	3.07903900	-0.65890700	H	-1.79564100	-3.86756400	-1.69708300
H	-5.39245200	1.51104800	-1.41930300	C	1.35065000	-4.02222400	0.58212400
H	-5.34060600	1.61226500	0.37663100	H	0.56820000	-2.25602100	1.54201100
C	-0.56350400	2.87828000	-0.50718400	C	1.16735300	-4.97688400	-0.42461300
C	0.19493300	2.41250200	0.44806600	H	-0.11171400	-5.65338300	-2.03237300
C	0.76657300	3.06366500	1.63934400	H	2.23603500	-4.06284200	1.22152700
C	1.27940400	4.37202400	1.53520400	H	1.90877400	-5.76596400	-0.57334300
C	0.82231700	2.42100300	2.88985000	C	0.89482900	0.57385200	0.29050300
C	1.81997400	5.01661300	2.64813000	N	2.01266600	0.21059900	0.08903300
H	1.24682800	4.87784700	0.56745500	C	3.33574100	-0.00519700	-0.20332700
C	1.36292600	3.07025200	4.00289900	C	3.73425200	-0.08034600	-1.56097700
H	0.41848500	1.41042200	2.99083100	C	4.26437300	-0.15819300	0.85483500
C	1.86574700	4.36964900	3.88802000	C	5.08561700	-0.30423200	-1.84191800
H	2.21065100	6.03262100	2.54623900	C	2.72034100	0.07389100	-2.66341500
H	1.38442700	2.55789700	4.96846100	C	5.60642300	-0.38181500	0.52999900
H	2.28994200	4.87576200	4.75878700	C	3.80946900	-0.07784200	2.28728000
Pd	-1.01683800	0.58244300	0.39302300	C	6.00825000	-0.45266400	-0.80474400
P	-1.93198700	-1.56878100	0.24506200	H	5.41699000	-0.36346300	-2.88000800
C	-3.19591700	-1.73162800	-1.08339200	H	3.19408900	-0.00989400	-3.65117300
C	-4.26798700	-2.63593400	-0.99106800	H	1.93485900	-0.69685600	-2.59165400
C	-3.08904200	-0.90719900	-2.21590700	H	2.21139200	1.05031400	-2.60798900
C	-5.20709400	-2.72100200	-2.02197700	H	6.34056700	-0.49970600	1.32891800
H	-4.37649600	-3.27042600	-0.10858000	H	3.04496400	-0.84223800	2.50672400
C	-4.03114700	-0.99405200	-3.24467700	H	4.65014700	-0.22795700	2.97872000
H	-2.27845200	-0.17709200	-2.28217300	H	3.34971200	0.89936400	2.50973900
C	-5.09017800	-1.90129700	-3.14949400	Br	7.84396400	-0.76098700	-1.21886300
H	-6.03936400	-3.42468000	-1.93944700				
H	-3.94721700	-0.33527400	-4.11209500	<b>12</b>			
H	-5.83269400	-1.96111200	-3.94922900	C	-2.36846800	5.44948800	-1.28978900
C	-2.81891900	-2.02646200	1.79473700	O	-3.48391300	5.88594800	-1.54678100
C	-2.74368300	-3.30367700	2.37332200	C	-2.11159600	4.04172700	-0.90291700
C	-3.60370300	-1.03190000	2.40920200	C	-0.77071000	3.67628000	-0.54656200
C	-3.44808300	-3.58484700	3.54877000	H	-0.00683100	4.45264300	-0.66725700

C	-3.17000500	3.07039100	-0.91976400	H	-6.13543600	-3.96334400	1.88134400
O	-3.02711800	1.84832400	-0.59410200	H	-6.85199600	0.03459300	0.41914400
C	-1.18908500	6.42353200	-1.37043900	H	-7.70600800	-2.07377800	1.44455000
H	-0.70878700	6.57181600	-0.38972400	C	-1.28042500	-2.63659000	1.22125900
H	-0.41252300	6.07910900	-2.07225900	C	-0.94691400	-3.97085300	0.94018300
H	-1.58441100	7.38631900	-1.71802100	C	-0.96918200	-2.10749400	2.48547500
C	-4.56968700	3.42543200	-1.37308200	C	-0.32131400	-4.76237100	1.90991600
H	-5.02941500	4.15069300	-0.68598200	H	-1.17174200	-4.39600500	-0.04012100
H	-4.56677800	3.92230500	-2.35264900	C	-0.35226100	-2.90144100	3.45467200
H	-5.16689500	2.50426200	-1.40926200	H	-1.20869000	-1.06481000	2.71209500
C	-0.29140600	2.47323500	-0.14789200	C	-0.02641800	-4.23176800	3.16848400
C	0.65083400	1.76740100	0.60175900	H	-0.06481800	-5.79934800	1.67803500
C	1.20354400	2.16776700	1.92132500	H	-0.11979100	-2.47757300	4.43492100
C	0.73848800	3.32983500	2.56586100	H	0.46090200	-4.85219900	3.92496100
C	2.22958300	1.42117500	2.53161800	C	0.70948500	0.42246000	0.05705300
C	1.29495300	3.74195300	3.77661800	N	1.47099900	-0.50826500	-0.29159700
H	-0.07421400	3.90255300	2.11465300	C	2.86859600	-0.46391900	-0.46491900
C	2.78236200	1.83493600	3.74458600	C	3.48429100	0.44579500	-1.35945800
H	2.60990200	0.52218500	2.04590900	C	3.63500100	-1.44736000	0.20967000
C	2.31876600	2.99608100	4.37100900	C	4.87616900	0.38527600	-1.52299800
H	0.92189900	4.64624900	4.26399400	C	2.68590900	1.44073200	-2.16708400
H	3.58432900	1.24874100	4.20009500	C	5.02291400	-1.46514600	0.03608000
H	2.75219100	3.31781900	5.32132600	C	2.95993000	-2.45386600	1.10472000
Pd	-1.29250700	0.71118300	-0.09269300	C	5.63394100	-0.54910100	-0.82077900
P	-2.16085700	-1.54270000	0.01993100	H	5.36572600	1.07540100	-2.21277500
C	-2.01749100	-2.42028000	-1.59740200	H	3.26806400	1.79222600	-3.03110500
C	-3.11458200	-3.00706400	-2.24689600	H	1.74788300	1.00161500	-2.53929500
C	-0.75383000	-2.45002400	-2.21845300	H	2.40536900	2.32678400	-1.57488600
C	-2.94953900	-3.62194300	-3.49322200	H	5.62497600	-2.20693400	0.56405100
H	-4.10336600	-2.98465600	-1.78535500	H	2.14238200	-2.96697500	0.57426300
C	-0.59456400	-3.07377600	-3.45727400	H	3.67588300	-3.20656700	1.46465800
H	0.10555400	-1.98586100	-1.72575900	H	2.49483700	-1.97928500	1.98459700
C	-1.69171200	-3.65991600	-4.09885100	Br	7.52892700	-0.59651400	-1.05418100
H	-3.81234300	-4.07262900	-3.99045800				
H	0.39196400	-3.09569100	-3.92749600	<b>13-ts</b>			
H	-1.56555800	-4.14165300	-5.07190400	C	-6.09093900	0.35067900	-1.50688300
C	-3.93234400	-1.73880800	0.50499200	O	-7.08161900	-0.19061900	-1.03408400
C	-4.41834300	-2.92146700	1.09108000	C	-4.90945500	0.66681900	-0.68991000
C	-4.81883500	-0.67371700	0.26992900	C	-3.72949600	1.25169900	-1.16245100
C	-5.76962000	-3.04001300	1.42465200	H	-3.61138300	1.56636600	-2.20345200
H	-3.74124000	-3.75385300	1.29358400	C	-4.77360500	0.36494900	0.71838700
C	-6.17138100	-0.80042300	0.60423900	O	-3.69076100	0.71404300	1.24735000
H	-4.44738000	0.25888900	-0.16172400	C	-6.05938600	0.72173800	-2.98507600
C	-6.64949700	-1.98037000	1.17982800	H	-5.92235800	1.80669600	-3.12234200

H	-5.22969400	0.21701600	-3.50651300	C	1.85432400	-2.95212000	2.19043800
H	-7.01070100	0.41780200	-3.44028000	C	-0.00998000	-1.52973100	2.80618000
C	-5.80682700	-0.35584200	1.53680600	C	2.23912100	-3.02223200	3.53306700
H	-6.76275600	0.18719900	1.50621100	H	2.44054100	-3.47636700	1.43284700
H	-6.01893000	-1.34489100	1.10281100	C	0.37230500	-1.61014300	4.14780400
H	-5.44953800	-0.45587900	2.57025200	H	-0.88071300	-0.93175600	2.52009200
C	-2.61925700	1.40255200	-0.33232400	C	1.49826400	-2.35516800	4.51340100
C	-1.66781600	2.36599200	0.02406800	H	3.12288000	-3.60147400	3.81281400
C	-1.92684000	3.80238500	0.26905200	H	-0.20767500	-1.08070500	4.90783200
C	-3.25160000	4.28521600	0.29910800	H	1.80180600	-2.41112600	5.56197300
C	-0.88321400	4.72638300	0.47919200	C	-0.40656500	1.73074600	0.12164500
C	-3.51904100	5.63762200	0.51227100	N	0.77213900	1.99181200	0.38286500
H	-4.08129600	3.58846000	0.16618300	C	2.10586400	1.86652600	0.12326700
C	-1.15567300	6.07922400	0.69406500	C	2.58631700	1.93855400	-1.21540900
H	0.15133100	4.38101000	0.47438400	C	3.01000500	1.73736100	1.21257100
C	-2.47322200	6.54569100	0.70928300	C	3.96343200	1.85313000	-1.44034300
H	-4.55599000	5.98416600	0.53251200	C	1.62243300	2.10346300	-2.35912100
H	-0.32698200	6.77519800	0.85113300	C	4.37963800	1.64923100	0.94561700
H	-2.68413200	7.60460900	0.87845700	C	2.48366100	1.69480700	2.62153100
Pd	-1.21998300	-0.17777100	-0.33751300	C	4.84655600	1.70244100	-0.36913600
P	0.12600300	-2.09335400	0.07354700	H	4.34654600	1.90479600	-2.46107100
C	1.58304800	-2.61239600	-0.93795200	H	2.15256700	2.16568000	-3.31974700
C	1.64383700	-3.84422000	-1.60986700	H	0.91502700	1.25866800	-2.41024400
C	2.66683700	-1.72319200	-1.04757800	H	1.01363600	3.01506500	-2.24022400
C	2.76827000	-4.17832400	-2.37256900	H	5.08483100	1.54041000	1.77153800
H	0.81424300	-4.54990200	-1.54069800	H	1.84056400	0.81372400	2.78064800
C	3.79242800	-2.06436600	-1.79982400	H	3.30370600	1.65809400	3.35251500
H	2.63610300	-0.75699400	-0.54008100	H	1.86068700	2.57844200	2.83604800
C	3.84463200	-3.29288800	-2.46731600	Br	6.72026100	1.56241300	-0.71124100
H	2.80069800	-5.13964600	-2.89189100				
H	4.62783700	-1.36319500	-1.86572500	<b>14</b>			
H	4.72292000	-3.55744700	-3.06166800	C	-4.84358600	0.94309700	-2.62698300
C	-1.05385400	-3.51012300	-0.09370200	O	-6.05405100	0.81205900	-2.54623300
C	-1.13998300	-4.55580300	0.83941800	C	-4.02448800	1.46655900	-1.51102600
C	-1.91988600	-3.51538300	-1.20309800	C	-2.58589900	1.66211100	-1.48403200
C	-2.06949400	-5.58582000	0.66220300	H	-1.91592300	1.66047000	-2.34097000
H	-0.48445900	-4.56768100	1.71233000	C	-4.48714300	1.88932200	-0.28071600
C	-2.84169100	-4.54921700	-1.38187100	O	-3.45595100	2.31383500	0.48618800
H	-1.87360100	-2.70018000	-1.93160200	C	-4.10336600	0.57364000	-3.90085200
C	-2.91992800	-5.58649600	-0.44679400	H	-3.61098300	1.46116200	-4.33225900
H	-2.12890800	-6.39135800	1.39863100	H	-3.31233400	-0.16623600	-3.69642100
H	-3.50718900	-4.53901800	-2.24865900	H	-4.81753900	0.16518100	-4.62712600
H	-3.64725100	-6.39130100	-0.58007000	C	-5.83892000	1.93503800	0.33050800
C	0.72373500	-2.20728300	1.81596300	H	-6.58457000	1.63918200	-0.41565800

H	-5.89512300	1.24784600	1.19221500	C	0.04733800	-1.52853000	4.35939100
H	-6.05847200	2.94757900	0.70681000	H	-1.19268700	-0.67806500	2.80667600
C	-2.27517900	2.17966400	-0.22642700	C	1.04924300	-2.45475600	4.66799200
C	-1.01861500	2.68067400	0.35479500	H	2.36252500	-3.99131000	3.89520200
C	-0.86016600	4.08310400	0.79865000	H	-0.35854300	-0.87816400	5.13824900
C	-1.83541300	5.05190100	0.47972500	H	1.42733300	-2.53336000	5.69052700
C	0.25918400	4.50176200	1.54886500	C	-0.01750400	1.75035400	0.39555900
C	-1.69772800	6.37708700	0.89548700	N	1.13900800	1.47725100	0.78502400
H	-2.71374000	4.76621000	-0.10220200	C	2.38899000	1.27904600	0.23674200
C	0.39313000	5.82767900	1.96095500	C	2.69554000	1.53641200	-1.13100300
H	1.02786400	3.77427100	1.81487600	C	3.40327100	0.80689000	1.11774300
C	-0.58308800	6.77642500	1.63876500	C	3.99413300	1.28924500	-1.59161600
H	-2.46981000	7.10531800	0.63206600	C	1.65490500	2.06403300	-2.08157900
H	1.27074200	6.12238600	2.54302500	C	4.68959500	0.57724700	0.62269300
H	-0.47570400	7.81461600	1.96260400	C	3.08642400	0.56125100	2.56870400
Pd	-1.35668500	0.07358400	-0.23421400	C	4.97572000	0.81080600	-0.72333300
P	-0.63905000	-2.08501800	0.34365200	H	4.23856700	1.47928400	-2.63849000
C	0.59020700	-2.92811400	-0.75130000	H	2.07485300	2.19476900	-3.08903400
C	0.42420100	-4.24242000	-1.21784600	H	0.79445100	1.37760300	-2.15312600
C	1.73371900	-2.20742200	-1.14009600	H	1.25502200	3.03402300	-1.74575000
C	1.38564700	-4.82336000	-2.05201100	H	5.47062600	0.21227600	1.29197700
H	-0.45833400	-4.81848000	-0.93354400	H	2.28709500	-0.18715400	2.68187100
C	2.69766400	-2.79412700	-1.96258500	H	3.97429900	0.20997500	3.11379600
H	1.87599700	-1.18038100	-0.79743500	H	2.71853700	1.47918800	3.05462300
C	2.52411600	-4.10365700	-2.42354500	Br	6.73273900	0.47029800	-1.38771400
H	1.24132800	-5.84582400	-2.41078500				
H	3.58367800	-2.22113100	-2.24699400	<b>15</b>			
H	3.27440700	-4.56033700	-3.07410200	C	-2.63320800	-0.27291000	0.12212300
C	-2.07500900	-3.25516000	0.37045900	C	-2.38651700	-1.53882500	-0.33456700
C	-2.22024000	-4.27002600	1.33052100	C	-3.60645000	-2.29119100	-0.16658100
C	-3.06521800	-3.10909400	-0.61736400	C	-4.52361000	-1.40726200	0.37364000
C	-3.32871100	-5.12267500	1.29693700	O	-3.93708200	-0.20112100	0.55146400
H	-1.46916000	-4.39636500	2.11278600	H	-1.44713000	-1.88972500	-0.75442200
C	-4.16672100	-3.96675600	-0.65487300	C	-3.85531100	-3.70966500	-0.51146100
H	-2.97505700	-2.30820400	-1.35653800	O	-4.93733100	-4.24577700	-0.33880800
C	-4.30165300	-4.97566800	0.30456800	C	-2.68899600	-4.48539100	-1.09978100
H	-3.43109900	-5.90487700	2.05363000	H	-2.34279600	-4.01752400	-2.03615800
H	-4.92783300	-3.83841500	-1.42864800	H	-1.83353900	-4.49146600	-0.40448000
H	-5.16829700	-5.64131200	0.28247700	H	-3.00743400	-5.51626900	-1.30059200
C	0.08168600	-2.25014200	2.03611800	C	-2.28449400	2.29346700	0.00631400
C	1.09199500	-3.17309600	2.35225500	C	-3.38793900	2.51011000	-0.84110700
C	-0.42763300	-1.42053600	3.05036900	C	-1.64597000	3.41918900	0.56459600
C	1.57350800	-3.27166000	3.66196200	C	-3.83128200	3.80460600	-1.11977000
H	1.50861300	-3.81651800	1.57444900	H	-3.90391400	1.65850600	-1.28716400



