

Supporting Information

**Palladium Catalyzed C-H Activation of
Anisole with Electron-deficient Auxiliary
Ligands: a mechanistic investigation**

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Computational Methods

All of the quantum chemical calculations in this work were performed with Gaussian 16 program^{S1}. Single point energy calculations and geometry optimization were carried out at B3LYP-D3(BJ)/BS1-SMD(key words “eps=16.7, epsinf=1.631” were used)//B3LYP-D3(BJ)/BS2 level of theory^{S2-S4}. The basis set BS1 was designed as SDD for Pd, Ag, I and 6-311++G(d,p) for other atoms, while BS2 was designed as SDD for Pd, Ag, I and 6-31G(d) for other atoms^{S5-S7}. Several important conformations were evaluated manually. Frequency calculations (298.15K, ideal gas) were also performed to evaluate the nature of optimized structures. For transition states with one imaginary frequency, IRC calculations were also carried out to confirm its connectivity between corresponding substrates and products. Mulliken^{S8} and NPA^{S9} charge were calculated at the same level of geometry optimization through Gaussian program. Visualizations were completed through GaussView program^{S10}. For linear free energy relationship, the $\log(k/k_H)$ was calculated as follow (T=298.15K):

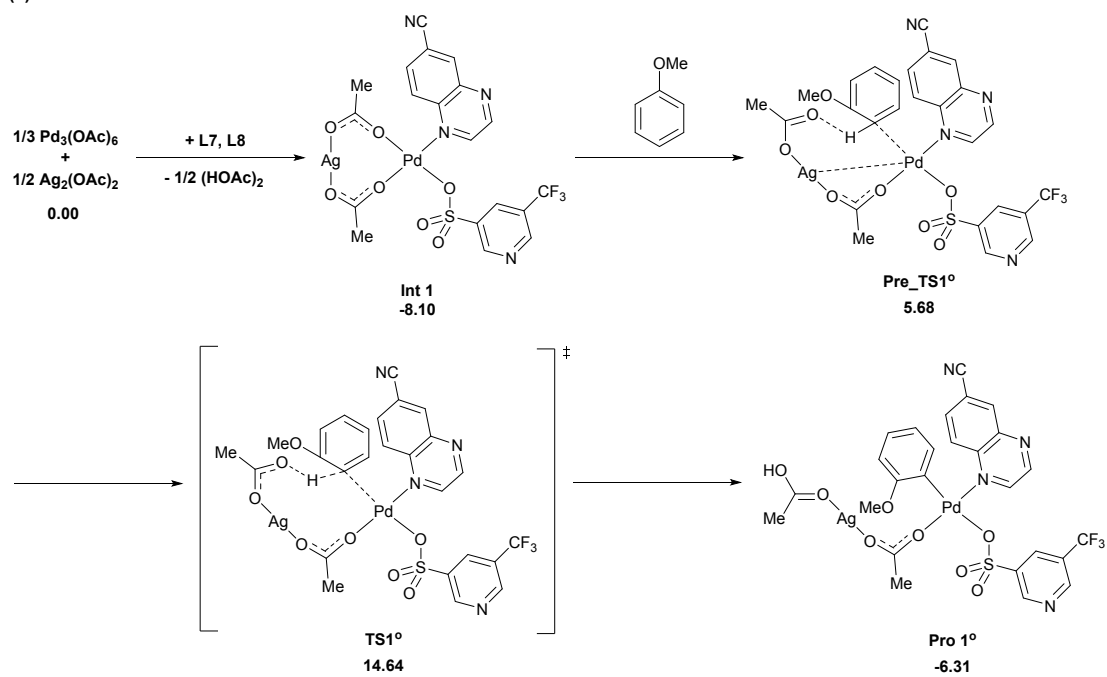
$$\log\left(\frac{k}{k_H}\right) = -\frac{\Delta G^* - \Delta G_H^*}{2.303RT}$$

In this equal, the ΔG^* represents the free energy barrier of C-H activation transition state formation with a series of substituted substrates; the ΔG_H^* represents the free energy barrier of C-H activation transition state formation with unsubstituted benzene substrate.

Overall catalytic cycle of Yu's meta-arylation reaction

In this section, further discussions were performed to support our assignment of the rate-determine step. The free energy profile of the all catalytic cycle will be discussed stage by stage. The first stage, which bears an activation energy barrier as 22.74 kcal/mol (scheme S1), has been well discussed and analyzed in the main text.

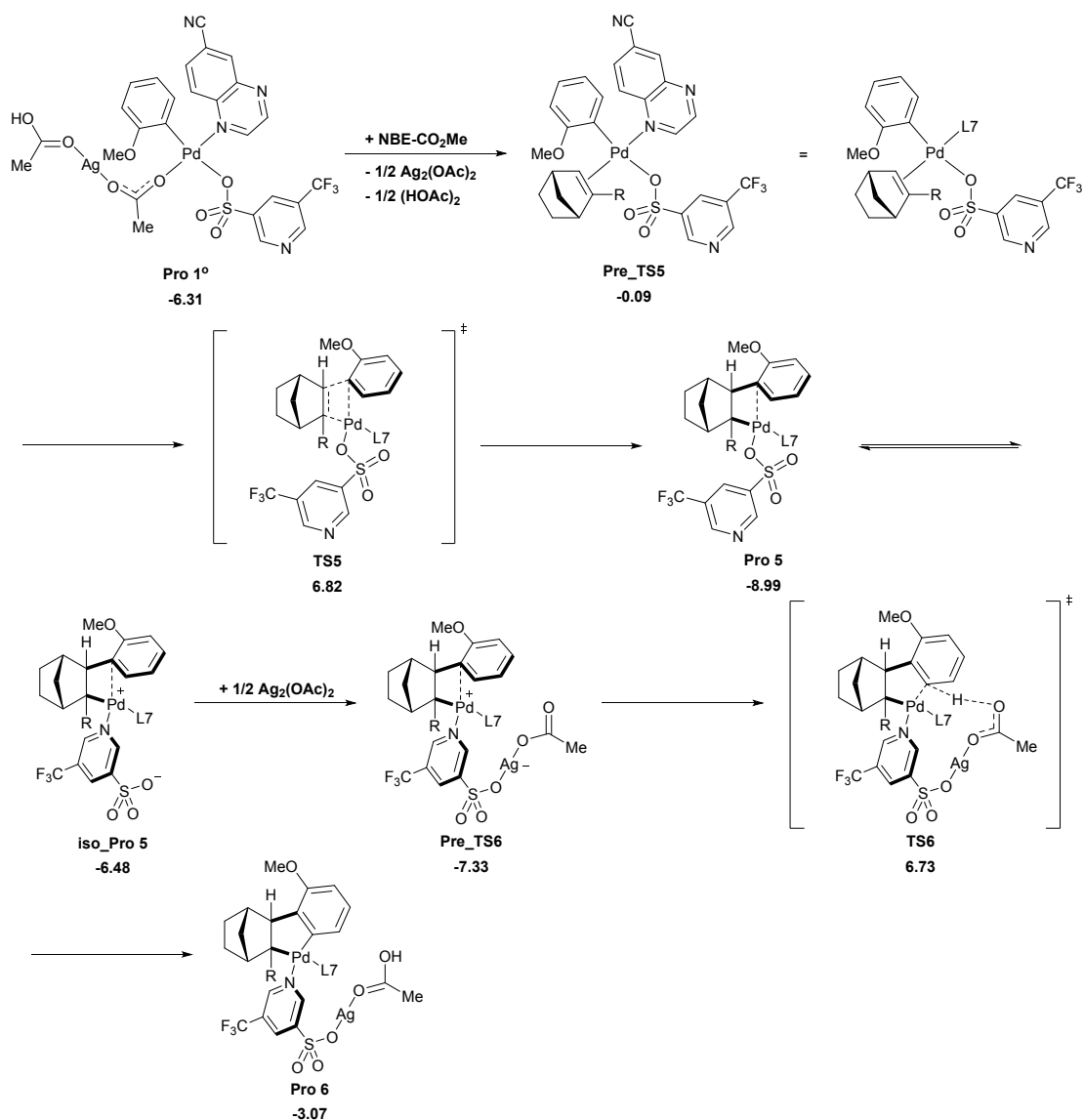
(1) The first C-H activation



Scheme S1. The first C-H activation.

The second stage of the overall catalytic cycle is norbornene insertion and the second C-H activation (scheme S2), which forms the key palladacycle intermediate **Pro 6**. After the first C-H activation step, the norbornene co-catalyst substitutes the silver acetate and acetic acid to form **Pre_TS5**. Then the norbornene co-catalyst insertion into C-Pd bond (via **TS5**) to afford the insertion product **Pro 5** and finally, isomerize to N-coordinated complex **iso_Pro 5**. With the advance of one molecular of silver acetate, the second C-H activation step is facile and via a macrocyclic transition state **TS6**. The highest activation energy barrier of this stage is 15.72 kcal/mol ($\Delta G_{\text{TS6}} - \Delta G_{\text{Pro 5}}$).

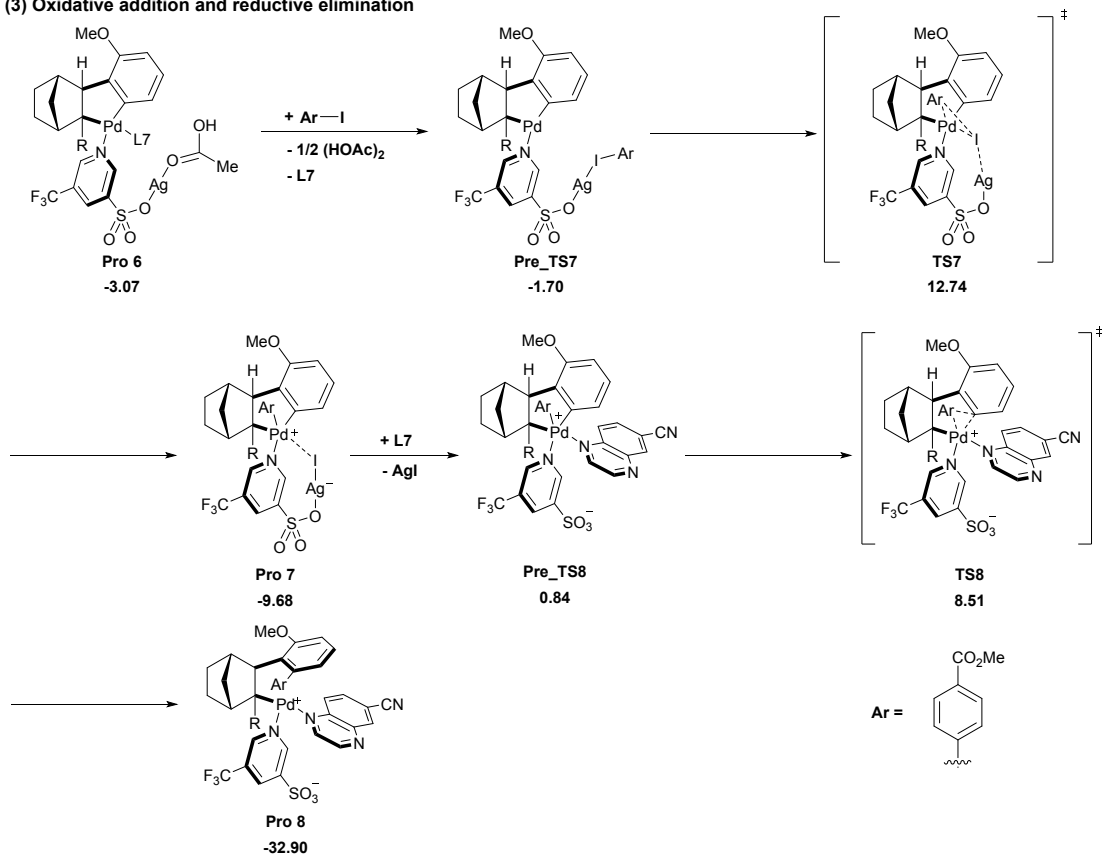
(2) Norbornene insertion and the second C-H activation



Scheme S2. Norbornene insertion and the second C-H activation (R = CO₂Me; similar hereinafter).