C	-2.08593600	4.71130800	0.27666300	H	-3.90557500	3.54490900	3.28409500
H	-0.80144700	3.27736900	1.24422700	H	-3.06928300	5.03840100	2.74036400
C	-3.18348300	4.91293000	-0.56681500	C	-1.73098100	2.71858300	-0.53588500
H	-4.69118400	3.94671000	-1.77982000	C	-0.52627200	2.57724000	-1.09076000
H	-1.57377400	5.56722100	0.72424300	C	0.63169100	3.44549300	-1.21421000
H	-3.53305800	5.92457900	-0.78683500	C	1.79058500	3.02049600	-1.90356700
C	-5.95222400	-1.52830200	0.76064000	C	0.62446700	4.76471200	-0.69812900
H	-6.57457900	-0.82317400	0.18399400	C	2.89328200	3.86043800	-2.05539900
H	-6.28946100	-2.55324500	0.56972300	H	1.80340600	2.01579500	-2.33138100
H	-6.08994300	-1.28617300	1.82789500	C	1.72245200	5.60867600	-0.86895600
C	-0.52815500	0.70976800	0.67860200	H	-0.25463100	5.11036800	-0.15223500
N	0.57569200	0.53277400	1.15516100	C	2.86606800	5.16279900	-1.54120500
C	1.87128800	0.26638000	0.68941800	H	3.77639700	3.50365100	-2.59299500
C	2.26622200	0.50859700	-0.64973500	H	1.68892100	6.62388400	-0.46333200
C	2.78800500	-0.22511700	1.64938900	H	3.72654000	5.82493000	-1.66813800
C	3.59410000	0.24339800	-1.00818300	Pd	-0.80814700	0.60487100	-0.43737600
C	1.30344800	1.04304600	-1.67702800	P	-1.91982100	-1.51973600	-0.07560900
C	4.10240300	-0.49105300	1.25198500	C	-3.10892700	-1.92569700	-1.43703500
C	2.34940200	-0.46424000	3.07082500	C	-4.26811100	-2.69662400	-1.24826800
C	4.49446600	-0.25514000	-0.06633600	C	-2.83164900	-1.41892600	-2.71974500
H	3.92295200	0.42639900	-2.03265000	C	-5.12591100	-2.95965700	-2.32106200
H	1.82268700	1.26781700	-2.61905800	H	-4.50945600	-3.08997700	-0.25897000
H	0.50055800	0.32083800	-1.89790300	C	-3.68451900	-1.69249200	-3.79265300
H	0.80777400	1.96526700	-1.33252200	H	-1.94430100	-0.79751200	-2.87437600
H	4.82180500	-0.87622600	1.97639600	C	-4.83527400	-2.46204400	-3.59482700
H	1.57749500	-1.24899000	3.12414500	H	-6.02750300	-3.55581000	-2.15810400
H	3.19655100	-0.77214800	3.69971100	H	-3.45376900	-1.29289500	-4.78345800
H	1.89883200	0.44291300	3.50259300	H	-5.50858900	-2.66755800	-4.43093900
Br	6.29169200	-0.61462500	-0.58760800	C	-2.89822200	-1.76797600	1.47312600
C	-1.79312100	0.91879300	0.29009600-	C	-3.09241100	-3.02588000	2.07137700
<b>16-ts</b>				C	-3.49311600	-0.63801000	2.05754900
C	-5.29299200	2.17058200	0.62734300	C	-3.87825400	-3.14582700	3.22122900
O	-5.95375500	2.52355400	1.59893500	H	-2.62671100	-3.91610100	1.64324700
C	-3.89442400	2.56829000	0.44870000	C	-4.29173600	-0.76191700	3.19820300
C	-3.01492600	2.16852900	-0.59826900	H	-3.33299200	0.34721400	1.61567200
H	-3.34000200	1.64584400	-1.49681700	C	-4.48365400	-2.01668100	3.78306000
C	-3.20367600	3.50256000	1.26401400	H	-4.02005300	-4.12844400	3.67891700
O	-1.99202600	3.72579800	0.91800500	H	-4.76361700	0.12777500	3.62212500
C	-5.91734100	1.28654900	-0.44336800	H	-5.10233300	-2.11567300	4.67870800
H	-5.87804200	1.77373200	-1.43144500	C	-0.77378200	-2.97492700	-0.05886800
H	-5.38077200	0.32804000	-0.53168100	C	-0.79394400	-3.98137300	-1.03676700
H	-6.96355000	1.09216000	-0.17401600	C	0.18397800	-3.04960600	0.97004400
C	-3.76289300	4.24082300	2.44168000	C	0.11876400	-5.04195500	-0.98340000
H	-4.76090200	4.64223100	2.21791300	H	-1.52644100	-3.94613900	-1.84531900

C	1.08450900	-4.11467100	1.02868800	C	0.78373900	3.43323500	-1.10077400
H	0.22049600	-2.27172300	1.73739700	C	1.96090500	2.96746100	-1.73624900
C	1.05611100	-5.11480600	0.04920100	C	0.85163100	4.71550800	-0.49667700
H	0.08874500	-5.81779100	-1.75289000	C	3.13968600	3.71158100	-1.74090400
H	1.81402600	-4.16298600	1.84133200	H	1.92067300	2.00466100	-2.25011300
H	1.76286500	-5.94735800	0.09341000	C	2.02638000	5.46984100	-0.52158400
C	1.08758400	0.14910200	-0.18117000	H	-0.03228700	5.11861400	-0.00215000
N	2.24203400	-0.04681500	-0.05520600	C	3.18240800	4.97273600	-1.13254900
C	3.60259000	-0.20546800	0.11416000	H	4.02846900	3.31587100	-2.24104800
C	4.26541200	-1.23115200	-0.59761000	H	2.04084300	6.45662200	-0.04925100
C	4.28300300	0.67119200	0.99113900	H	4.10173300	5.56413700	-1.14539100
C	5.64357600	-1.37636100	-0.40530800	Pd	-0.91657400	0.68955300	-0.49827600
C	3.50682100	-2.12941600	-1.53792300	P	-1.96667900	-1.43177800	-0.03624800
C	5.66090800	0.49073500	1.15576700	C	-3.19772800	-1.90664400	-1.33766500
C	3.54381600	1.76669200	1.71156000	C	-4.30981400	-2.72989000	-1.09363700
C	6.32579800	-0.52379700	0.46469700	C	-2.99364700	-1.40780800	-2.63682200
H	6.18440700	-2.15878200	-0.93993300	C	-5.19388200	-3.04983600	-2.12849300
H	4.17541500	-2.86523200	-2.00553500	H	-4.49658700	-3.11844200	-0.09098300
H	2.70563400	-2.67476300	-1.01376400	C	-3.87281000	-1.73799300	-3.67210600
H	3.02277100	-1.54705600	-2.33922600	H	-2.14327500	-0.74786600	-2.83319900
H	6.21459900	1.14998000	1.82615800	C	-4.97660000	-2.55813900	-3.41921700
H	2.71948200	1.36129100	2.32075700	H	-6.05895200	-3.68552200	-1.92263500
H	4.21778800	2.32796300	2.37282800	H	-3.69907900	-1.34337800	-4.67642000
H	3.09086300	2.47407100	0.99748300	H	-5.67091500	-2.80846500	-4.22541500
Br	8.20199600	-0.74802700	0.70958900	C	-2.85753100	-1.66112500	1.56824800
<b>17</b>				C	-3.07775800	-2.92606300	2.14474700
C	-5.12351800	2.00885500	0.54142300	C	-3.34022500	-0.52102700	2.23041500
O	-5.80319400	2.37344900	1.49114200	C	-3.78295500	-3.04217000	3.34531100
C	-3.74712600	2.49592300	0.31006700	H	-2.69093600	-3.82544000	1.66052900
C	-2.79240700	2.05899300	-0.71164600	C	-4.05651400	-0.63997000	3.42541300
H	-3.09826700	1.66262500	-1.67883800	H	-3.15282300	0.46830900	1.81000600
C	-3.17324600	3.58484700	0.93468200	C	-4.27909000	-1.90065200	3.98460900
O	-1.94854200	3.86038000	0.43925700	H	-3.94593700	-4.03035000	3.78350900
C	-5.68314200	1.03483800	-0.47850500	H	-4.44020200	0.25916300	3.91307600
H	-5.69620800	1.49247800	-1.48172400	H	-4.83464100	-1.99547700	4.92114800
H	-5.05925500	0.13061300	-0.54935400	C	-0.79213000	-2.86564700	-0.03073800
H	-6.70429500	0.75722200	-0.18737200	C	-0.77755000	-3.84707700	-1.03381100
C	-3.66939100	4.50073500	1.99500500	C	0.15382100	-2.94592700	1.00853300
H	-4.69319100	4.22867000	2.27325900	C	0.15710000	-4.88901900	-0.99447200
H	-3.02188200	4.43740000	2.88630100	H	-1.50029700	-3.80763900	-1.85077300
H	-3.62844100	5.54436700	1.64145700	C	1.07821700	-3.99098000	1.05143000
C	-1.65770700	2.92108300	-0.58151200	H	0.16168000	-2.18902200	1.79724500
C	-0.44305000	2.64070600	-1.17401200	C	1.08359700	-4.96696200	0.04762600
				H	0.15282800	-5.64634000	-1.78271900

H	1.79893500	-4.04333200	1.87156500	C	-1.60287500	2.50612000	5.22088900
H	1.80774200	-5.78493100	0.08055100	H	-0.58429200	0.62757800	5.57940500
C	0.96624300	0.16583200	-0.22664200	H	-2.46064800	4.37087900	4.54161200
N	2.11246000	-0.06618700	-0.09956900	H	-2.00521900	2.58526500	6.23382500
C	3.46988000	-0.25696200	0.06180500	P	2.86091500	-0.93176400	-0.04754500
C	4.12080300	-1.23554300	-0.72326500	C	4.36731200	-1.08368100	1.01800900
C	4.15900300	0.54287900	1.00292300	C	2.23520600	-2.67388900	-0.12878800
C	5.49671600	-1.41215600	-0.54082100	C	3.53745800	-0.62768800	-1.74234200
C	3.35348800	-2.05238400	-1.72847700	C	4.86961800	0.08706500	1.61300300
C	5.53419300	0.33318800	1.15479100	C	5.01946600	-2.30376000	1.26227800
C	3.43311800	1.59185300	1.80151100	C	2.49785900	-3.54408100	-1.19853300
C	6.18779300	-0.63522200	0.39076500	C	1.44368900	-3.13087900	0.94048300
H	6.02849300	-2.15897900	-1.13248100	C	2.66411500	-0.10209900	-2.71170800
H	4.01723700	-2.75035900	-2.25694200	C	4.87175000	-0.88361600	-2.09829900
H	2.55432300	-2.63598600	-1.24393300	C	6.00811300	0.04158500	2.42111700
H	2.86730000	-1.40601400	-2.47755000	H	4.35691500	1.03946300	1.44786700
H	6.09488500	0.93391400	1.87255600	C	6.15556300	-2.34804300	2.07671000
H	2.59366600	1.15546900	2.36711200	H	4.63777200	-3.22694700	0.82125400
H	4.11020800	2.08332400	2.51325400	C	1.98447600	-4.84632200	-1.19474400
H	3.00564000	2.36358200	1.14034000	H	3.10387200	-3.20721000	-2.04205300
Br	8.06076200	-0.89928600	0.62035000	C	0.94279700	-4.43440500	0.94867500
<b>18-ts</b>				H	1.21324500	-2.45595300	1.76946600
C	-0.40860700	3.04973700	0.14745300	C	3.10983300	0.14248600	-4.01258700
C	0.25061100	3.63465200	-0.90938400	H	1.63075100	0.12813600	-2.43817500
C	-0.72276900	4.26987400	-1.75297200	C	5.31857800	-0.62826900	-3.39916100
C	-1.94937700	4.04508200	-1.14222400	H	5.57055100	-1.27824500	-1.35780900
O	-1.77699000	3.32524800	-0.02212900	C	6.65339500	-1.17690700	2.65511800
H	1.32961400	3.61835100	-1.03716300	H	6.38568500	0.96014200	2.87735900
C	-0.49004600	5.02612600	-3.00265300	H	6.65142300	-3.30453700	2.26165100
O	-1.39676000	5.52566400	-3.64980200	C	1.21065200	-5.29562100	-0.12163000
C	0.95304600	5.16050400	-3.45997100	H	2.19404000	-5.51200500	-2.03614900
H	1.55340800	5.68580100	-2.69902000	H	0.33356500	-4.77635500	1.78926000
H	1.41320000	4.16941700	-3.60474200	C	4.43973400	-0.11915600	-4.35903300
H	0.98072500	5.72299300	-4.40206700	H	2.41858000	0.54874100	-4.75549600
C	0.06193500	2.23230600	1.23876300	H	6.36100500	-0.82732700	-3.66115200
Pd	1.33057200	0.71478800	0.65704000	H	7.53935400	-1.21463300	3.29418800
C	-0.54739400	2.29998500	2.57387900	H	0.81205500	-6.31334200	-0.11999000
C	-0.28090000	1.32093300	3.56588600	H	4.79194100	0.08087000	-5.37423200
C	-1.35099600	3.39798300	2.97378900	C	-3.33621700	4.45301600	-1.48713700
C	-0.80978100	1.41092400	4.84982000	H	-3.77193900	5.06745300	-0.68105400
H	0.36623500	0.47852000	3.30752800	H	-3.32291500	5.02773600	-2.41997600
C	-1.85414000	3.50093500	4.27289200	H	-3.98401900	3.56817800	-1.60769300
H	-1.57628800	4.18863600	2.25795600	C	-0.59208400	0.28196900	0.53527400
				N	-1.56648100	-0.34189200	0.28405500