The third stage is oxidative addition and reductive elimination (scheme S3), which achieves the C-C bond formation at the meta site of anisole. In this stage, the aryl iodide substrate coordinates with silver atom and then oxidative addition through a cyclic transition state **TS7**. Silver iodide extrusion and **L7** coordination offers the Pd (IV) intermediate **Pre_TS8**. Finally, the highly exergonic reductive elimination step takes place to form the C-C bond formation product **Pro 8**. The highest energy transition state of this stage is the oxidative addition transition state **TS7**, which correspond to an energy barrier valued 21.73 kcal/mol ($\Delta G_{TS7} - \Delta G_{Pro5}$).

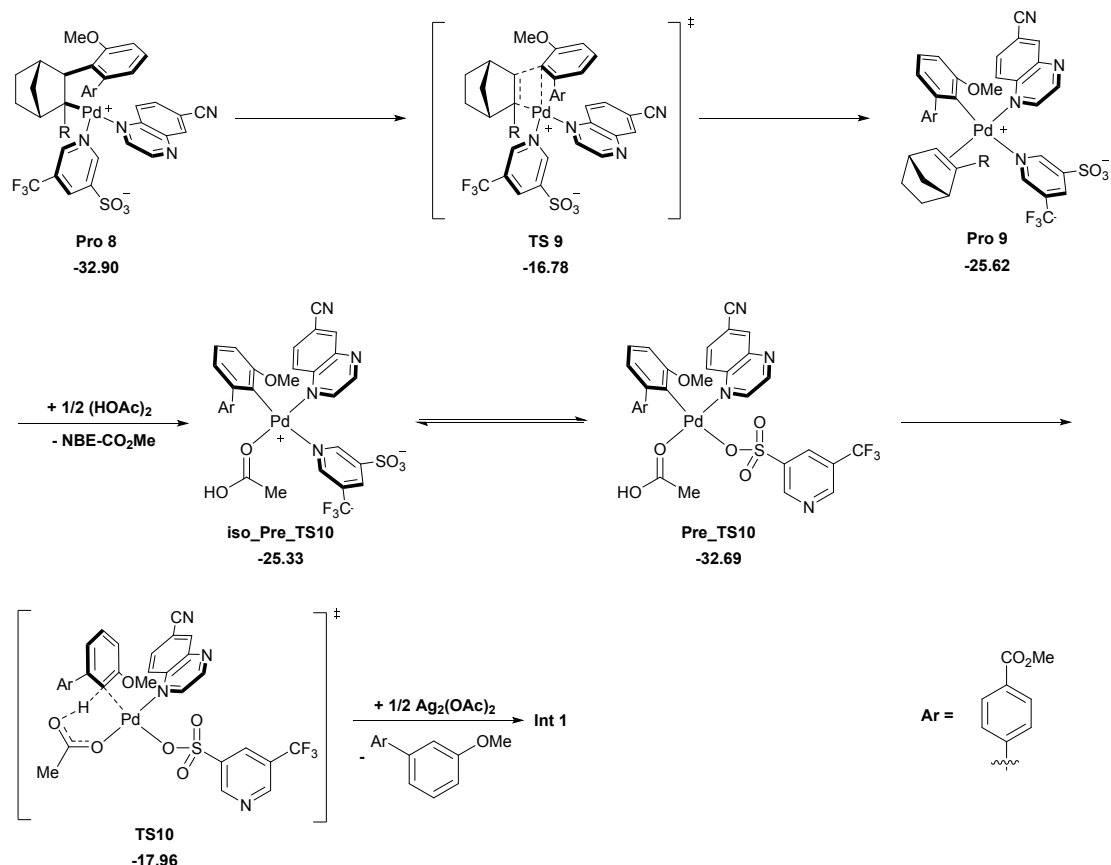
(3) Oxidative addition and reductive elimination



Scheme S3. Oxidative addition and reductive elimination.

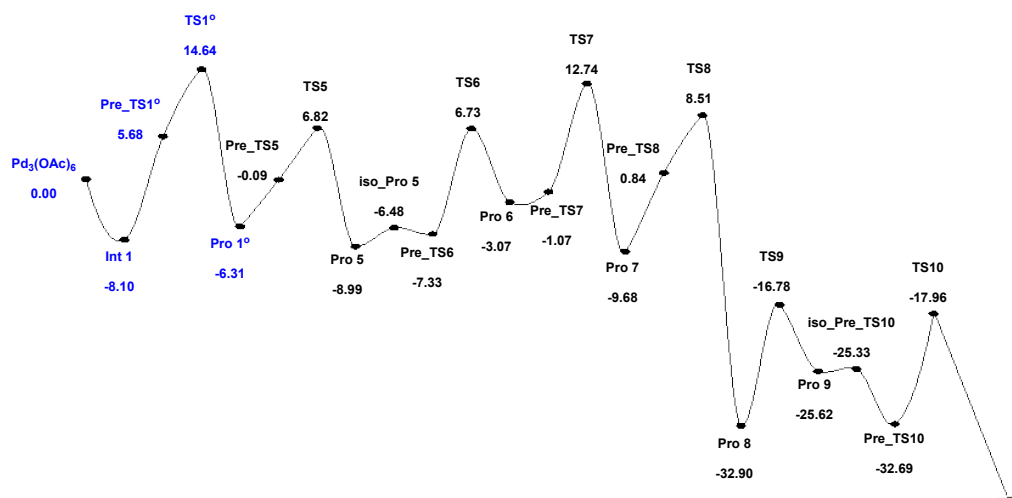
The final stage is norbornene extrusion and protodemallation (scheme S4), which releases the coupling product and regenerates the activate catalyst. The highest activation energy barrier of this stage is 16.12 kcal/mol ($\Delta G_{TS9} - \Delta G_{Pro8}$).

(4) Norbornene extrusion and protodemetalation



Scheme S4. Norbornene extrusion and protodemetalation.

The Gibbs free energy profile of the overall catalytic cycle was represented in scheme S5 (geometry structures of **TS5** – **TS10** can be found in figure S6); our calculation results supported that the first C-H activation step (22.74 kcal/mol) is the actual rate-determine step (although the activation energy barrier of oxidative addition is comparable; 21.73 kcal/mol) of this meta-arylation reaction and thus can have significant impact on the rate of desired product formation.



Scheme S5. The Gibbs free energy profile of the overall catalytic cycle.

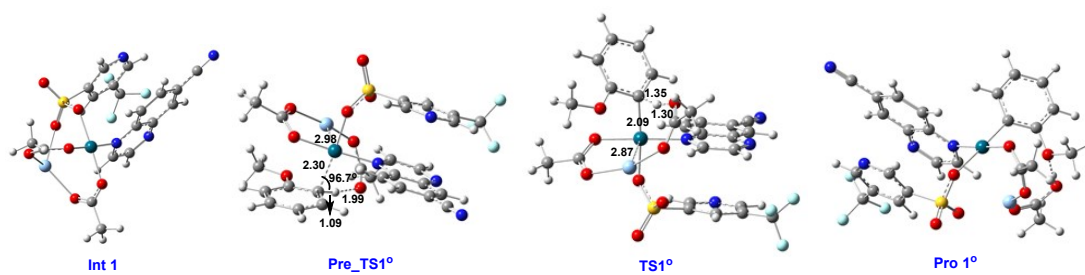


Figure S1. Geometry structures of **Int 1 – Pro 1°**.

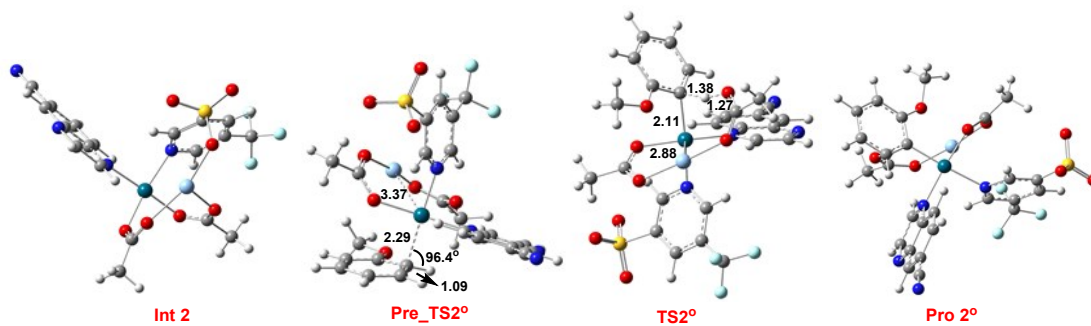


Figure S2. Geometry structures of **Int 2 – Pro 2°**.

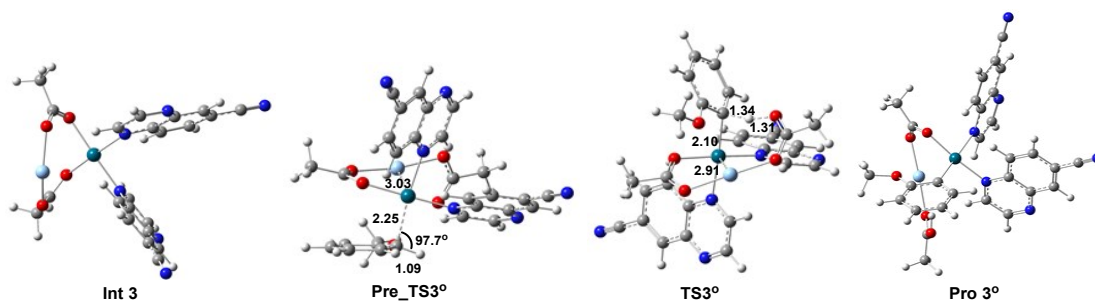


Figure S3. Geometry structures of **Int 3 – Pro 3°**.

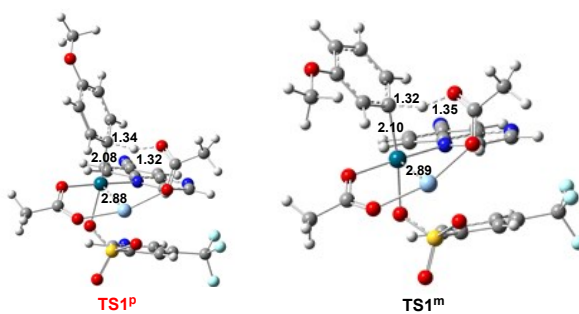


Figure S4. Geometry structures of **TS1^m** and **TS1^p**.