C	-2.77436400	-0.96207100	0.04486300	H	1.69719400	6.26805300	1.31597900
C	-3.91116100	-0.56059400	0.78783500	H	2.19923300	3.84847000	4.85326400
C	-2.83879700	-1.97434900	-0.94159400	H	2.54274200	6.01667800	3.65402300
C	-5.12400300	-1.20960500	0.53028400	Pd	0.69921300	0.15109500	0.26299400
C	-3.81422000	0.53538100	1.81347700	P	2.70015000	0.93620900	-0.87084200
C	-4.07150900	-2.59469300	-1.17098600	P	0.37747000	-2.20292900	-0.22913400
C	-1.61276500	-2.36518000	-1.72280300	C	2.51832100	2.64385400	-1.55949800
C	-5.19590500	-2.21400100	-0.43645000	C	1.40497000	2.88317400	-2.38572300
H	-6.01704300	-0.92235400	1.08761800	C	3.39918200	3.70380500	-1.29379500
H	-4.79320400	0.73594300	2.26976000	C	1.19668200	4.13962800	-2.95998100
H	-3.10602900	0.27729000	2.61729200	H	0.69169900	2.07655800	-2.57507300
H	-3.43884900	1.46896400	1.36455500	C	3.18316600	4.96471300	-1.85911600
H	-4.15047700	-3.37829100	-1.92625400	H	4.25484600	3.55554900	-0.63382000
H	-0.80632500	-2.71173500	-1.05706700	C	2.08725800	5.18570800	-2.69769000
H	-1.83939500	-3.16864000	-2.43695900	H	0.32855500	4.30538400	-3.60317700
H	-1.21070300	-1.50768700	-2.28741600	H	3.87752900	5.77958200	-1.63821400
Br	-6.86243000	-3.07912700	-0.76242100	H	1.92203000	6.17198100	-3.13906800
<b>19-ts</b>				C	4.06934600	1.03477000	0.37127000
C	-2.60532900	-0.94838100	4.54687000	C	5.40256200	1.28743100	-0.00407900
O	-2.61226000	-1.83571700	5.39060600	C	3.77430100	0.81638900	1.72670700
C	-1.42859900	-0.65948000	3.69384000	C	6.41205500	1.34165700	0.95901700
C	-1.48616800	0.39057200	2.77955700	H	5.65732400	1.43091600	-1.05667200
H	-2.38708000	1.01798900	2.82357800	C	4.78924500	0.86691800	2.68870700
C	-0.15447900	-1.40934600	3.84059000	H	2.74964300	0.58996300	2.03212400
O	0.86182500	-1.01645500	3.26563600	C	6.10630800	1.13309200	2.30893800
C	-3.87489000	-0.11064100	4.37523900	H	7.44286500	1.54030000	0.65377000
H	-3.69351000	0.95460600	4.59139400	H	4.54184400	0.69150900	3.73847800
H	-4.27888600	-0.17880600	3.35288700	H	6.89841800	1.17079200	3.06154000
H	-4.62056600	-0.49372600	5.08353300	C	3.56284700	0.04755500	-2.26190100
C	-0.07252900	-2.65038100	4.70486700	C	3.64115600	0.55035500	-3.57123000
H	-0.27186700	-2.40104600	5.75709900	C	4.11977400	-1.21740000	-1.99302800
H	-0.84232700	-3.38350600	4.42630400	C	4.25827000	-0.19295400	-4.58462000
H	0.93337300	-3.07899900	4.59694800	H	3.22832000	1.53211900	-3.80911300
C	-0.57684600	0.81379000	1.81311500	C	4.74125000	-1.95273300	-3.00369100
C	-0.01995700	1.89690400	1.28680900	H	4.07319900	-1.63307500	-0.98379100
C	0.68326500	3.05087700	1.88500600	C	4.81062700	-1.44490300	-4.30567400
C	0.88860500	4.27330700	1.22185800	H	4.31329700	0.21860000	-5.59610900
C	1.17568100	2.91801700	3.20202800	H	5.16866200	-2.93097500	-2.77007200
C	1.55142300	5.32763900	1.85444200	H	5.29520900	-2.02239500	-5.09713600
H	0.52091300	4.39199500	0.20233200	C	-0.98218200	-3.07536300	0.68174000
C	1.83398100	3.97519700	3.83041500	C	-0.82770800	-4.34384500	1.26364300
H	1.03654200	1.96882400	3.72355300	C	-2.23617700	-2.44538200	0.75830400
C	2.02653400	5.18861500	3.16133800	C	-1.90587200	-4.96931000	1.89999300
				H	0.13769700	-4.85148000	1.22312900

C	-3.31583300	-3.07819400	1.37714100	H	-3.76292700	4.30255600	0.74554400
H	-2.36452400	-1.44568600	0.33610800	N	-2.22580600	2.30730600	-0.47797300
C	-3.15288600	-4.34207500	1.95430600	C	-1.12668200	2.58836400	-0.12372500
H	-1.76704000	-5.95384200	2.35432200				
H	-4.28611000	-2.57671800	1.42073300	<b>20</b>			
H	-3.99362000	-4.83106600	2.45255100	C	0.39453900	-4.76997300	1.83887900
C	1.84733200	-3.28279500	0.09050800	O	-0.28265700	-5.56669900	2.48597100
C	2.27175100	-4.28761700	-0.79401500	C	-0.16697700	-3.66648500	1.04795400
C	2.57552500	-3.05869900	1.27454500	C	0.71789800	-2.79053700	0.28636300
C	3.40469300	-5.05514500	-0.50223800	H	1.67886500	-3.24176200	0.00965500
H	1.72163400	-4.47222900	-1.71861500	C	-1.55749700	-3.52028000	0.88639900
C	3.70286800	-3.83305100	1.56308600	O	-2.09940100	-2.53055300	0.25777700
H	2.25063000	-2.28592000	1.97743500	C	1.91772100	-4.92616900	1.88275300
C	4.12309600	-4.82971300	0.67551900	H	2.32408800	-5.19159900	0.89236600
H	3.72468700	-5.83340100	-1.20038000	H	2.41880500	-3.99876400	2.20217600
H	4.25870300	-3.65011800	2.48628000	H	2.15253500	-5.73344400	2.58867600
H	5.00900300	-5.42916000	0.90142000	C	-2.56150300	-4.53317000	1.39152300
C	-0.07362500	-2.59536200	-1.99160400	H	-2.26959900	-5.56074000	1.13720200
C	-0.98819400	-3.60532700	-2.33937800	H	-2.60507000	-4.51381900	2.49156700
C	0.52236800	-1.84747600	-3.02215700	H	-3.54745500	-4.28868100	0.97282400
C	-1.29441900	-3.85931900	-3.68032900	C	0.51518700	-1.55332800	-0.22440900
H	-1.46901500	-4.20009300	-1.56112500	C	1.41825600	-0.98717500	-1.26887600
C	0.22338500	-2.10822700	-4.36216700	C	1.12657600	-1.19657300	-2.71900100
H	1.23250400	-1.05779400	-2.77629900	C	1.79857700	-0.47075100	-3.72619700
C	-0.68923100	-3.11351000	-4.69597100	C	0.17082500	-2.14915100	-3.12521800
H	-2.00935800	-4.64783700	-3.93005500	C	1.53459800	-0.69515500	-5.07731300
H	0.70690300	-1.51932000	-5.14568500	H	2.53886800	0.28207600	-3.44476300
H	-0.92828100	-3.31504400	-5.74353000	C	-0.09160300	-2.37011200	-4.48072700
C	-6.09606500	1.17464100	-1.43201000	H	-0.35792500	-2.72925400	-2.36763200
C	-5.88096400	2.06449800	-0.37753000	C	0.58551700	-1.64757600	-5.46671000
C	-4.58275300	2.45928500	-0.03952700	H	2.07551200	-0.12001200	-5.83412300
C	-3.50538400	1.92974000	-0.79367300	H	-0.82714400	-3.12769500	-4.76578900
C	-3.71557000	1.03707200	-1.87421500	H	0.38101600	-1.82554100	-6.52543200
C	-5.02939900	0.66523700	-2.17584000	Pd	-1.27744500	-0.63217000	0.08499200
H	-6.72808800	2.45623200	0.18792700	P	-3.76146100	0.00067600	-0.16772600
H	-5.21802300	-0.02457200	-3.00006200	P	-0.27393400	1.39218500	0.67866700
Br	-7.87657400	0.65192200	-1.86606800	C	-4.44807600	-1.20072500	-1.39772400
C	-2.55155000	0.52723900	-2.67978900	C	-3.63698400	-1.58228900	-2.47964900
H	-1.77443600	0.08319500	-2.03801700	C	-5.74324600	-1.73311100	-1.30086500
H	-2.86988100	-0.23146700	-3.40720000	C	-4.11943800	-2.45749600	-3.45597600
H	-2.06925500	1.35094900	-3.23369600	H	-2.61387200	-1.20683000	-2.55756100
C	-4.32704000	3.42051900	1.09008600	C	-6.21962000	-2.61890100	-2.27192900
H	-5.26908900	3.76574400	1.53761900	H	-6.38696800	-1.46532300	-0.46128100
H	-3.72015200	2.95553500	1.88544800	C	-5.41178900	-2.97998500	-3.35378900

H	-3.47479300	-2.73900500	-4.29215200	H	-2.68054200	5.51478800	2.33443000
H	-7.22845300	-3.02954400	-2.17924200	H	-3.07619000	1.94668600	4.73062900
H	-5.78595800	-3.67298200	-4.11177400	H	-3.57404400	4.37003900	4.36618100
C	-4.82772000	-0.22684200	1.32546300	C	0.23517100	2.54939700	-0.66401200
C	-6.08436600	0.38257000	1.48896100	C	0.84586600	3.80149000	-0.44936600
C	-4.35669800	-1.08924100	2.33102700	C	-0.04458400	2.15907700	-1.98394200
C	-6.84534200	0.14099400	2.63665000	C	1.17840300	4.62589300	-1.52686300
H	-6.47525700	1.05222900	0.72047600	H	1.04853700	4.15354900	0.56265500
C	-5.12218500	-1.33336100	3.47463900	C	0.28493200	2.98683300	-3.06161000
H	-3.39192900	-1.58290600	2.20238800	H	-0.52150800	1.19495600	-2.16921500
C	-6.36638200	-0.71584600	3.63225400	C	0.90067600	4.21941700	-2.83631100
H	-7.81965000	0.62362000	2.75029100	H	1.65099900	5.59378100	-1.34061800
H	-4.74317500	-2.01100100	4.24388500	H	0.06169100	2.65761200	-4.07894500
H	-6.96372700	-0.90372700	4.52823500	H	1.16007000	4.86711600	-3.67773600
C	-4.29035900	1.63332100	-0.86979800	C	7.61625400	0.05683900	0.09352300
C	-4.46071500	1.80817000	-2.25500300	C	6.78126500	-0.97869700	0.51167800
C	-4.44624000	2.75096800	-0.03013900	C	5.40755500	-0.93918800	0.23931400
C	-4.78195300	3.06210100	-2.78245900	C	4.88917600	0.18197300	-0.45366800
H	-4.35304200	0.95930100	-2.93213700	C	5.73594300	1.23913600	-0.86731700
C	-4.77763400	4.00089000	-0.55956900	C	7.10572600	1.15768600	-0.59424000
H	-4.31931800	2.64960300	1.04848000	H	7.19787600	-1.83126100	1.05088600
C	-4.94540300	4.16293200	-1.93763100	H	7.77216600	1.96073000	-0.91363400
H	-4.91300700	3.17379500	-3.86193500	Br	9.48407400	-0.03072000	0.47400200
H	-4.90204300	4.85267400	0.11402500	C	5.17065900	2.42300300	-1.60836700
H	-5.20385300	5.14139700	-2.35047400	H	4.29054600	2.83337100	-1.09008700
C	1.17763100	1.10639000	1.81091000	H	5.92337600	3.21650200	-1.72109200
C	1.09510600	0.00542300	2.68250300	H	4.82732300	2.13629600	-2.61663700
C	2.30146900	1.94272000	1.89496800	C	4.52037300	-2.07035300	0.68514500
C	2.09078600	-0.23026100	3.63420400	H	5.07469700	-2.77617200	1.31937900
H	0.25937400	-0.69231300	2.60268100	H	3.65131900	-1.70466300	1.25427200
C	3.30283600	1.69988400	2.83997900	H	4.12324900	-2.63181300	-0.17562800
H	2.42545000	2.77846600	1.20917000	N	3.52379500	0.34257000	-0.72166700
C	3.19720300	0.61924300	3.71908900	C	2.55421200	-0.36533200	-0.93650000
H	2.00328000	-1.09133500	4.30146700				
H	4.17373200	2.35871900	2.88183000	<b>21</b>			
H	3.98034500	0.43267000	4.45830700	C	-3.82138900	-0.69406900	0.00699500
C	-1.35687700	2.40622100	1.80614900	O	-4.79289200	0.04158200	0.02471300
C	-1.66993000	3.75788400	1.59414400	C	-2.42483300	-0.15293100	0.00166100
C	-1.88344500	1.76753600	2.94440300	C	-1.37292800	-1.03605300	0.00033800
C	-2.45646900	4.46009100	2.51482900	H	-1.60854400	-2.10471500	-0.00067800
H	-1.31625300	4.27536400	0.70315200	C	-2.13871800	1.33315600	-0.00024500
C	-2.67647300	2.46574900	3.85624300	O	-0.98208200	1.71469900	0.02121600
H	-1.67573100	0.71113600	3.12484800	C	-4.03965300	-2.20393200	-0.00833900
C	-2.95918400	3.82020300	3.64916500	H	-3.59707600	-2.67174800	-0.90194000

H	-3.59767600	-2.68845700	0.87670400	N	-1.08949000	-0.01991400	1.07906600
H	-5.12217500	-2.38241700	-0.00946300	N	1.08942900	-0.02010000	1.07910800
C	-3.26407500	2.34387300	-0.03293400	C	-0.00001700	-0.00467700	0.27940500
H	-3.90995400	2.19398700	-0.91020400	C	-0.68169800	-0.04448900	2.40345900
H	-3.92341300	2.23132600	0.83983900	H	-1.39756700	-0.05865000	3.22056100
H	-2.81245500	3.34471900	-0.05020800	C	0.68158300	-0.04464500	2.40348900
C	0.00359100	-0.76543700	-0.00023600	H	1.39743000	-0.05895000	3.22061500
C	1.22397600	-0.66591200	-0.00112200	C	-2.47450100	-0.01427400	0.64241700
C	2.61404100	-0.36538500	-0.00079200	C	-3.11686500	1.23136900	0.46681200
C	3.59320600	-1.38339700	-0.00726000	C	-4.45816100	1.20201500	0.05884600
C	3.02570300	0.98801200	0.00628100	H	-4.99412000	2.14184500	-0.08896000
C	4.94731000	-1.05358400	-0.00667400	C	-5.12176300	-0.00481000	-0.15648200
H	3.27605200	-2.42832500	-0.01271700	H	-6.16780000	-0.00112000	-0.47189100
C	4.38192300	1.30630400	0.00678600	C	-4.45913300	-1.21650200	0.03361700
H	2.26077600	1.76730000	0.01133700	H	-4.99604500	-2.15250400	-0.13347900
C	5.34417800	0.28891900	0.00030400	C	-3.11765100	-1.25559100	0.43974900
H	5.69960300	-1.84615700	-0.01168900	C	-2.42964800	-2.60043200	0.66135100
H	4.69344000	2.35375600	0.01230700	H	-1.37291400	-2.40927400	0.90488900
H	6.40722800	0.54311000	0.00070400	C	-2.44605900	-3.47258400	-0.60661100
<b>CuOTf</b>				H	-3.47058500	-3.75355000	-0.89670700
S	-0.21673800	0.78843200	0.00011600	H	-1.88618100	-4.40550200	-0.43611900
O	-0.86986100	2.08465100	0.00035000	H	-1.98784400	-2.95291700	-1.46342900
O	0.61175400	0.41463100	-1.21613100	C	-3.04141900	-3.34815300	1.86113800
C	-1.57294200	-0.50049600	0.00015100	H	-4.09890200	-3.59869400	1.68185900
F	-2.32898200	-0.36900000	1.08300900	H	-2.99475200	-2.74663500	2.78247900
F	-2.32945200	-0.36857600	-1.08232800	H	-2.50233600	-4.29111800	2.04367900
F	-1.02264500	-1.71879600	-0.00020400	C	-2.42738800	2.57123600	0.71272700
O	0.61206600	0.41435200	1.21606500	H	-1.37972400	2.37270600	0.98734500
Cu	2.11046600	-0.37288500	-0.00032200	C	-3.06808400	3.32251000	1.89470800
<b>AgOTf</b>				H	-2.52497200	4.25944200	2.09544400
S	-0.67894600	0.78600000	0.00000000	H	-3.05503500	2.71842300	2.81542800
O	-1.37345000	2.06321200	-0.00000300	H	-4.11688000	3.58526800	1.68469600
O	0.14761600	0.44636400	-1.22378100	C	-2.40197900	3.44301100	-0.55551600
C	-2.00411100	-0.53526700	0.00000100	H	-1.91748700	2.92118900	-1.39668600
F	-2.76342600	-0.41916900	1.08279000	H	-1.84648500	4.37551600	-0.36898200
F	-2.76338300	-0.41920800	-1.08282300	H	-3.41691000	3.72348200	-0.87820900
F	-1.43125800	-1.74306000	0.00003500	C	2.47445900	-0.01456000	0.64255300
O	0.14761900	0.44637200	1.22378000	C	3.11716400	1.23103400	0.46775600
Ag	2.00289600	-0.20806500	0.00000000	C	4.45845900	1.20158700	0.05980500
<b>IPr-Au<sup>+</sup></b>				H	4.99463500	2.14137400	-0.08739500
Au	0.00008900	0.03955800	-1.71165500	C	5.12176100	-0.00524500	-0.15628900
				H	6.16777900	-0.00160600	-0.47169300
				C	4.45884100	-1.21689000	0.03303600
				H	4.99549800	-2.15292800	-0.13465700

C	3.11734400	-1.25591400	0.43914300	H	5.89482400	-1.67438200	1.18602800
C	2.42902300	-2.60073200	0.65994200	H	6.05106100	-1.61720600	-0.55604000
H	1.37220700	-2.40949500	0.90309600	H	6.29656800	-0.09920900	0.39529400
C	2.44585100	-3.47244000	-0.60835100	C	1.32795700	-0.02905700	-0.12155700
H	3.47043500	-3.75396300	-0.89772500	C	0.94589300	1.17111700	-0.11153600
H	1.98865200	-2.95218700	-1.46536100	C	0.99104400	2.60360000	-0.02662800
H	1.88524400	-4.40505800	-0.43861100	C	-0.18693200	3.37676400	-0.12693800
C	3.04014700	-3.34904000	1.85967600	C	2.23854400	3.24331100	0.16151200
H	2.50095200	-4.29208400	2.04146200	C	-0.11586800	4.76526700	-0.03915500
H	2.99300000	-2.74798300	2.78129800	H	-1.14951100	2.88062500	-0.27337900
H	4.09771700	-3.59950700	1.68083300	C	2.29199200	4.63240300	0.24681900
C	2.42793300	2.57093300	0.71426700	H	3.13860900	2.63232600	0.23669400
H	1.38053200	2.37240500	0.98991300	C	1.12066600	5.39415500	0.14735800
C	3.06971400	3.32241300	1.89550900	H	-1.02867800	5.36015300	-0.11724800
H	3.05772700	2.71841400	2.81629800	H	3.25525800	5.12728900	0.39217200
H	2.52662200	4.25925500	2.09671600	H	1.17217200	6.48383800	0.21515300
H	4.11823700	3.58538700	1.68442200				
C	2.40130500	3.44248000	-0.55412200	<b>22b</b>			
H	1.84628300	4.37518200	-0.36716600	S	-3.40690200	-0.69279900	-0.74176300
H	1.91571100	2.92061100	-1.39463600	O	-4.36949800	-0.96504600	-1.79690100
H	3.41595700	3.72255600	-0.87802200	O	-2.24832300	-1.65910700	-0.60005000
				C	-4.33170900	-0.90219000	0.87035500
<b>22a</b>				F	-5.32942400	-0.02713300	0.94142600
S	-3.16567400	-0.71652700	-0.72994600	F	-4.82381600	-2.13306500	0.96285200
O	-4.15915400	-1.06015100	-1.72919500	F	-3.50140800	-0.69191500	1.89806300
O	-1.91865400	-1.57543900	-0.64010100	O	-2.84614700	0.70340100	-0.64458900
C	-3.97909100	-0.95754800	0.93746400	C	3.99752100	-3.09300100	0.19943600
F	-5.04760100	-0.17621500	1.03835300	O	5.16818200	-3.40484800	0.31081700
F	-4.34620900	-2.22524500	1.08425900	C	3.59333100	-1.64717700	0.10157400
F	-3.11473900	-0.64050300	1.90434800	C	2.25886900	-1.33404000	0.08488300
O	-2.66996700	0.71506600	-0.67688000	H	1.54932500	-2.16306000	0.11940200
Cu	-0.69586000	0.08990600	-0.40990400	C	4.61598800	-0.53678000	0.03724700
C	3.51544400	-3.18294500	0.01546200	O	4.22792600	0.61493300	0.13862400
O	4.65754700	-3.57377200	0.17063900	C	2.92716100	-4.17338400	0.16866900
C	3.19094400	-1.71415500	0.03056400	H	2.24432900	-4.09105300	1.02942300
C	1.88050800	-1.33343900	-0.10915600	H	2.31803300	-4.12197400	-0.74751600
H	1.13997700	-2.12769900	-0.22987900	H	3.43245100	-5.14609000	0.21170200
C	4.26100900	-0.66050100	0.19852100	C	6.08077900	-0.82974300	-0.17155100
O	3.92386000	0.51091900	0.23704400	H	6.49325400	-1.36279000	0.69735400
C	2.39782400	-4.19453600	-0.19505900	H	6.24042600	-1.49756900	-1.03063200
H	1.64310000	-4.13979600	0.60548900	H	6.59974300	0.12656500	-0.31815100
H	1.87797500	-4.03729600	-1.15319700	C	1.66516400	-0.05071700	0.02846300
H	2.84864300	-5.19456600	-0.19086200	C	1.20810300	1.11470100	0.02080400
C	5.71983600	-1.02981200	0.31256800	C	1.15657200	2.54751700	0.07872800



C	-0.06538500	3.25607300	0.05625800	C	1.12995900	-1.31125500	0.05665600
C	2.37799200	3.25781600	0.16490400	C	2.93382600	-2.65841000	0.14459700
C	-0.06318900	4.64760200	0.12227300	H	3.99146500	-2.90558000	0.14888200
H	-1.01170700	2.71376800	-0.01412200	C	1.82782100	-3.44636500	0.23228000
C	2.36227200	4.64858300	0.23005100	H	1.72081000	-4.52284800	0.32915600
H	3.31426300	2.69888800	0.17742300	C	3.36968700	-0.20680800	-0.07871600
C	1.14717100	5.34495400	0.20926900	C	3.76240300	0.21372800	-1.36940200
H	-1.01090000	5.19018400	0.10409300	C	4.64877700	1.29811900	-1.44645300
H	3.30561000	5.19575600	0.29662700	H	4.97943700	1.65169800	-2.42528400
H	1.14370500	6.43671900	0.25955900	C	5.12495000	1.92494300	-0.29555700
Ag	-0.64377100	-0.06471200	-0.33211500	H	5.82438700	2.76025200	-0.38114700
<b>22c</b>				C	4.71993500	1.48486400	0.96404100
C	-5.65774000	0.56852500	-0.33173200	H	5.10572100	1.98364200	1.85563000
O	-6.79657600	0.96892800	-0.19473500	C	3.83343100	0.40722600	1.10661100
C	-4.49855000	1.51662500	-0.20204100	C	3.42884900	-0.06361900	2.50129400
C	-3.21290300	1.04721700	-0.25201600	H	2.68169500	-0.86333600	2.38686800
H	-3.05357000	-0.02481100	-0.38726300	C	2.76089000	1.05867200	3.31514100
C	-4.67760000	3.00009000	-0.00747800	H	3.45837600	1.88601400	3.52000200
O	-3.65981600	3.67493400	0.04587700	H	2.41650500	0.67257200	4.28749400
C	-5.38874800	-0.89363000	-0.64133000	H	1.88994300	1.47752500	2.78684800
H	-4.83801000	-1.01052700	-1.58818000	C	4.62668400	-0.66785000	3.25768800
H	-4.79467200	-1.37481200	0.15177300	H	5.41286700	0.08305900	3.43557000
H	-6.35604400	-1.40494400	-0.72168800	H	5.08296300	-1.50014900	2.69909000
C	-6.03257800	3.63711000	0.11706900	H	4.30741800	-1.05295100	4.23901800
H	-6.64550100	3.42678400	-0.77199900	C	3.28279800	-0.46462800	-2.65043800
H	-6.58913200	3.20835100	0.96336500	H	2.58059400	-1.26428400	-2.37057200
H	-5.89677000	4.71828300	0.24758300	C	4.44960900	-1.12963000	-3.40415900
C	-2.03306200	1.81402500	-0.14763700	H	4.07867300	-1.66098200	-4.29479400
C	-0.91196400	2.39017300	-0.10329500	H	4.98017700	-1.85774200	-2.77083100
C	-0.09454700	3.57645500	-0.04939300	H	5.18703300	-0.38577000	-3.74508500
C	1.31425400	3.52148200	-0.13445800	C	2.51271700	0.50970800	-3.55974000
C	-0.73525900	4.83209300	0.08469000	H	1.65815200	0.96477000	-3.03422000
C	2.06370100	4.69434600	-0.08834100	H	2.12520300	-0.01857800	-4.44517400
H	1.81808900	2.55928500	-0.24180900	H	3.15698900	1.32679200	-3.92121200
C	0.02763000	5.99570700	0.13196300	C	-0.64136500	-3.07077500	0.23244100
H	-1.82233000	4.87026500	0.14790100	C	-1.27308000	-3.44418300	-0.97566300
C	1.42392200	5.93195900	0.04555700	C	-2.58185700	-3.94037800	-0.88650200
H	3.15212300	4.64216400	-0.15739700	H	-3.10119100	-4.25095200	-1.79567400
H	-0.47080500	6.96213900	0.23597700	C	-3.22726000	-4.05874800	0.34434300
H	2.01509900	6.85027200	0.08208700	H	-4.24348700	-4.45804100	0.38936900
Au	-0.03495300	0.36644400	-0.04352800	C	-2.57695800	-3.68103700	1.51834100
N	2.48692000	-1.35005500	0.03648200	H	-3.09296000	-3.78644300	2.47504000
N	0.72797400	-2.60264100	0.17618500	C	-1.26560400	-3.18220700	1.49455700
				C	-0.57532300	-2.80428000	2.80281700

H	0.43311000	-2.43563600	2.56215900
C	-1.31139900	-1.66038400	3.52281400
H	-2.32649800	-1.95831700	3.83008300
H	-1.40127100	-0.77186600	2.87765300
H	-0.76550300	-1.36463400	4.43255400
C	-0.40096200	-4.02703500	3.72234700
H	0.15069900	-3.74647300	4.63342300
H	0.15743800	-4.83422600	3.22291100
H	-1.37217200	-4.44001900	4.03787600
C	-0.58244400	-3.35978000	-2.33467500
H	0.38951400	-2.86425900	-2.19093700
C	-0.29775600	-4.76302600	-2.90301600
H	0.30863200	-5.36729000	-2.21024600
H	0.24955600	-4.68909900	-3.85602700
H	-1.23050600	-5.31639100	-3.09677700
C	-1.37685900	-2.50432200	-3.33692100
H	-0.82108100	-2.40888100	-4.28295300
H	-1.55779900	-1.48930900	-2.94890000
H	-2.35338500	-2.95408200	-3.57694400

**23a-ts**

S	2.86587100	-1.20542900	-0.74515800
O	3.97693400	-1.76530900	-1.49597000
O	2.31811200	0.11114200	-1.14881200
C	3.49651700	-0.90242700	0.99074700
F	3.94164600	-2.02346800	1.54407600
F	4.47850900	-0.00521500	0.97057600
F	2.49676500	-0.41727400	1.74643000
O	1.73986000	-2.20934200	-0.47365200
Cu	0.00368300	-1.44820500	-0.30270700
C	0.52252600	3.97998700	-0.17888900
O	0.20169900	5.15491600	-0.12753800
C	-0.51417800	2.91198800	-0.08604200
C	-0.23404200	1.57327900	-0.18291600
H	0.78320000	1.19790100	-0.35335400
C	-1.95651000	3.15539100	0.11103800
O	-2.66781500	2.14180600	0.15798900
C	1.97036900	3.55951700	-0.32435300
H	2.30272900	2.99665500	0.56336300
H	2.12468800	2.89370100	-1.18754500
H	2.58637700	4.46089200	-0.43270500
C	-2.56086800	4.51843100	0.24931500
H	-2.09280400	5.05738500	1.08665400
H	-2.33546600	5.12158100	-0.64301600

H	-3.64432100	4.42625700	0.39764200
C	-1.25507400	0.61083900	-0.09076500
C	-1.73683500	-0.58664400	-0.09432500
C	-2.99524100	-1.29250500	0.01852900
C	-3.02005700	-2.70281400	-0.06394800
C	-4.21347500	-0.59795800	0.20898300
C	-4.22096900	-3.40077700	0.03972100
H	-2.08217100	-3.24423500	-0.21217500
C	-5.40977800	-1.30302000	0.31200000
H	-4.19820700	0.48979700	0.27235400
C	-5.41815800	-2.70148100	0.22792100
H	-4.22501200	-4.49109700	-0.02640000
H	-6.34622500	-0.75951700	0.45887500
H	-6.36151100	-3.24741900	0.30937400

**23b-ts**

S	-3.47819900	-0.73211400	-0.69746600
O	-4.44258900	-1.09799900	-1.72444500
O	-2.27521300	-1.66429700	-0.57285600
C	-4.34520700	-1.00240300	0.93770200
F	-5.40395000	-0.20231300	1.03053100
F	-4.74514800	-2.26550300	1.05175100
F	-3.51050200	-0.72508900	1.94696800
O	-3.00526400	0.67953900	-0.62804900
C	4.52776800	-2.78955500	0.06063300
O	5.73337100	-2.92277200	0.17188500
C	3.91209100	-1.43235000	0.07237500
C	2.56308600	-1.21022500	-0.04660900
H	1.86969900	-2.04500000	-0.15645000
C	4.67633200	-0.17048900	0.21288100
O	3.99845400	0.86019500	0.20331700
C	3.62084200	-3.99702100	-0.09247400
H	2.88677600	-4.05250700	0.72752200
H	3.05889000	-3.95812100	-1.03959300
H	4.24250700	-4.90088400	-0.08009800
C	6.16701500	-0.11302400	0.35816300
H	6.48603000	-0.68850500	1.24008000
H	6.65300000	-0.60237900	-0.49910100
H	6.48169900	0.93511400	0.44058200
C	2.00780700	0.08289300	-0.03335300
C	1.12946800	1.01108400	-0.07083100
C	0.92081500	2.43862700	-0.01118400
C	-0.37856500	2.99156700	-0.10472300
C	2.03036200	3.30770600	0.14233000

C	-0.55969300	4.37199400	-0.04621000	H	4.02688900	-2.86766200	0.14568600
H	-1.24754000	2.33899600	-0.22428200	C	1.86788100	-3.42872000	0.21320600
C	1.83487600	4.68390300	0.19912000	H	1.77042200	-4.50698100	0.29979400
H	3.03073000	2.88217600	0.21412400	C	3.38105500	-0.17254800	-0.06382700
C	0.54301900	5.21924600	0.10514700	C	3.77416800	0.26187200	-1.34981700
H	-1.56750600	4.78624500	-0.12035100	C	4.64810100	1.35710700	-1.41542900
H	2.69472800	5.34763700	0.31716300	H	4.97834800	1.72189800	-2.39033300
H	0.39709100	6.30159400	0.14998600	C	5.11239300	1.98117400	-0.25816200
Ag	-0.60358900	-0.27837200	-0.33553200	H	5.80210700	2.82543900	-0.33491500
<b>23c-ts</b>				C	4.70791500	1.52693800	0.99657600
C	-5.69886000	0.50458600	-0.28890700	H	5.08417000	2.02360900	1.89344500
O	-6.84049200	0.90811200	-0.18570900	C	3.83352500	0.43798900	1.12765800
C	-4.54619200	1.45808300	-0.17541300	C	3.42975100	-0.04816300	2.51732700
C	-3.25061500	1.01579300	-0.21582800	H	2.68966200	-0.85311800	2.39427100
H	-3.05605300	-0.05249600	-0.33268200	C	2.75087000	1.06141700	3.33947700
C	-4.72018300	2.93958700	-0.00816600	H	3.44105100	1.89283700	3.55242800
O	-3.69211500	3.60400700	0.03813100	H	2.40824700	0.66420700	4.30798200
C	-5.41768100	-0.96574100	-0.53926100	H	1.87724600	1.47720000	2.81320000
H	-4.86171000	-1.11370000	-1.47874700	C	4.63117400	-0.64873900	3.27100700
H	-4.82094200	-1.40910800	0.27355400	H	5.41068200	0.10725100	3.45671800
H	-6.37956000	-1.48933400	-0.60402000	H	5.09555800	-1.47241600	2.70630800
C	-6.06727900	3.59192600	0.10004500	H	4.31331100	-1.04486800	4.24841600
H	-6.67551800	3.37276800	-0.79023200	C	3.30677000	-0.41179800	-2.63783300
H	-6.63208600	3.17680900	0.94782300	H	2.61782100	-1.22569700	-2.36643700
H	-5.92565900	4.67376000	0.21737600	C	4.48440200	-1.05044600	-3.39745000
C	-2.10363100	1.82840600	-0.12325900	H	4.12206100	-1.57975900	-4.29284300
C	-0.95246300	2.35853900	-0.08984700	H	5.02681900	-1.77551500	-2.77065800
C	-0.15658600	3.56318300	-0.04551500	H	5.20966500	-0.29184200	-3.73188200
C	1.25339700	3.52595600	-0.12919300	C	2.52051900	0.55857400	-3.53740400
C	-0.80985400	4.81368700	0.07769000	H	1.65596800	0.98992000	-3.00820700
C	1.99006800	4.70718000	-0.09242400	H	2.14541100	0.03391800	-4.43034400
H	1.76856500	2.56886900	-0.22865800	H	3.14983300	1.39243900	-3.88674000
C	-0.06077400	5.98638200	0.11620700	C	-0.60437300	-3.07581000	0.20132600
H	-1.89691000	4.84243900	0.13997600	C	-1.22662400	-3.43713400	-1.01536900
C	1.33633300	5.93841400	0.03118300	C	-2.53067900	-3.94792700	-0.94038100
H	3.07905900	4.66641500	-0.16056400	H	-3.04237900	-4.24990200	-1.85676000
H	-0.57042600	6.94777600	0.21220600	C	-3.18073900	-4.09196000	0.28527400
H	1.91677800	6.86382700	0.06075200	H	-4.19293200	-4.50246900	0.31914500
Au	-0.02383100	0.37324400	-0.03778000	C	-2.53996700	-3.72563200	1.46811200
N	2.50876400	-1.32493100	0.03935400	H	-3.05923300	-3.85101500	2.42070100
N	0.76065000	-2.59443000	0.15886400	C	-1.23379600	-3.21286900	1.45837000
C	1.15117300	-1.29811400	0.05270700	C	-0.55380700	-2.84852600	2.77584200
C	2.96709200	-2.63001900	0.13822700	H	0.44974900	-2.46072400	2.54562100
				C	-1.30870000	-1.72861100	3.51374500