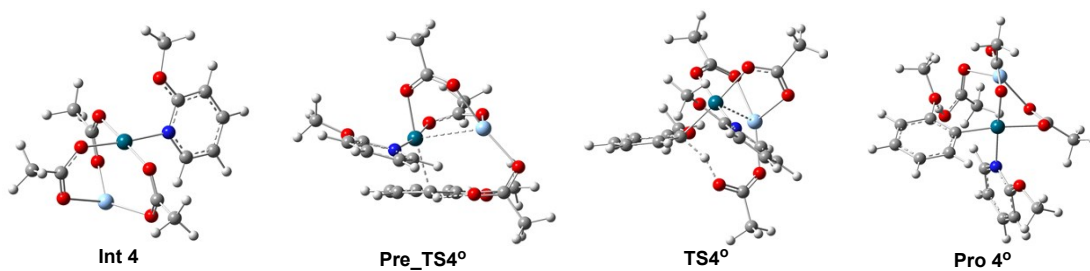


Figure S5. Geometry structures of **Int 4 – Pro 4°**.

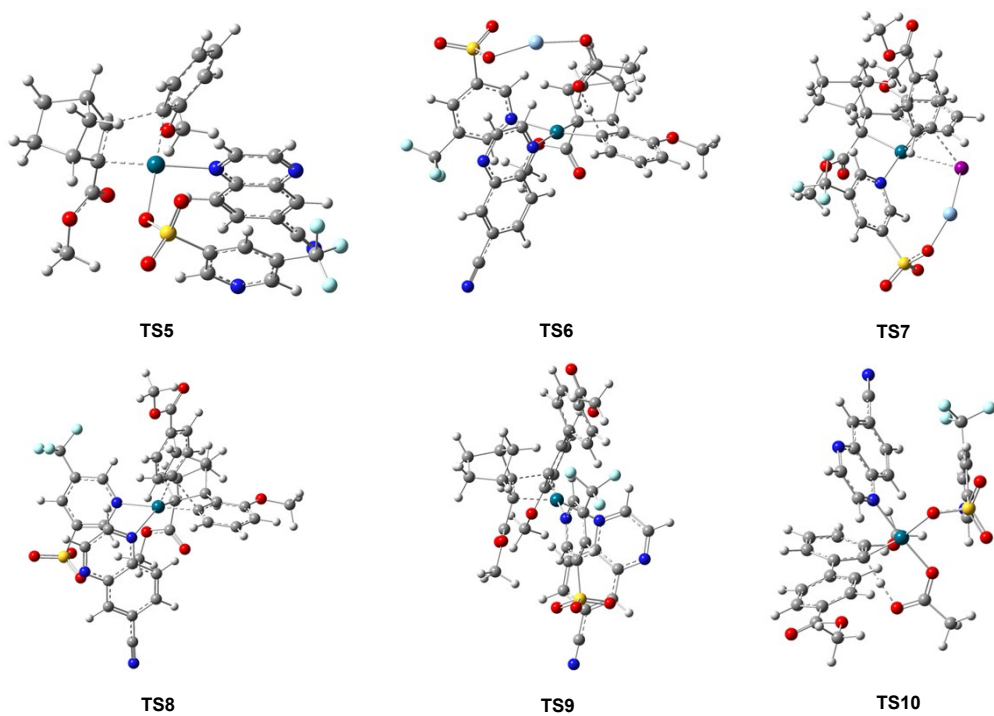


Figure S6. Geometry structures of **TS5 – TS10**.

Table S1. Free energy barriers of C-H activation transition states formation with a series of substituted substrates (kcal/mol; for ligands L7/L8).

R	Free energy barrier	σ	σ^+
OMe	23.41	-0.27	-0.78
NHAc	24.16	0	-0.60
Me	26.01	-0.14	-0.31
H	27.80	0	0
Cl	28.08	0.24	0.11
CN	30.53	0.70	0.66
NO ₂	30.90	0.81	0.79

Table S2. Free energy barriers of C-H activation transition states formation with a series of substituted substrates (kcal/mol; for ligands L3).

R	Free energy barrier	σ	σ^+
OMe	27.19	-0.27	-0.78
NHAc	28.20	0	-0.60
Me	29.01	-0.14	-0.31
H	30.15	0	0
Cl	29.46	0.24	0.11
CN	30.86	0.70	0.66
NO ₂	30.96	0.81	0.79

Table S3. Calculated energies and imaginary frequencies

Stationary point	Single-point energy at B3LYP-D3(BJ)/BS1-SMD (in a.u.) (1)	Thermal correction to Gibbs free energy at B3LYP-D3(BJ)/BS2 (in a.u.) (2)	Gibbs free energies (G) (in a.u.) (3)=(1)+(2)	Imaginary frequencies
Int 1	-2451.483984	0.255135	-2451.228849	
Pre_TS1^o	-2798.391759	0.379578	-2798.012181	
TS1^o	-2798.372269	0.37436	-2797.997909	-1289.14 <i>i</i>
Pro 1^o	-2798.410034	0.378737	-2798.031297	
Int 2	-2451.481202	0.254825	-2451.226377	
Pre_TS2^o	-2798.389276	0.377824	-2798.011452	
TS2^o	-2798.367672	0.37278	-2797.994892	-1573.13 <i>i</i>
Pro 2^o	-2798.389641	0.375453	-2798.014188	
Int 3	-1752.862651	0.283631	-1752.57902	
L8⁻	-1209.003787	0.055473	-1208.948314	
Pre_TS3^o	-2099.775858	0.409962	-2099.365896	
TS3^o	-2099.753227	0.403009	-2099.350218	-1245.42 <i>i</i>
Pro 3^o	-2099.778096	0.406351	-2099.371745	
Pd₃(OAc)₆	-1755.439642	0.244793	-1755.194849	
Ag₂(OAc)₂	-751.278556	0.058278	-751.220278	
(HOAc)₂	-458.386959	0.089612	-458.297347	
L7	-510.394046	0.088892	-510.305154	
L8	-1209.451881	0.067515	-1209.384366	
Anisole	-346.908134	0.102833	-346.805301	
Pre_TS1^m	-2798.395075	0.378234	-2798.016841	
TS1^m	-2798.364082	0.37287	-2797.991212	-1131.76 <i>i</i>
Pro 1^m	-2798.404828	0.375779	-2798.029049	
Pre_TS1^p	-2798.39609	0.377511	-2798.018579	
TS1^p	-2798.370084	0.373247	-2797.996837	-1222.15 <i>i</i>
Pro 1^p	-2798.402173	0.376175	-2798.025998	
Int Pd1	-1605.958590	0.285064	-1605.673526	
Pre_TS^{Pd1}	-1442.448723	0.298179	-1442.150544	
TS^{Pd1}	-1442.422696	0.293325	-1442.129371	-1195.79 <i>i</i>
Pro^{Pd1}	-1442.442356	0.297866	-1442.14449	
Int Pd2	-2191.117155	0.376350	-2190.740805	
Pre_TS^{Pd2}	-2027.605887	0.387342	-2027.218545	
TS^{Pd2}	-2027.584523	0.384315	-2027.200208	-1218.27 <i>i</i>
Pro^{Pd2}	-2027.609391	0.391095	-2027.218296	
Int 4	-1323.760567	0.217713	-1323.542854	