H	-2.32120500	-2.04576800	3.81016100	C	0.87779500	0.79937800	-0.12258100
H	-1.40681200	-0.82916900	2.88522600	C	0.60750400	2.22610000	-0.06845500
H	-0.77125100	-1.44313900	4.43176400	C	-0.74610200	2.63749400	-0.23224800
C	-0.36494900	-4.08532500	3.67345600	C	1.58262500	3.24389800	0.13866400
H	0.17850800	-3.81360800	4.59211600	C	-1.10288200	3.98260800	-0.19400600
H	0.20769800	-4.87458900	3.16165900	H	-1.52380400	1.88578300	-0.39739200
H	-1.33118900	-4.51878900	3.97654700	C	1.21825800	4.58398200	0.18016900
C	-0.53035000	-3.32489900	-2.36951200	H	2.62735200	2.97347300	0.27039300
H	0.43613300	-2.82272200	-2.21307300	C	-0.12331300	4.95853600	0.01320000
C	-0.22994600	-4.71615500	-2.95880700	H	-2.14886100	4.26751600	-0.32638000
H	0.37887900	-5.32576800	-2.27288500	H	1.98130600	5.34890000	0.34355000
H	0.32111100	-4.62179600	-3.90784400	H	-0.40167000	6.01531900	0.04591500
H	-1.15655900	-5.27491300	-3.16594600				
C	-1.32790500	-2.46066100	-3.36167500	<b>24b</b>			
H	-0.76909000	-2.34597000	-4.30378400	S	-3.56716900	-0.67462800	-0.70195200
H	-1.51877600	-1.45335500	-2.95864900	O	-4.54890200	-1.15037100	-1.66787500
H	-2.29961800	-2.91481300	-3.61272600	O	-2.31151700	-1.54826100	-0.61853900
				C	-4.32711600	-0.98279000	0.97960100
<b>24a</b>				F	-5.44217700	-0.26722100	1.11637500
S	-3.35400000	-0.99899400	-0.76727700	F	-4.62142900	-2.27123200	1.13846500
O	-4.24305400	-1.82989000	-1.56526100	F	-3.47111500	-0.62133500	1.94546900
O	-1.99238800	-1.65629100	-0.49302200	O	-3.21666900	0.76219300	-0.68408700
C	-4.07714100	-0.97807900	0.95819800	C	4.76800700	-2.67993500	0.07334100
F	-5.26841100	-0.38456400	0.94855800	O	5.97614500	-2.70126100	0.21002700
F	-4.21501800	-2.21310600	1.43355200	C	4.01312100	-1.39221600	0.07485800
F	-3.26808100	-0.29350500	1.77929700	C	2.62493100	-1.19270600	-0.06847500
O	-3.19093300	0.42749500	-1.11117900	H	1.85634400	-1.95009300	-0.20598800
Cu	-0.56561900	-0.41094200	-0.32783400	C	4.56000600	-0.10852200	0.22385600
C	4.73354400	-2.48967600	0.06967500	O	3.59996200	0.81008300	0.17713600
O	5.94323100	-2.43756200	0.18568600	C	3.96152500	-3.94767100	-0.10571500
C	3.90259500	-1.25113700	0.05817300	H	3.21116200	-4.05053800	0.69538200
C	2.50045500	-1.13787200	-0.06553600	H	3.41526700	-3.93149900	-1.06319000
H	1.77635000	-1.94276100	-0.17360200	H	4.63932300	-4.81010800	-0.08548600
C	4.37329000	0.06473400	0.16705400	C	5.95221900	0.36173100	0.41531900
O	3.35698900	0.92339700	0.11705000	H	6.03614800	0.91704100	1.36458000
C	4.00207700	-3.80742000	-0.07001500	H	6.63227800	-0.49649900	0.42445300
H	3.27411500	-3.93911300	0.74737300	H	6.23180900	1.05632000	-0.39430600
H	3.43811500	-3.84307500	-1.01662000	C	2.35815700	0.17917700	-0.00609300
H	4.73101300	-4.62704300	-0.04680500	C	1.12503700	0.84517500	-0.09968800
C	5.73724300	0.62466000	0.31938000	C	0.94408300	2.28335600	-0.02480400
H	5.81095200	1.19083700	1.26320000	C	-0.38338000	2.79137500	-0.13132600
H	6.47051600	-0.18864500	0.31774700	C	1.99459900	3.23344800	0.14581200
H	5.95172500	1.32947700	-0.50101900	C	-0.64473800	4.15729100	-0.07102800
C	2.15616300	0.21511700	-0.02860500	H	-1.22027900	2.09941800	-0.26429000

C	1.72621100	4.59467400	0.20410700	C	-3.43889000	0.00917500	-0.30897500
H	3.02316500	2.89340200	0.23194000	C	-3.95278800	0.68050900	0.82279700
C	0.40772100	5.06213900	0.09618000	C	-4.73835500	1.81927600	0.59185200
H	-1.67362600	4.51305600	-0.15655600	H	-5.15732200	2.36277500	1.44145100
H	2.54709200	5.30391400	0.33445400	C	-5.00082000	2.26553100	-0.70261600
H	0.20500700	6.13546100	0.14269600	H	-5.62164100	3.15144700	-0.85796200
Ag	-0.56363700	-0.36285000	-0.36519500	C	-4.48308600	1.57890600	-1.80015600
<b>24c</b>				H	-4.70372400	1.93522000	-2.80875100
C	5.89352000	0.12082700	-0.43186900	C	-3.69304800	0.43183900	-1.63275300
O	7.00036400	0.61335000	-0.52444400	C	-3.16599600	-0.30888500	-2.85953800
C	4.69920000	1.00514300	-0.30137300	H	-2.54810600	-1.14921500	-2.51003300
C	3.34089800	0.67611600	-0.17550500	C	-2.25781100	0.58631500	-3.72095400
H	2.89839500	-0.31775700	-0.14919000	H	-2.80928900	1.44191400	-4.14214300
C	4.75162500	2.41305800	-0.30044800	H	-1.84453800	0.01339300	-4.56622300
O	3.53209100	2.91592800	-0.16986300	H	-1.41447000	0.98350900	-3.13410700
C	5.66244300	-1.37214300	-0.44476500	C	-4.31621700	-0.90742100	-3.69029200
H	5.15123900	-1.69736000	0.47605900	H	-4.97293700	-0.12222100	-4.09737100
H	5.01599100	-1.65651000	-1.29138700	H	-4.94207300	-1.58447000	-3.08791700
H	6.62820900	-1.88541400	-0.53205900	H	-3.91772800	-1.48134100	-4.54196800
C	5.88811400	3.35202900	-0.42133200	C	-3.70390800	0.20924000	2.25329800
H	6.56551900	3.23484700	0.44054100	H	-3.02912000	-0.65872100	2.21244600
H	6.49421000	3.10203200	-1.30514900	C	-5.00878700	-0.26166900	2.92225700
H	5.52963800	4.38787800	-0.47804500	H	-4.80583500	-0.64779800	3.93380600
C	2.60458500	1.86954100	-0.08264200	H	-5.49489600	-1.06345800	2.34441700
C	1.22573700	2.08728000	0.02864800	H	-5.73294800	0.56281600	3.02034300
C	0.65266200	3.41799800	0.18381800	C	-2.99812100	1.28547300	3.09680100
C	-0.69273000	3.63073800	-0.22144800	H	-2.05254400	1.60471500	2.63116700
C	1.34840900	4.52013900	0.75369700	H	-2.76934600	0.89532500	4.10132700
C	-1.29080800	4.88201700	-0.11689000	H	-3.62807900	2.17961000	3.22799900
H	-1.25594600	2.79558600	-0.64178500	C	0.36067700	-3.05178100	0.37756700
C	0.73177000	5.75869900	0.89362900	C	0.87886500	-3.15322000	1.68761800
H	2.36520300	4.39200600	1.11851600	C	2.15966000	-3.70805400	1.83072200
C	-0.58195800	5.94980100	0.44590200	H	2.59141400	-3.80929600	2.82882400
H	-2.31819600	5.02265100	-0.45930600	C	2.88457000	-4.14767900	0.72385400
H	1.27688500	6.58549900	1.35462100	H	3.87382100	-4.59131100	0.86204500
H	-1.05632400	6.92908100	0.54771600	C	2.34510100	-4.03689700	-0.55772400
N	-2.63955700	-1.18064100	-0.10373100	H	2.91956400	-4.39594400	-1.41455100
N	-0.97261400	-2.51953700	0.19825900	C	1.07084600	-3.48747500	-0.76399300
C	-1.28583600	-1.20646000	0.02867900	C	0.49711400	-3.40848500	-2.17652800
C	-3.16667700	-2.46017600	-0.01753500	H	-0.45760400	-2.86451300	-2.12358100
H	-4.23276200	-2.65108000	-0.09934300	C	1.40904000	-2.61553400	-3.12891200
C	-2.11626100	-3.30457200	0.17396800	H	2.38016500	-3.11430400	-3.27717900
H	-2.07795500	-4.38329400	0.29487800	H	1.60197600	-1.59982200	-2.74899400
				H	0.93708600	-2.52060900	-4.11959400

C	0.19293000	-4.81147100	-2.73458400	H	-2.00404900	4.23002800	5.74447500
H	-0.27047500	-4.73813600	-3.73122700	Pd	0.86862500	-0.01218600	-0.07757200
H	-0.49671400	-5.36820100	-2.08095100	P	1.40957200	2.20443800	-1.03528200
H	1.11051900	-5.41276400	-2.83733500	P	0.70539600	-2.25706700	-0.99001500
C	0.10675800	-2.70289600	2.92504000	C	1.35589300	3.74812900	-0.02161700
H	-0.86571200	-2.30965500	2.59402200	C	0.22052600	3.97571700	0.77416000
C	-0.18151500	-3.88191100	3.87241800	C	2.39217100	4.69637100	-0.01282200
H	-0.72784300	-4.68944600	3.36036300	C	0.11525500	5.13065100	1.55201300
H	-0.79233300	-3.54731000	4.72576200	H	-0.58676100	3.24145700	0.79766300
H	0.74648100	-4.31396800	4.27972800	C	2.28772500	5.84995800	0.77088500
C	0.82729700	-1.55658500	3.65701000	H	3.28742400	4.53598900	-0.61633300
H	0.22573300	-1.20976300	4.51218500	C	1.15015000	6.07106500	1.55210000
H	0.99335400	-0.69709200	2.98816700	H	-0.77014700	5.28150100	2.17383600
H	1.80584600	-1.87564100	4.05038900	H	3.10337500	6.57780900	0.77092500
Au	-0.01061400	0.42335600	0.00645100	H	1.07397900	6.97063700	2.16832000
<b>25-ts</b>				C	3.16298800	2.13312000	-1.61982700
C	3.42593800	-2.29238300	4.44679100	C	3.55843900	2.45831800	-2.92785800
O	4.64507300	-2.41437900	4.55045900	C	4.13278600	1.69779500	-0.69551500
C	2.78888800	-1.31566000	3.56993300	C	4.90211200	2.35669100	-3.30440000
C	1.37085500	-1.20467500	3.40069600	H	2.81985500	2.79315000	-3.65852500
H	0.70067200	-1.87941900	3.94512600	C	5.47421700	1.60840100	-1.07636900
C	3.48779600	-0.34417800	2.78838900	H	3.82993200	1.42211800	0.32047500
O	2.80212100	0.46631400	2.10573800	C	5.86288600	1.93574100	-2.38053400
C	2.52551300	-3.19790300	5.29272500	H	5.19722700	2.61236800	-4.32551600
H	1.88538800	-2.61036200	5.97109300	H	6.21837100	1.27315600	-0.34917200
H	1.85909200	-3.81353800	4.66677500	H	6.91277400	1.86168100	-2.67620800
H	3.16898000	-3.85943600	5.88710500	C	0.46531300	2.66822400	-2.55814700
C	4.99535600	-0.25459300	2.74165900	C	0.19503800	4.00021600	-2.91498300
H	5.42038900	-0.27508700	3.75410200	C	0.01112400	1.63571600	-3.39631000
H	5.41567300	-1.13685400	2.23291700	C	-0.50646300	4.28988700	-4.08971800
H	5.29325900	0.66113600	2.21193600	H	0.53242000	4.81746900	-2.27439200
C	0.75327300	-0.35735400	2.56464300	C	-0.67904000	1.92721300	-4.57597100
C	-0.30598100	0.45406200	2.25303900	H	0.19058100	0.59520500	-3.11546300
C	-0.79561100	1.51472000	3.18409400	C	-0.94113700	3.25603100	-4.92461700
C	-2.10478000	2.03258300	3.12712000	H	-0.71206700	5.33071700	-4.35330600
C	0.07190500	2.01387900	4.17693800	H	-1.02250900	1.10995500	-5.21504500
C	-2.53325000	3.00002800	4.04133100	H	-1.48859000	3.48558500	-5.84253800
H	-2.80904100	1.67064000	2.37785800	C	0.01857900	-3.64856100	0.01777500
C	-0.36054800	2.97626400	5.08889600	C	0.63177500	-3.93214500	1.25281200
H	1.09924600	1.64744400	4.21145900	C	-1.09079800	-4.41229800	-0.38050800
C	-1.66642800	3.47598000	5.02887800	C	0.15348600	-4.96746900	2.05820100
H	-3.55856500	3.37555900	3.98345300	H	1.49275300	-3.34631900	1.58358800
H	0.33342300	3.34731200	5.84793500	C	-1.57603800	-5.43894100	0.43770200
				H	-1.58052400	-4.21348200	-1.33511400

C	-0.95495700	-5.72142500	1.65625500	C	-0.87350600	0.29658100	0.93126300
H	0.64895500	-5.18565200	3.00761900				
H	-2.44070100	-6.02358300	0.11290500	<b>26</b>			
H	-1.33074300	-6.52729100	2.29178700	C	4.54039700	-4.46137700	0.98461100
C	2.38364300	-2.87707000	-1.46211400	O	5.60649000	-4.26346600	0.42432400
C	3.35760200	-1.93864500	-1.84397100	C	3.50412200	-3.41375800	1.12413100
C	2.72027900	-4.24225200	-1.46371100	C	2.20616300	-3.53056100	1.74100200
C	4.63526400	-2.35401100	-2.22876100	H	1.77088800	-4.41430200	2.19949200
H	3.12316600	-0.87115100	-1.83453500	C	3.59591700	-2.10701400	0.67969600
C	4.00031400	-4.65525300	-1.84394000	O	2.45386200	-1.44614800	0.99197500
H	1.98350100	-4.98948800	-1.16237300	C	4.22009400	-5.82315000	1.57884200
C	4.95975600	-3.71338800	-2.22834100	H	4.02425200	-5.74068200	2.66049200
H	5.37856300	-1.60707800	-2.51719800	H	3.31213000	-6.24708900	1.11916600
H	4.24890600	-5.71965600	-1.83609700	H	5.06822000	-6.49850100	1.40801000
H	5.96150800	-4.03906700	-2.52009800	C	4.66624900	-1.34523400	-0.01221000
C	-0.26080300	-2.36938400	-2.56652500	H	5.47954600	-2.03302600	-0.27032400
C	0.19325100	-3.07259200	-3.69486400	H	4.28276200	-0.85938000	-0.92343500
C	-1.50559100	-1.71669400	-2.63012700	H	5.06811600	-0.55200100	0.64228400
C	-0.58463900	-3.12781800	-4.85597200	C	1.59451700	-2.30854600	1.64153700
H	1.15892600	-3.58052000	-3.67195400	C	0.28704300	-1.83106600	2.09332500
C	-2.28751700	-1.78604400	-3.78632900	C	-0.21679500	-2.31299400	3.41605100
H	-1.86273300	-1.14429800	-1.77202300	C	-1.59279100	-2.39903200	3.71649900
C	-1.82797000	-2.49092200	-4.90388800	C	0.68733400	-2.65451700	4.44742700
H	-0.21553500	-3.67631400	-5.72651800	C	-2.04028500	-2.81106100	4.97405400
H	-3.25634700	-1.28096600	-3.81297800	H	-2.33304100	-2.14511300	2.95943500
H	-2.43649700	-2.54138200	-5.81052600	C	0.23854500	-3.06646800	5.70277000
C	-6.05326300	-0.12748600	0.11664800	H	1.76032900	-2.58119000	4.26545700
C	-5.29483000	-0.98309900	0.91565600	C	-1.13004800	-3.15171300	5.97745100
C	-3.90889100	-0.81792400	1.02227700	H	-3.11528300	-2.87000800	5.16502100
C	-3.29310500	0.23256700	0.28809400	H	0.96952300	-3.31593300	6.47705300
C	-4.06631500	1.09812300	-0.53092800	H	-1.48104500	-3.47764200	6.95978800
C	-5.44994800	0.90899000	-0.59738400	Pd	0.27313600	0.36581600	-0.10245600
H	-5.78305800	-1.78617900	1.47056700	P	0.99993200	2.57031400	0.81361100
H	-6.05706400	1.57351300	-1.21464600	P	0.50938100	-0.60746800	-2.27774800
Br	-7.94089600	-0.37781700	-0.00241500	C	1.27902500	2.62922700	2.64560700
C	-3.40131700	2.21111100	-1.29543700	C	0.47688900	1.80890700	3.45907300
H	-2.58432200	1.83116200	-1.92861100	C	2.25027300	3.44556600	3.25182100
H	-4.12214700	2.74066000	-1.93413600	C	0.63725900	1.81369200	4.84768100
H	-2.94521300	2.94857300	-0.61413100	H	-0.27472300	1.16024800	3.00507500
C	-3.10052100	-1.73460700	1.90106700	C	2.40990900	3.44496700	4.64090900
H	-3.72818100	-2.53737100	2.31191800	H	2.89106100	4.08285400	2.63912300
H	-2.26961100	-2.20283200	1.34961200	C	1.60413800	2.62996900	5.44170500
H	-2.65056700	-1.18826700	2.74561700	H	0.01089300	1.16354300	5.46344600
N	-1.92455900	0.41467600	0.30253700	H	3.17069100	4.08352400	5.09784500

H	1.73458200	2.62660000	6.52707900	H	5.53462900	0.31114800	-4.95045500
C	2.57614700	3.29658300	0.16129100	C	-0.68748300	0.28530900	-3.38279400
C	2.65230100	4.54374000	-0.47902000	C	-0.36419700	0.71869500	-4.67941100
C	3.74885600	2.52688600	0.28077500	C	-1.97928200	0.54056000	-2.88617100
C	3.87297000	5.01302500	-0.97911500	C	-1.31233100	1.38797200	-5.46077600
H	1.75707200	5.15852800	-0.58856200	H	0.63236700	0.53495800	-5.08526600
C	4.96778300	3.00294400	-0.20430100	C	-2.92932700	1.19618500	-3.67351200
H	3.70493300	1.54501500	0.75918600	H	-2.24363200	0.22388500	-1.87369200
C	5.03405600	4.24929600	-0.83913100	C	-2.59643400	1.62533700	-4.96291800
H	3.91325600	5.98650500	-1.47502300	H	-1.04359400	1.72259000	-6.46625500
H	5.86930700	2.39472200	-0.09348900	H	-3.93011700	1.37634700	-3.27299200
H	5.98747300	4.62106100	-1.22331500	H	-3.33603600	2.14603200	-5.57676600
C	-0.22826300	3.92732300	0.51771500	C	-5.50837200	-0.57535400	0.10311400
C	-0.43107300	4.99148500	1.41253400	C	-4.64761300	-1.64455200	-0.13585400
C	-0.99558300	3.87666500	-0.65970900	C	-3.31349900	-1.60125200	0.29203200
C	-1.37351600	5.98514300	1.13045300	C	-2.84687500	-0.43596900	0.96869100
H	0.14564900	5.04446300	2.33812700	C	-3.74198700	0.64303900	1.22341400
C	-1.92953100	4.87654300	-0.94559800	C	-5.06534100	0.55970800	0.78312000
H	-0.87071700	3.03963300	-1.35225400	H	-5.01190700	-2.53002900	-0.65971300
C	-2.12193900	5.93254800	-0.04959500	H	-5.75276100	1.38517000	0.97557800
H	-1.52358600	6.80458000	1.83836900	Br	-7.31597400	-0.66534900	-0.50323100
H	-2.51576800	4.82030400	-1.86628000	C	-3.27419000	1.86241400	1.97097100
H	-2.85884000	6.71014100	-0.26705900	H	-2.44438800	2.36108300	1.44753600
C	0.14256800	-2.39110900	-2.63824400	H	-4.09155900	2.58752000	2.09170000
C	0.81137100	-3.37190900	-1.88257200	H	-2.89624800	1.59411200	2.97003900
C	-0.78347200	-2.80504800	-3.60984700	C	-2.43010700	-2.79116800	0.03245600
C	0.56968500	-4.72915500	-2.10400300	H	-2.94131800	-3.52217500	-0.60932700
H	1.52509100	-3.08044400	-1.10932300	H	-1.48946600	-2.50620700	-0.45905500
C	-1.03250600	-4.16573500	-3.82190100	H	-2.14716200	-3.29989900	0.96762700
H	-1.31744000	-2.06509000	-4.20851000	N	-1.54476700	-0.26716300	1.43097800
C	-0.35591700	-5.13156500	-3.07289800	C	-0.47850200	-0.96311200	1.36662700
H	1.10218300	-5.47488200	-1.50843800				
H	-1.75845000	-4.46895000	-4.58103400	<b>27-ts</b>			
H	-0.55026800	-6.19406000	-3.24049700	C	-2.67214300	4.71745000	1.10786700
C	2.12813500	-0.37106600	-3.15633100	O	-2.75463200	5.61039100	1.94271500
C	2.85191600	0.80535200	-2.89715900	C	-1.37849600	4.19103500	0.65637700
C	2.65514800	-1.30149100	-4.06835700	C	-1.16774000	3.14781900	-0.27359000
C	4.06406600	1.05519000	-3.54548600	H	-1.97189800	2.64492300	-0.80931300
H	2.46731100	1.52608700	-2.17224700	C	-0.10668700	4.66986100	1.08650500
C	3.87537400	-1.05644100	-4.70699000	O	0.88921300	4.10024400	0.53175100
H	2.11514400	-2.22548700	-4.28241400	C	-3.93159800	4.11401500	0.50130400
C	4.58087800	0.12254200	-4.45074900	H	-3.93685900	4.22156400	-0.59548200
H	4.60956600	1.97664700	-3.32819700	H	-4.00143400	3.03598100	0.72016000
H	4.27486000	-1.79355100	-5.40850800	H	-4.80568000	4.62708400	0.92275600



C	0.13560200	5.74601000	2.10016500	C	0.30168200	-1.99820400	2.74484900
H	-0.35787300	6.67922500	1.78933100	C	1.29880700	-4.60009900	2.61699700
H	-0.32745600	5.47892900	3.06215200	H	2.47735700	-3.91586800	0.94581100
H	1.21539700	5.90404800	2.22342400	C	-0.13427500	-2.95745800	3.66067700
C	0.14683500	2.81161400	-0.54594100	H	-0.10392000	-0.98456300	2.79377100
C	0.95642000	1.98435500	-1.22732300	C	0.36132200	-4.26492100	3.59735000
C	2.23443700	2.24265600	-1.87814100	H	1.69457800	-5.61789400	2.56204600
C	2.88266900	1.21862000	-2.60543600	H	-0.87072600	-2.68390600	4.42035200
C	2.84310300	3.52204200	-1.85725800	H	0.01696800	-5.01887800	4.30990800
C	4.08726400	1.45300400	-3.26683900	C	-3.24503600	-0.02330900	-1.60994900
H	2.41481000	0.23380200	-2.64745000	C	-4.63915300	-0.06976100	-1.43629600
C	4.04044800	3.75656500	-2.53214900	C	-2.72186100	0.69948900	-2.69648200
H	2.36383500	4.32489200	-1.29649000	C	-5.48813900	0.58876700	-2.33053600
C	4.67145100	2.72452400	-3.23650400	H	-5.06904900	-0.61880500	-0.59617400
H	4.56790000	0.64104800	-3.81868400	C	-3.57323400	1.35028000	-3.59552500
H	4.48945100	4.75336300	-2.50519700	H	-1.63692400	0.76285700	-2.82724300
H	5.61114800	2.91182900	-3.76309300	C	-4.95818100	1.29831000	-3.41316100
Pd	0.06952200	0.28367900	-0.47257100	H	-6.56996900	0.54803800	-2.17865100
P	1.77204700	-0.96474700	0.60002400	H	-3.14918900	1.90699800	-4.43516900
P	-2.05169400	-0.88008500	-0.46735100	H	-5.62402500	1.81423800	-4.10983200
C	2.86434900	-1.84684000	-0.60436300	C	-3.00555500	-0.95875800	1.11952900
C	2.24694400	-2.68638500	-1.55243200	C	-3.88414900	-2.00149700	1.45787100
C	4.25435300	-1.66460500	-0.66799000	C	-2.83853900	0.10514000	2.02447300
C	3.00599000	-3.34508800	-2.52094100	C	-4.58194400	-1.97667500	2.67001500
H	1.16248400	-2.82442800	-1.53385500	H	-4.02509100	-2.84186100	0.77509200
C	5.01161600	-2.31796100	-1.64755200	C	-3.54429900	0.13415800	3.23041300
H	4.75399300	-1.00478200	0.04284700	H	-2.14220200	0.91357300	1.78371600
C	4.39305600	-3.16154100	-2.57267100	C	-4.41663600	-0.90926000	3.55740000
H	2.51010300	-3.99775700	-3.24407800	H	-5.26019200	-2.79692600	2.91981600
H	6.09281500	-2.16107000	-1.68507300	H	-3.40525100	0.97132900	3.91923700
H	4.98680400	-3.67066400	-3.33628400	H	-4.96395100	-0.89144300	4.50339000
C	2.94048600	-0.03248000	1.70102000	C	-2.08784900	-2.62399600	-1.09395500
C	3.80216400	-0.70211800	2.59093000	C	-2.59460100	-2.95863300	-2.36092300
C	2.95599800	1.37007800	1.67022700	C	-1.50575200	-3.63961300	-0.31122900
C	4.66869000	0.01731600	3.41603700	C	-2.52497800	-4.27482500	-2.83084200
H	3.79443600	-1.79300100	2.64488700	H	-3.04940600	-2.19157100	-2.98990800
C	3.82407000	2.08893200	2.49971700	C	-1.44824300	-4.95439500	-0.77871600
H	2.28413000	1.91228900	1.00476900	H	-1.09704000	-3.40483600	0.67351600
C	4.68236100	1.41633400	3.37146800	C	-1.95562700	-5.27706800	-2.04215200
H	5.33251700	-0.51670100	4.10117700	H	-2.92413700	-4.51485200	-3.81985500
H	3.81712700	3.18082300	2.45938500	H	-0.99864300	-5.72814600	-0.15126500
H	5.35819300	1.97837300	4.02157200	H	-1.90627900	-6.30548500	-2.40915900
C	1.24760300	-2.32345200	1.75565500				
C	1.74252900	-3.63669500	1.70298400	<b>28</b>			

C	-5.36307300	-0.39366900	-2.94186800	C	-1.34701100	-3.33079500	-0.51671800
O	-6.56901200	-0.46304600	-3.11108800	C	-0.16360800	-5.39045300	-1.98472200
C	-4.75911800	-0.20676400	-1.60181600	H	1.70786100	-4.38874300	-1.61388600
C	-3.37687800	-0.11570800	-1.26545700	C	-2.13582400	-4.35687100	-1.04457400
H	-2.52203500	-0.17284400	-1.93383100	H	-1.80663000	-2.51292400	0.04329000
C	-5.44543100	-0.10060300	-0.39177100	C	-1.54702500	-5.38814800	-1.78270200
O	-4.57884900	0.04808500	0.61268000	H	0.30515300	-6.19239700	-2.56139800
C	-4.40411500	-0.50133500	-4.11430100	H	-3.21709100	-4.34387400	-0.88431700
H	-3.78482100	0.40696000	-4.19536700	H	-2.16469100	-6.18630600	-2.20292000
H	-3.71671300	-1.35221100	-3.97734000	C	2.63269900	-2.09090700	-0.89095800
H	-4.98038700	-0.63759200	-5.03831600	C	3.79762600	-2.66626700	-0.35651800
C	-6.89065900	-0.13045200	-0.05001500	C	2.67862000	-1.56539600	-2.19571700
H	-7.19054300	0.81184500	0.43905500	C	4.97644600	-2.71632300	-1.10979700
H	-7.47952000	-0.27420600	-0.96245600	H	3.78917800	-3.07958000	0.65374500
H	-7.10015000	-0.94519600	0.66328100	C	3.85173100	-1.62664000	-2.95060300
C	-3.26946800	0.04790000	0.10681000	H	1.79051400	-1.09378300	-2.62377600
C	-2.13500500	0.13725600	0.97080900	C	5.00713400	-2.20030200	-2.40806500
C	-2.39561600	0.37068200	2.40687100	H	5.87409400	-3.16691500	-0.67764700
C	-1.69451400	-0.36992800	3.38644400	H	3.86477700	-1.21312900	-3.96210300
C	-3.28632500	1.37261500	2.86397400	H	5.92856900	-2.24140300	-2.99469700
C	-1.88955900	-0.13871900	4.74789900	C	0.25772600	3.56700500	-0.10414800
H	-0.99238600	-1.13782100	3.05592500	C	0.61090000	4.71286000	-0.83819100
C	-3.44935000	1.62807400	4.22624100	C	-0.76216400	3.66635000	0.85571000
H	-3.84135000	1.96884400	2.13757500	C	-0.04028500	5.92886200	-0.61292900
C	-2.76115600	0.86818500	5.17783300	H	1.39589300	4.65983300	-1.59538700
H	-1.34397900	-0.74115200	5.47927900	C	-1.40339100	4.88696400	1.08988000
H	-4.13011800	2.42122000	4.54842400	H	-1.06159900	2.77555700	1.41251100
H	-2.90074200	1.06101600	6.24472900	C	-1.04683700	6.02027900	0.35399700
Pd	-0.24480200	0.06061200	0.29147900	H	0.24072300	6.80934500	-1.19702700
P	1.03278700	-1.94195200	0.04247900	H	-2.19126600	4.94529700	1.84528700
P	1.10576600	1.92558200	-0.33393900	H	-1.55497100	6.97234700	0.52886200
C	1.47981300	-2.58756300	1.72092700	C	1.62986100	2.02538900	-2.11035500
C	2.05401700	-1.68673000	2.63740600	C	2.87951200	2.49745700	-2.54364100
C	1.24711500	-3.91117100	2.12880100	C	0.69683900	1.60551500	-3.07622800
C	2.40113500	-2.10515800	3.92392100	C	3.18691100	2.54816900	-3.90798400
H	2.22542700	-0.64842800	2.34202500	H	3.62314200	2.82696700	-1.81540400
C	1.58448900	-4.32458500	3.42234700	C	1.00071300	1.66451800	-4.43809900
H	0.79705800	-4.62551700	1.43693200	H	-0.27489900	1.22478200	-2.75021200
C	2.16390600	-3.42560000	4.32152200	C	2.25006100	2.13420000	-4.85862500
H	2.84946000	-1.39264100	4.62111200	H	4.16523200	2.91740600	-4.22722400
H	1.39168400	-5.35684500	3.72652300	H	0.26157500	1.33783800	-5.17439200
H	2.42609400	-3.75105800	5.33163500	H	2.49144700	2.17663100	-5.92390700
C	0.04602400	-3.32814500	-0.70670600	C	2.68138000	2.17013800	0.61320200
C	0.62881000	-4.36984400	-1.44999600	C	2.84302100	3.20161100	1.55361300