Pre_TS4°	-1670.667227	0.343617	-1670.323610	
TS4°	-1670.641636	0.337519	-1670.304117	-1412.69 <i>i</i>
Pro 4°	-1670.671695	0.342581	-1670.329114	
L3	-362.958211	0.091129	-362.867082	
TS1P_NHAc	-2891.908435	0.3899	-2891.518535	-1209.15 <i>i</i>
TS1P_Me	-2723.134237	0.368076	-2722.766161	-1128.24 <i>i</i>
TS1P_H	-2683.79756	0.343612	-2683.453948	-1110.37 <i>i</i>
TS1P_Cl	-3143.425539	0.332038	-3143.093501	-1113.40 <i>i</i>
TS1P_CN	-2776.070115	0.33958	-2775.730535	-1073.39 <i>i</i>
TS1P_NO₂	-2888.366823	0.34206	-2888.024763	-1061.47 <i>i</i>
TS4P	-1670.639447	0.336049	-1670.303398	-1352.44 <i>i</i>
TS4P_NHAc	-1764.178533	0.353863	-1763.824670	-1334.06 <i>i</i>
TS4P_Me	-1595.404943	0.330984	-1595.073959	-1290.48 <i>i</i>
TS4P_H	-1556.069389	0.306608	-1555.762781	-1273.26 <i>i</i>
TS4P_Cl	-2015.698351	0.294471	-2015.403880	-1264.29 <i>i</i>
TS4P_CN	-1648.344944	0.302358	-1648.042586	-1223.59 <i>i</i>
TS4P_NO₂	-1760.642077	0.304824	-1760.337253	-1213.06 <i>i</i>
PhNHAc	-440.448145	0.119963	-440.328182	
PhMe	-271.676611	0.097849	-271.578762	
PhH	-232.342796	0.073396	-232.2694	
PhCl	-691.97096	0.061552	-691.909408	
PhCN	-324.619621	0.069279	-324.550342	
PhNO₂	-436.917125	0.071962	-436.845163	
Pre_TS5	-2694.373456	0.465195	-2693.908261	
TS5	-2694.364539	0.467288	-2693.897251	-210.06 <i>i</i>
Pro 5	-2694.393604	0.471157	-2693.922447	
iso_Pro 5	-2694.388635	0.470197	-2693.918438	
Pre_TS6	-3070.041703	0.511775	-3069.529928	
TS6	-3070.012054	0.50453	-3069.507524	-1408.93 <i>i</i>
Pro 6	-3070.032694	0.509543	-3069.523151	
Pre_TS7	-2801.551046	0.460497	-2801.090549	
TS7	-2801.528356	0.460813	-2801.067543	-179.06 <i>i</i>
Pro 7	-2801.568005	0.464745	-2801.10326	
Pre_TS8	-3153.433868	0.583183	-3152.850685	
TS8	-3153.417978	0.579528	-3152.83845	-80.46 <i>i</i>
Pro 8	-3153.48591	0.58146	-3152.90445	
TS 9	-3153.460935	0.582179	-3152.878756	-265.53 <i>i</i>
Pro 9	-3153.474453	0.581614	-3152.892839	
iso_Pre_TS10	-2881.845186	0.449814	-2881.395372	
Pre_TS10	-2881.857543	0.450443	-2881.4071	
TS10	-2881.828471	0.44485	-2881.383621	-1202.58 <i>i</i>
(AgI)₂	-317.044774	-0.03718	-317.081954	
NBE-CO₂Me	-500.807392	0.161703	-500.645689	

Arl	-471.118572	0.095157	-471.023415	
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Cartesian coordinate of optimized structures