C	3.71859000	1.22902500	0.46303300	H	-4.34606800	-4.05481800	3.49501200
C	4.01163400	3.29260400	2.31793200	Cu	-0.11047700	-0.01813900	0.01683500
H	2.05347200	3.94158200	1.69458000				
C	4.88900600	1.33000700	1.21787800	<b>Ag<sup>+</sup>-PPh<sub>3</sub></b>			
H	3.61484600	0.41080400	-0.25229600	P	-2.52466300	0.00022600	0.00088200
C	5.03902700	2.36116500	2.15190100	C	-3.15811200	1.64260400	0.48618100
H	4.11671400	4.10175100	3.04558600	C	-2.57564500	2.30343200	1.58343200
H	5.68407300	0.59297900	1.07827900	C	-4.22715900	2.24135500	-0.20157300
H	5.95238600	2.43615200	2.74772800	C	-3.06550500	3.54351500	1.99375200
				H	-1.74011700	1.84994500	2.12553400
				C	-4.70904900	3.48659900	0.21334300
<b>Cu<sup>+</sup>-PPh<sub>3</sub></b>				H	-4.68495600	1.74202300	-1.05764200
P	-2.33301200	-0.00194100	0.00124500	C	-4.13173300	4.13685600	1.30730600
C	-2.96389800	1.62903900	0.52322400	H	-2.61103400	4.05147800	2.84733500
C	-2.32899300	2.28743500	1.59187100	H	-5.53984800	3.94913900	-0.32436500
C	-4.07127600	2.22349400	-0.10376000	H	-4.50952900	5.11151000	1.62487500
C	-2.80621800	3.52017400	2.03768300	C	-3.17282600	-0.39385900	-1.66017300
H	-1.46062900	1.83659200	2.08247400	C	-4.24642500	-1.28422300	-1.83014200
C	-4.54051900	3.46180700	0.34509800	C	-2.59476600	0.22606800	-2.78340800
H	-4.56715000	1.72695300	-0.94033400	C	-4.73726600	-1.54289200	-3.11360800
C	-3.91215300	4.10863500	1.41293700	H	-4.70060300	-1.77596100	-0.96782800
H	-2.31088600	4.02650800	2.86926900	C	-3.09335200	-0.03407400	-4.05998800
H	-5.40100000	3.92244700	-0.14551100	H	-1.75578700	0.91868300	-2.66508400
H	-4.28077300	5.07766500	1.75735100	C	-4.16430800	-0.92057700	-4.22584400
C	-2.96660100	-0.35686800	-1.67285800	H	-5.57169100	-2.23611800	-3.24185500
C	-4.08792300	-1.17872500	-1.87440000	H	-2.64220200	0.45107000	-4.92847600
C	-2.32142800	0.22848100	-2.77726000	H	-4.54904400	-1.12912400	-5.22684700
C	-4.56086300	-1.40117700	-3.17126100	C	-3.17714800	-1.23571800	1.17651100
H	-4.59137700	-1.64718800	-1.02617200	C	-4.22077800	-0.91939500	2.06243600
C	-2.80216900	0.00586000	-4.06779800	C	-2.62899800	-2.53192900	1.17708900
H	-1.44213200	0.86379000	-2.63171500	C	-4.71257800	-1.89687700	2.93313400
C	-3.92233900	-0.81026800	-4.26511100	H	-4.65145200	0.08359900	2.07737600
H	-5.43228900	-2.04169100	-3.32512400	C	-3.12850300	-3.50229200	2.04578000
H	-2.29887900	0.46410600	-4.92216700	H	-1.81329300	-2.79027400	0.49486600
H	-4.29408900	-0.98989500	-5.27657300	C	-4.16996200	-3.18448600	2.92602700
C	-2.98900000	-1.26770200	1.14124200	H	-5.52382400	-1.64698700	3.62066800
C	-4.06336900	-0.99672200	2.00416300	H	-2.70089500	-4.50743200	2.04075400
C	-2.40070000	-2.54572700	1.13683500	H	-4.55515200	-3.94337700	3.61104100
C	-4.54754600	-2.00272100	2.84638200	Ag	-0.09290400	-0.01970400	-0.00355000
H	-4.52217700	-0.00613200	2.02445400				
C	-2.89258400	-3.54536800	1.97613200	<b>Pd-PPh<sub>3</sub></b>			
H	-1.55804500	-2.76512700	0.47373700	Pd	-0.00382700	-0.00770000	2.57623800
C	-3.96617300	-3.27342500	2.83272600	P	-0.00087700	-0.00032600	0.36283500
H	-5.38282300	-1.78882100	3.51709700	C	-1.55921100	-0.61474000	-0.43484100
H	-2.43416500	-4.53685300	1.96748300				

C	-2.20519100	-1.71804500	0.15084900	H	6.12208700	1.37424200	-1.96401900
C	-2.12035500	-0.03307500	-1.58330200	H	5.18754300	1.44970900	-4.27363100
C	-3.37335300	-2.23897600	-0.40877700	C	2.59316300	0.30504000	1.63032500
H	-1.78818900	-2.16021500	1.06023800	C	3.50319100	-0.47253500	2.36574500
C	-3.29832500	-0.54854700	-2.13570500	C	2.23349200	1.58108500	2.09883600
H	-1.64038900	0.82926100	-2.05050100	C	4.05109800	0.02873500	3.55008000
C	-3.92529100	-1.65307900	-1.55346300	H	3.78120900	-1.47119900	2.02171700
H	-3.86169600	-3.09877600	0.05741300	C	2.78792800	2.07847800	3.27958100
H	-3.72656000	-0.08145200	-3.02661600	H	1.51688700	2.19149300	1.54093200
H	-4.84613400	-2.05310700	-1.98587500	C	3.69670400	1.30193200	4.00630300
C	0.24671300	1.66083100	-0.42428000	H	4.75654400	-0.58088200	4.11953100
C	1.03898900	1.86482700	-1.56593000	H	2.50416200	3.07085400	3.63746600
C	-0.39261000	2.76720100	0.16315500	H	4.12518100	1.68839500	4.93405700
C	1.18231600	3.14623000	-2.10993400	C	1.95542100	-2.11451900	0.08582100
H	1.55269600	1.02312000	-2.03487400	C	2.88023800	-2.83354800	-0.68656800
C	-0.25830900	4.04293800	-0.38790000	C	1.05563300	-2.80998100	0.91533300
H	-0.99005100	2.62023000	1.06754100	C	2.90689200	-4.23120900	-0.62359700
C	0.53267500	4.23654100	-1.52596700	H	3.58125500	-2.30904800	-1.33898700
H	1.80696900	3.29004200	-2.99560300	C	1.09284000	-4.20374800	0.98057200
H	-0.76385200	4.89194800	0.07973900	H	0.33025900	-2.26174800	1.52454100
H	0.64731000	5.23684700	-1.95166000	C	2.01806600	-4.91652500	0.20819900
C	1.31441200	-1.04025800	-0.43031400	H	3.62968500	-4.78447000	-1.22780000
C	1.09420500	-1.82404500	-1.57457000	H	0.39974300	-4.73605600	1.63654100
C	2.59272600	-1.04051700	0.15592000	H	2.04435200	-6.00768300	0.25630600
C	2.13205700	-2.58678400	-2.12193800	Cu	-0.27165500	0.41768600	-0.21212700
H	0.10778800	-1.84501100	-2.04207800	C	-4.37874200	-3.07937200	-0.39634200
C	3.63029300	-1.79224100	-0.39855100	O	-5.39709200	-3.57671400	0.03823600
H	2.76409500	-0.45224500	1.06197900	C	-4.10366600	-1.61009100	-0.19734500
C	3.40158900	-2.57075400	-1.53874400	C	-2.88714400	-1.10020200	-0.55780100
H	1.94405500	-3.19676300	-3.00955500	H	-2.14792500	-1.77951400	-0.99040300
H	4.61881700	-1.77979000	0.06804300	C	-5.12676100	-0.66254600	0.40148800
H	4.21036200	-3.16865800	-1.96693800	O	-4.84686100	0.52432300	0.42260200
				C	-3.36850400	-3.93007200	-1.14831900
				H	-3.17849600	-3.53719600	-2.15968100
				H	-2.40401700	-3.97701600	-0.61693400
				H	-3.77568600	-4.94561900	-1.22716100
				C	-6.43519600	-1.15764900	0.95305700
				H	-7.02142300	-1.66304800	0.17111300
				H	-6.27518200	-1.91491500	1.73430600
				H	-6.98672300	-0.29639800	1.35115300
				C	-2.46748600	0.24607800	-0.43638400
				C	-2.06102400	1.42596500	-0.45072200
				C	-2.08237500	2.85639000	-0.35886200
				C	-0.98930300	3.64835000	-0.77560400
<b>29a</b>							
P	1.86264800	-0.28199700	0.05772800				
C	2.95276200	0.29112400	-1.29850600				
C	2.42705400	0.34723500	-2.60222300				
C	4.28756500	0.66608100	-1.07473600				
C	3.23050400	0.75505700	-3.66864700				
H	1.38609100	0.06687700	-2.79023600				
C	5.08528600	1.08139200	-2.14519800				
H	4.70666800	0.64031900	-0.06675000				
C	4.56065000	1.12375500	-3.44030100				
H	2.81583100	0.79172600	-4.67872500				

C	-3.24506700	3.47467000	0.15897200	H	-3.15052400	-1.45446200	5.57637800
C	-1.05774300	5.03555800	-0.67422900	Ag	0.26139300	0.33545700	-0.26807100
H	-0.09835000	3.17076300	-1.19187200	C	4.62260000	-3.18735700	-0.45267500
C	-3.29808200	4.86298200	0.25371400	O	5.57405000	-3.72163300	0.07911400
H	-4.08326700	2.84905700	0.47070500	C	4.32303400	-1.73230400	-0.19325600
C	-2.20983000	5.64284900	-0.15904200	C	3.15670700	-1.19243000	-0.66076000
H	-0.21524800	5.64822200	-1.00238100	H	2.47386700	-1.83611100	-1.22095300
H	-4.19544600	5.34314100	0.65032500	C	5.26887000	-0.83346400	0.58150400
H	-2.26122000	6.73162400	-0.08266900	O	5.00645800	0.35689800	0.62225900
<b>29b</b>				C	3.72269400	-3.97734600	-1.38852400
P	-2.06163800	-0.28570300	0.07408800	H	2.70190700	-4.06902400	-0.98285400
C	-3.21755700	1.03643600	-0.45596800	H	3.65211700	-3.50639000	-2.38159700
C	-2.93353900	2.36413000	-0.08697300	H	4.14731500	-4.98324500	-1.49458300
C	-4.37344800	0.75779700	-1.20278000	C	6.48302300	-1.38026300	1.28087200
C	-3.80067200	3.39538100	-0.45101400	H	6.20956300	-2.17744900	1.98728200
H	-2.03553300	2.59657300	0.49359900	H	7.16785000	-1.85076600	0.55966500
C	-5.23459800	1.79681900	-1.57059800	H	6.98144500	-0.55142800	1.79960200
H	-4.60487100	-0.26646300	-1.50151400	C	2.73106300	0.14873000	-0.51289000
C	-4.95152200	3.11270900	-1.19564100	C	2.33921400	1.33070200	-0.52615700
H	-3.57662100	4.42308400	-0.15566600	C	2.38192800	2.75910100	-0.40615400
H	-6.13132000	1.57353700	-2.15336400	C	1.38145100	3.59488000	-0.95016800
H	-5.62679200	3.92110600	-1.48574700	C	3.48807000	3.33253800	0.26557100
C	-2.51249200	-1.79193900	-0.87072300	C	1.48501000	4.97786500	-0.82240600
C	-3.28953900	-2.81630400	-0.30625500	H	0.53623600	3.15541500	-1.48599100
C	-2.07005200	-1.91122500	-2.20104600	C	3.57610100	4.71706400	0.38709800
C	-3.62205100	-3.94149900	-1.06754900	H	4.25917500	2.67561500	0.67164100
H	-3.63543200	-2.74149500	0.72651300	C	2.57915800	5.53956800	-0.15272300
C	-2.41090900	-3.03333600	-2.95802800	H	0.71499700	5.62308000	-1.25094000
H	-1.46292100	-1.12116800	-2.65369600	H	4.43043100	5.16014600	0.90372600
C	-3.18624400	-4.05116700	-2.39066600	H	2.65724500	6.62503500	-0.05505400
H	-4.22556600	-4.73539500	-0.62139500	<b>29c</b>			
H	-2.06859800	-3.11555000	-3.99229700	C	-3.96487500	-3.50011400	0.61437000
H	-3.44820300	-4.93204900	-2.98154200	O	-4.88999100	-4.17936800	0.19919000
C	-2.43095400	-0.62933900	1.83607200	C	-3.80230800	-2.07023900	0.21498700
C	-3.65628200	-0.26253800	2.41746700	C	-2.76157900	-1.34010100	0.74556700
C	-1.46569900	-1.29120000	2.61576900	H	-2.07620900	-1.86244700	1.41798000
C	-3.91000000	-0.56111900	3.75952400	C	-4.75836900	-1.41822200	-0.74645300
H	-4.41305500	0.25982900	1.82857000	O	-4.83196200	-0.20125400	-0.79138100
C	-1.72706900	-1.59229600	3.95356800	C	-2.96426600	-4.12716100	1.58020900
H	-0.50328600	-1.57496400	2.17919200	H	-1.93572100	-4.08975800	1.18803600
C	-2.94939500	-1.22574100	4.52714400	H	-2.96679800	-3.61462200	2.55517800
H	-4.86367900	-0.27033700	4.20614300	H	-3.25631300	-5.17450600	1.72763100
H	-0.97211300	-2.10729800	4.55207800	C	-5.60328900	-2.25664500	-1.68163500

H	-5.01748300	-3.05475800	-2.16049600	H	3.95312700	-2.34854500	0.19681700
H	-6.39755000	-2.76713900	-1.11787700	C	2.76219000	-1.36838100	3.76601900
H	-6.04111900	-1.58586700	-2.43326400	H	1.47183000	0.06184300	2.78282300
C	-2.40612500	0.00659600	0.52193900	C	3.71234800	-2.38132400	3.59794100
C	-2.28216700	1.26137900	0.43306400	H	4.86957900	-3.52580900	2.17256100
C	-2.74745500	2.62228600	0.34608800	H	2.42144700	-1.09588100	4.76822800
C	-1.92247600	3.70250800	0.72485100	H	4.11823400	-2.90317700	4.46841800
C	-4.05296700	2.88335600	-0.12877000				
C	-2.39266300	5.01217800	0.63702500	<b>30a-ts</b>			
H	-0.91489000	3.49531600	1.09198400	C	4.36981500	-3.20898600	-0.12755100
C	-4.51139200	4.19710200	-0.21406500	O	5.49569500	-3.64514900	0.00913100
H	-4.67680400	2.04107400	-0.43089000	C	4.12294200	-1.73463400	-0.06060100
C	-3.68719900	5.26276200	0.16808300	C	2.88010200	-1.17216700	-0.17441900
H	-1.74785900	5.84230100	0.93640800	H	1.99882900	-1.79827300	-0.33244300
H	-5.52154300	4.39303600	-0.58294000	C	5.19572700	-0.71799000	0.13618200
H	-4.05429200	6.29023900	0.09968400	O	4.81596000	0.45450000	0.13740500
Pd	-0.32567100	0.51111400	0.21760500	C	3.19264200	-4.13530700	-0.36781000
P	1.92043100	-0.10715900	-0.05782100	H	2.44348400	-4.04641900	0.43578100
C	2.31935600	-1.13830000	-1.54143300	H	2.69165900	-3.90734900	-1.32256600
C	1.33663500	-2.02362700	-2.01566800	H	3.56478600	-5.16694500	-0.39531200
C	3.55457300	-1.07217700	-2.20834100	C	6.63941700	-1.06300900	0.32403800
C	1.59023300	-2.84041000	-3.12067500	H	6.76356100	-1.73014900	1.19034300
H	0.36222800	-2.05839100	-1.52066400	H	7.00793600	-1.63796700	-0.53903500
C	3.80370500	-1.88464200	-3.31859300	H	7.21823100	-0.14010700	0.45408700
H	4.32528300	-0.37841800	-1.86485200	C	2.66795700	0.21953400	-0.11128500
C	2.82437600	-2.77240900	-3.77444200	C	2.05250900	1.33749000	-0.14996200
H	0.81608000	-3.52369800	-3.47908200	C	2.21351800	2.77136200	-0.12680500
H	4.76703700	-1.82051200	-3.83130100	C	1.10830100	3.62326600	-0.35547100
H	3.01979100	-3.40459200	-4.64447100	C	3.48488900	3.34348400	0.12100100
C	3.03465400	1.35832100	-0.25244400	C	1.26577100	5.00618900	-0.33829500
C	4.23705300	1.51913100	0.45396800	H	0.12571000	3.18964300	-0.56171800
C	2.62988800	2.36782900	-1.14559200	C	3.63046500	4.72767000	0.14186200
C	5.02157200	2.66257500	0.26439400	H	4.33833100	2.68751500	0.29174200
H	4.56553000	0.75343500	1.15975600	C	2.52679600	5.56007500	-0.08676100
C	3.41874100	3.50310200	-1.33899400	H	0.40767800	5.65604600	-0.52288600
H	1.68658100	2.26386000	-1.68975200	H	4.61272800	5.16457400	0.33541300
C	4.61735400	3.65412800	-0.63263200	H	2.65090100	6.64560400	-0.07122500
H	5.95400900	2.77598900	0.82359700	P	-1.91527300	-0.23604400	0.02735900
H	3.09207500	4.27713300	-2.03819200	C	-2.35570200	-0.88656900	1.68232200
H	5.23147300	4.54649700	-0.77825600	C	-3.13623900	1.07958100	-0.35221700
C	2.66256800	-1.04504300	1.35486300	C	-2.20442800	-1.58888300	-1.17802700
C	3.61486900	-2.06485500	1.19534500	C	-1.34727100	-1.47974700	2.46150100
C	2.23411500	-0.71165200	2.65230000	C	-3.66679400	-0.81997600	2.18348400
C	4.13328500	-2.72986800	2.31171500	C	-4.19302600	0.88814300	-1.25537700



H	-1.66983400	-2.44747500	-4.39476900	C	-2.86555900	-2.23270700	4.10907500
H	-4.29544500	-4.44647900	-1.61089800	H	-0.84392900	-2.99163700	3.95660100
H	-3.78888400	-2.25346600	5.12772200	H	-4.82084100	-1.31368600	3.99243300
H	-5.51423600	4.21437900	-1.19257900	H	-3.06450300	-2.72301800	5.06560100
H	-3.21879600	-4.32769200	-3.85597800	C	-3.16390500	1.21734600	-0.08180500
<b>30c-ts</b>				C	-4.38490300	1.11455900	-0.76720600
C	4.28054400	-3.44331800	-0.26897100	C	-2.84004300	2.43228400	0.54903100
O	5.32300800	-3.97112700	0.09034400	C	-5.26609800	2.20090700	-0.81259100
C	4.07023600	-1.98911700	-0.14462800	H	-4.65184600	0.18495900	-1.27417900
C	2.92396100	-1.28895200	-0.51838200	C	-3.72538900	3.51132500	0.51222400
H	2.06050000	-1.75885500	-0.98673000	H	-1.88046200	2.53184000	1.06493500
C	5.04296600	-1.05558500	0.37171800	C	-4.94152600	3.39864400	-0.17084000
O	4.67527000	0.14844200	0.35591500	H	-6.21115300	2.10768000	-1.35423500
C	3.15407000	-4.27641300	-0.85988200	H	-3.46056500	4.44757000	1.01053900
H	2.23340700	-4.18181500	-0.26149400	H	-5.63107500	4.24600600	-0.20810600
H	2.91304100	-3.94834200	-1.88409600	C	-2.53403100	-1.38118600	-1.22429500
H	3.46831200	-5.32770900	-0.88012300	C	-3.41430200	-2.43444400	-0.92744000
C	6.39796100	-1.41489300	0.89691000	C	-2.06516000	-1.23973800	-2.54291600
H	6.30511100	-2.13125500	1.72705700	C	-3.82246300	-3.32102700	-1.93017100
H	6.97576800	-1.94156400	0.12253400	H	-3.78191100	-2.57103600	0.09164700
H	6.92234800	-0.50747600	1.22360400	C	-2.48366900	-2.11804900	-3.54486300
C	2.90001800	0.09083700	-0.31197200	H	-1.35701500	-0.43911700	-2.77566200
C	2.21369800	1.21548200	-0.40997100	C	-3.36237600	-3.16335800	-3.24014500
C	2.54446100	2.62686400	-0.30261800	H	-4.50372700	-4.13959100	-1.68306400
C	1.55290900	3.59154800	-0.60077500	H	-2.11321600	-1.99243900	-4.56564000
C	3.82276000	3.08520400	0.10184200	H	-3.68201500	-3.85773900	-4.02156700
C	1.81899500	4.95524500	-0.48686500	<b>31a</b>			
H	0.57308100	3.23907700	-0.93088900	Cu	0.19985800	0.56161600	-0.01022400
C	4.08448500	4.44930600	0.20859000	C	4.50099600	-3.25803300	-0.02986600
H	4.59574300	2.35479200	0.33656200	O	5.66072400	-3.61574600	-0.03058200
C	3.08630900	5.38802900	-0.08279400	C	4.14949700	-1.80319300	-0.01106000
H	1.03916800	5.68394300	-0.72199300	C	2.87690300	-1.20811200	-0.01067200
H	5.07528100	4.78686500	0.52380200	H	1.91310100	-1.71322800	-0.02892600
H	3.29945500	6.45714900	0.00087100	C	5.06278700	-0.73100000	-0.00532700
Pd	0.27867800	0.50812700	-0.20854000	O	4.41147300	0.42756600	0.00002100
P	-1.92947500	-0.16083300	0.03277700	C	3.35432200	-4.24408100	-0.04899000
C	-2.35203100	-0.96056000	1.65094600	H	2.71251700	-4.11443400	0.83806500
C	-1.36514300	-1.74680900	2.27084800	H	2.72238100	-4.09148500	-0.93948500
C	-3.59626800	-0.81078100	2.28581000	H	3.75889900	-5.26374400	-0.05969600
C	-1.62205900	-2.38422600	3.48710600	C	6.54174700	-0.68836900	-0.00151400
H	-0.38390400	-1.84404700	1.79768800	H	6.90004200	-0.27331600	0.95681500
C	-3.84952000	-1.44282000	3.50760900	H	6.94432200	-1.69881400	-0.12756300
H	-4.37193900	-0.19202500	1.82956600	H	6.90412100	-0.02079500	-0.79979400



C	3.03122800	0.18739700	0.00104400	H	-3.44049700	-2.19695900	5.17405600
C	2.05234900	1.18521600	-0.01862100	H	-5.68493400	3.93760200	-1.30566400
C	2.32425400	2.60955600	-0.01592200	H	-2.63207800	-4.44056700	-3.78421900
C	1.24078600	3.48095800	-0.31930400				
C	3.58159500	3.21074900	0.27797700	<b>31b</b>			
C	1.39999300	4.86112700	-0.35745100	C	4.70322500	-3.38056900	-0.00233600
H	0.26499400	3.04246200	-0.54634700	O	5.87652500	-3.69176000	-0.04445900
C	3.73177500	4.59247500	0.26432300	C	4.32302100	-1.93704700	-0.00872600
H	4.43484100	2.58637400	0.53252100	C	3.05789700	-1.33612200	0.02141600
C	2.64824300	5.42120100	-0.06005800	H	2.09161800	-1.83558000	0.05419100
H	0.55448700	5.50454300	-0.61001500	C	5.24605600	-0.87175000	-0.06829400
H	4.70098800	5.03454600	0.50596200	O	4.60835500	0.28885800	-0.06100300
H	2.77769800	6.50630900	-0.07537600	C	3.58974000	-4.40033000	0.05828500
P	-1.94124400	-0.19994100	0.01494100	H	2.98355100	-4.26141000	0.96878500
C	-2.45899100	-0.81292000	1.66433200	H	2.91467200	-4.29275400	-0.80692000
C	-3.16195400	1.09220300	-0.44708900	H	4.02336100	-5.40809700	0.05923500
C	-2.18713600	-1.58652000	-1.16432300	C	6.72285400	-0.86335900	-0.14192000
C	-1.47918000	-1.35322700	2.51507900	H	7.14615200	-1.35932300	0.74643500
C	-3.79574700	-0.76636700	2.09492800	H	7.06097700	-1.46569300	-0.99948400
C	-4.19648700	0.86486000	-1.36767200	H	7.10194800	0.16351000	-0.22092900
C	-3.03856300	2.35780500	0.15573600	C	3.22171400	0.06135200	-0.00213600
C	-1.55942200	-1.50341700	-2.42107100	C	2.27145800	1.08107300	-0.01365800
C	-2.96689600	-2.71310600	-0.85773900	C	2.60043500	2.49393000	0.00514200
C	-1.83160500	-1.85487200	3.76977000	C	1.61456400	3.41987800	-0.43523900
H	-0.43261700	-1.37600200	2.19716000	C	3.83953400	3.02859500	0.46082200
C	-4.14366700	-1.26545000	3.35316800	C	1.86117200	4.78760600	-0.46773200
H	-4.56648500	-0.33510700	1.45215500	H	0.64963100	3.03679000	-0.77694000
C	-5.09870200	1.88937600	-1.67386000	C	4.06845100	4.39964800	0.46300500
H	-4.30132500	-0.10910200	-1.84993400	H	4.61121500	2.36245500	0.83999900
C	-3.94628800	3.37380600	-0.14717700	C	3.08918400	5.28252800	-0.01240300
H	-2.23413500	2.54917800	0.87252300	H	1.09427400	5.47345600	-0.83401400
C	-1.72490400	-2.52231400	-3.36120800	H	5.01813100	4.78951200	0.83627500
H	-0.94330600	-0.63448100	-2.67181100	H	3.28075500	6.35843600	-0.01738600
C	-3.12292600	-3.73504800	-1.79978200	Ag	0.20508400	0.47839900	-0.01196000
H	-3.45247800	-2.79875600	0.11641200	P	-2.13902800	-0.19855400	0.01453600
C	-3.16485600	-1.81120000	4.18969300	C	-2.77452200	-0.53804600	1.70344300
H	-1.06329400	-2.27211400	4.42499600	C	-3.25290000	1.08228700	-0.68988100
H	-5.18464100	-1.22434100	3.68243500	C	-2.43543500	-1.72509600	-0.96494800
C	-4.97732900	3.14081300	-1.06454800	C	-1.90553600	-1.10556300	2.65180100
H	-5.90128200	1.70499200	-2.39193700	C	-4.10303800	-0.25989800	2.06697100
H	-3.84812600	4.35122500	0.33128900	C	-4.26310700	0.77601700	-1.61525000
C	-2.50631400	-3.64072800	-3.05053200	C	-3.07794800	2.41552000	-0.27544000
H	-1.23994100	-2.44527000	-4.33731100	C	-1.80449700	-1.84870400	-2.21684400
H	-3.73111500	-4.60855000	-1.55302800	C	-3.26528600	-2.76156600	-0.50807700

C	-2.36027100	-1.40208400	3.93839300	C	1.64399700	3.32411800	-0.60237800
H	-0.86527500	-1.31591800	2.38611400	C	3.59701600	2.94205600	0.77854600
C	-4.55231300	-0.55307700	3.35780100	C	1.93102500	4.68702600	-0.63253900
H	-4.78885800	0.19053500	1.34630800	H	0.76621600	2.92684900	-1.11661900
C	-5.08740000	1.79018400	-2.11445200	C	3.85200100	4.31302000	0.78849000
H	-4.41037800	-0.25222200	-1.95131300	H	4.25027500	2.27355000	1.33984700
C	-3.90843300	3.42216700	-0.77043700	C	3.03135400	5.19034000	0.07164000
H	-2.29463800	2.66944700	0.44521900	H	1.28098700	5.36565800	-1.19099600
C	-2.01352100	-2.98287800	-3.00361600	H	4.70413200	4.70015100	1.35363000
H	-1.15111700	-1.05178700	-2.58488100	H	3.24313400	6.26282900	0.06929700
C	-3.46432800	-3.89978700	-1.29633200	Pd	0.20562800	0.39900100	0.22357500
H	-3.75795200	-2.68598200	0.46325800	P	-2.05441200	-0.19562200	0.01926400
C	-3.68453000	-1.12471800	4.29301200	C	-2.86781300	-0.75046700	1.58966600
H	-1.67745200	-1.84317700	4.66835500	C	-2.10642700	-1.53694700	2.47301900
H	-5.58597000	-0.33102800	3.63351600	C	-4.18366100	-0.41322300	1.94638400
C	-4.91331700	3.11089800	-1.69351100	C	-2.65476000	-1.99237600	3.67390100
H	-5.87021500	1.54308100	-2.83547900	H	-1.07128700	-1.78025500	2.21735900
H	-3.76953100	4.45362000	-0.43779400	C	-4.72844300	-0.86278700	3.15411900
C	-2.84300700	-4.01153500	-2.54300000	H	-4.78811000	0.20845800	1.28266100
H	-1.52513400	-3.06574300	-3.97753300	C	-3.96806000	-1.65521100	4.01817100
H	-4.11097300	-4.70173200	-0.93227600	H	-2.05003600	-2.60288500	4.34960100
H	-4.03893200	-1.34953800	5.30179200	H	-5.75287400	-0.58889000	3.42011100
H	-5.55928400	3.90007800	-2.08549400	H	-4.39474900	-2.00295700	4.96261600
H	-3.00262300	-4.90152300	-3.15640500	C	-3.16047300	1.16800300	-0.57278800
				C	-4.25240500	0.96791100	-1.43275300
<b>31c</b>				C	-2.87213300	2.47224400	-0.13255800
C	4.92549000	-3.26300200	0.04893300	C	-5.04544100	2.04845900	-1.83424200
O	6.10861800	-3.51504700	-0.10437200	H	-4.48505000	-0.03472400	-1.79763700
C	4.43474100	-1.86649700	0.01560600	C	-3.67153900	3.54797300	-0.52563900
C	3.11725600	-1.36688000	0.15925000	H	-2.00496700	2.63950200	0.51296500
H	2.19564500	-1.92127000	0.31900200	C	-4.75992500	3.33867300	-1.37942800
C	5.24237200	-0.74372800	-0.20020700	H	-5.88989200	1.87891900	-2.50760700
O	4.50705400	0.36222800	-0.17727100	H	-3.43670800	4.55553400	-0.17253700
C	3.90020300	-4.35540500	0.27858400	H	-5.38004400	4.18163600	-1.69556400
H	3.38115000	-4.20578500	1.23959200	C	-2.41349900	-1.57831000	-1.16104300
H	3.13011900	-4.33725400	-0.51004400	C	-3.40840300	-2.54649600	-0.94814500
H	4.40398700	-5.33034300	0.27963500	C	-1.63043200	-1.65405400	-2.32684900
C	6.70058200	-0.60939100	-0.44524500	C	-3.62082000	-3.56268500	-1.88630100
H	7.27200300	-1.00981600	0.40689700	H	-4.01926700	-2.51424300	-0.04333300
H	7.00175800	-1.21154900	-1.31615500	C	-1.85162900	-2.66255800	-3.26750400
H	6.96119200	0.44498100	-0.60806300	H	-0.83438700	-0.92054100	-2.48432800
C	3.15977100	0.01997700	0.05022800	C	-2.84709000	-3.62096700	-3.04862400
C	2.12555200	0.98589300	0.10236200	H	-4.39553100	-4.31257200	-1.70513700
C	2.48086500	2.41200300	0.08483400	H	-1.23684700	-2.70636300	-4.17041100

H -3.01454100 -4.41605300 -3.77998400