Int 1

0 1

Pd	-1.59125300	1.03019000	-0.01026100
O	-3.25600000	1.49236500	-1.04903100
C	-4.08799200	0.64774800	-1.55632200
O	-4.16995900	-0.57335200	-1.30169300
Ag	-2.92504600	-1.47413700	0.32981000
O	-2.86005000	-0.48994500	2.39998600
C	-2.91013700	0.75818100	2.54244900
O	-2.46744400	1.63878700	1.71460500
C	-3.55454100	1.32538900	3.79036100
H	-3.23910000	2.35471100	3.96801900
H	-4.64184400	1.31071900	3.65171000
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H	-5.94063400	0.65204500	-2.64924600
H	-5.26110200	2.28674300	-2.33654700
H	-4.52695800	1.23193100	-3.55621600
N	0.19549000	0.74727000	0.97657300
C	1.31393800	1.46348500	0.63015100
C	0.30380200	-0.18705900	1.90906600
C	1.26376100	2.47487300	-0.35868700
C	2.55070000	1.16564900	1.28166600
C	1.54712900	-0.45331100	2.53374700
H	-0.59729900	-0.72726600	2.17386700
C	2.40897900	3.15224300	-0.69862400
H	0.32076700	2.68904800	-0.84856900
C	3.71711900	1.87602500	0.91484800
N	2.64774700	0.19929400	2.23395200
H	1.61237100	-1.23787700	3.28215600
C	3.64898900	2.84982600	-0.06401200
H	2.38389200	3.92053600	-1.46303400
H	4.64767900	1.62035300	1.40757200
C	4.83100200	3.55786500	-0.45569100
N	5.78655900	4.13685600	-0.77590400
O	-0.75107700	0.35986200	-1.77260300
S	-0.30493800	-1.11554300	-1.89145700
C	1.46166900	-1.01088000	-1.59749500
O	-0.51869400	-1.60763200	-3.24840100
O	-0.81540200	-1.94753500	-0.76030900
C	2.23506600	-0.09838000	-2.32225900
C	2.06353500	-1.80514800	-0.63007600

N	3.54396000	0.06455900	-2.11318100
H	1.77512200	0.53123200	-3.07869000
C	3.42853900	-1.63225200	-0.40809800
H	1.47425000	-2.50897400	-0.05526200
C	4.12179700	-0.68941200	-1.17089900
C	4.14931800	-2.43388200	0.63957900
H	5.18227200	-0.52176100	-1.00299800
F	3.29714000	-2.88117400	1.59160700
F	4.75909300	-3.51427700	0.11229500
F	5.09864500	-1.69585600	1.25100400

Pre_TS1°

0 1

C	-3.67618500	1.15585400	1.35200000
C	-4.34069500	2.32364600	0.99438300
C	-3.63291200	3.53392700	0.94922700
C	-2.28389100	3.60926600	1.27842400
C	-1.61269400	2.43932500	1.65879700
H	-5.39570200	2.31298000	0.75011900
H	-1.76179900	4.55978400	1.26110200
H	-0.59618500	2.49458600	2.03426800
C	-2.27777800	1.18435900	1.65857600
H	-1.86878800	0.30163200	2.15654200
Pd	-1.10150600	0.95375700	-0.30392500
O	-2.63829300	1.61638300	-1.41961900
C	-3.40395200	0.77793100	-2.02398800
O	-3.48990100	-0.45028300	-1.79407600
Ag	-2.48865100	-1.68574400	-0.30303400
O	-1.96537000	-2.98718900	1.29001000
C	-1.75137500	-2.63060500	2.51265100
O	-1.43269700	-1.48859900	2.89789000
C	-1.89405700	-3.75967600	3.52640600
H	-1.52963200	-3.44805100	4.50719100
H	-2.95118700	-4.03818100	3.60609600
H	-1.35310900	-4.64725500	3.18388000
C	-4.25842800	1.38091200	-3.11631400
H	-5.13543400	0.75761600	-3.29994000
H	-4.55174700	2.40172100	-2.86077900
H	-3.65859100	1.42055800	-4.03282200
H	-4.16467500	4.43585200	0.65982400
O	-4.24947800	-0.05729300	1.45365300
C	-5.59536200	-0.22346300	1.01015100
H	-6.28516800	0.37309400	1.61778100
H	-5.68563300	0.04676500	-0.04726200

H	-5.81331100	-1.28333900	1.13754300
N	0.58107300	0.34328000	0.71461600
C	1.66110900	1.17799900	0.88713400
C	0.65031500	-0.89197700	1.17999700
C	1.68817800	2.47327300	0.32219600
C	2.79071000	0.69574400	1.61281400
C	1.78126800	-1.32276500	1.92673900
H	-0.16425800	-1.56541500	0.96874200
C	2.80739300	3.25896500	0.46519500
H	0.83586100	2.81461200	-0.25571700
C	3.92727000	1.52190700	1.75570200
N	2.81958600	-0.55666100	2.15259600
H	1.79151800	-2.33183600	2.32714800
C	3.93822500	2.78440400	1.18733700
H	2.84752300	4.24315300	0.01242600
H	4.78142700	1.12655100	2.29248800
C	5.09646500	3.61862500	1.30824000
N	6.03128700	4.30281100	1.40400200
N	4.03645400	0.99038300	-1.95527200
C	2.78777100	0.70929000	-2.34148700
C	4.67988700	0.07269400	-1.22653000
C	2.14302700	-0.48639300	-2.01269000
H	2.26608900	1.47133300	-2.91324900
C	4.11809900	-1.15506100	-0.86379500
H	5.68338100	0.33264600	-0.89985000
C	2.81957400	-1.44951200	-1.27386400
S	0.43183100	-0.74583900	-2.49560200
C	4.91083400	-2.12011800	-0.02721100
H	2.32957200	-2.37702400	-1.00220600
O	0.38818300	-0.92962400	-3.94483500
O	-0.07136500	-1.83010500	-1.62357500
O	-0.20595900	0.62242600	-2.13227700
F	5.80719400	-2.80429300	-0.76677900
F	4.11279600	-3.02588900	0.57858900
F	5.60333100	-1.47058700	0.93485200

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C	-3.74120100	1.57542600	0.56050400
C	-4.54809600	2.71679200	0.60465700
C	-3.95424500	3.96274300	0.80167100
C	-2.57247000	4.09238600	0.98530800
C	-1.78224800	2.95261000	0.93962400
H	-5.62311900	2.64768000	0.48911000

H	-2.13141000	5.06898400	1.15786900
H	-0.71077800	3.04625600	1.09229400
C	-2.32443300	1.65978800	0.71562400
H	-2.03708700	0.81110600	1.72032600
Pd	-1.14359600	0.57314700	-0.62445800
O	-2.66072500	0.59006700	-1.97392100
C	-3.23595400	-0.49088200	-2.36290700
O	-3.20912000	-1.60779500	-1.79426100
Ag	-2.34177200	-1.89970300	0.19956800
O	-2.10303700	-1.88433400	2.37700500
C	-2.12741200	-0.92676800	3.19211700
O	-1.94950200	0.31312300	2.91926700
C	-2.37255600	-1.24051400	4.65577600
H	-1.77549500	-0.58469200	5.29413000
H	-3.42885600	-1.05072200	4.88056800
H	-2.15442500	-2.28942400	4.86383900
C	-4.00380600	-0.36352100	-3.66299700
H	-4.81290200	-1.09568500	-3.70018400
H	-4.38910800	0.65028700	-3.79309000
H	-3.31096000	-0.57251300	-4.48629800
H	-4.58627600	4.84638600	0.82711500
O	-4.23375000	0.32565800	0.43835200
C	-5.61403200	0.13484500	0.14773300
H	-6.24525300	0.47767000	0.97571500
H	-5.89103300	0.65931900	-0.77366800
H	-5.73481300	-0.93921700	0.00862400
N	0.53431900	0.63914900	0.57638700
C	1.56328700	1.50401100	0.29144800
C	0.70236500	-0.23553900	1.55424900
C	1.47529800	2.41509000	-0.78729200
C	2.75048900	1.45215700	1.08322600
C	1.88863700	-0.24642900	2.33085600
H	-0.08618100	-0.95233300	1.72959300
C	2.53964300	3.23357000	-1.07804300
H	0.57244900	2.42974700	-1.38899600
C	3.83066100	2.30893500	0.77140700
N	2.88847400	0.57705700	2.11697000
H	1.99362700	-0.97333700	3.13111700
C	3.72986100	3.18224400	-0.29639500
H	2.49001600	3.92026900	-1.91547800
H	4.72927200	2.23766900	1.37275800
C	4.82877400	4.03815700	-0.63094300
N	5.71448400	4.73941000	-0.90454700
N	4.16060100	0.13701400	-2.03207900

C	2.92573100	-0.31469100	-2.27104700
C	4.81309400	-0.37047100	-0.98018200
C	2.30251700	-1.28194500	-1.47534300
H	2.39474500	0.12336500	-3.11101700
C	4.27186800	-1.34297700	-0.13600900
H	5.80472600	0.03069100	-0.78823700
C	2.98797700	-1.82072100	-0.39441400
S	0.60979900	-1.77940000	-1.82669000
C	5.06082500	-1.84141300	1.04145600
H	2.51323000	-2.55793100	0.24212600
O	0.62583700	-2.64298100	-3.00656100
O	0.11169200	-2.36340000	-0.54984000
O	-0.05466200	-0.42818600	-2.13333300
F	5.92086100	-2.82068100	0.69373000
F	4.25195900	-2.34395900	2.00283600
F	5.78996600	-0.84923000	1.59598400

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C	-3.20467300	1.76259400	1.12982100
C	-3.79797900	2.56836000	2.10376400
C	-3.16093300	3.73590400	2.51868700
C	-1.93030900	4.08013900	1.95861700
C	-1.34185800	3.25042500	1.00116600
H	-4.75091600	2.27278800	2.53410700
H	-1.42316200	4.98963100	2.26868200
H	-0.37822800	3.53293000	0.58642000
C	-1.96563000	2.07139700	0.56232100
H	-3.93209500	-0.51440700	1.96698400
Pd	-1.05072200	0.91272800	-0.77318600
O	-2.54515700	1.17266100	-2.14071100
C	-3.23906900	0.21180700	-2.62957300
O	-3.39009400	-0.93762000	-2.14693700
Ag	-2.37176900	-1.61938300	-0.31457100
O	-2.23884500	-2.19894700	1.91812400
C	-3.05379700	-2.00577300	2.82601400
O	-3.99629300	-1.08468500	2.79406100
C	-3.05387100	-2.81855600	4.09205400
H	-2.95489900	-2.15698400	4.95841500
H	-4.01222800	-3.33952600	4.18897600
H	-2.23935000	-3.54233500	4.07109300
C	-3.93854100	0.53163400	-3.93630600
H	-4.83820600	-0.07708600	-4.04720800
H	-4.17714900	1.59538200	-4.00228100

H	-3.25308300	0.28470300	-4.75538800
H	-3.61981300	4.36512500	3.27529700
O	-3.87231800	0.58550000	0.74811400
C	-5.08838300	0.80371900	0.00858800
H	-5.85527000	1.25239300	0.64854700
H	-4.87728500	1.45811200	-0.83944100
H	-5.41157000	-0.17482800	-0.34681400
N	0.53357000	0.72930100	0.53379500
C	1.69196200	1.43977700	0.34596700
C	0.47832800	-0.12497100	1.54340500
C	1.82547000	2.34238100	-0.73593400
C	2.77888200	1.24941100	1.25187800
C	1.57970000	-0.29577500	2.41813000
H	-0.43215800	-0.69519300	1.67358200
C	3.00313200	3.02565700	-0.91351100
H	0.99392200	2.45792900	-1.42423000
C	3.98302600	1.96349400	1.05133600
N	2.70184700	0.37638700	2.29263700
H	1.51036300	-1.01559400	3.22912100
C	4.09407500	2.83639400	-0.01536900
H	3.12211500	3.70673000	-1.74843400
H	4.80428500	1.78272500	1.73451500
C	5.31830400	3.54672200	-0.23629200
N	6.30834500	4.12792500	-0.41845300
N	4.24803300	-0.09664700	-1.94065100
C	2.99372700	-0.43708300	-2.25447200
C	4.78160400	-0.64287100	-0.84307700
C	2.23393100	-1.32686300	-1.48991700
H	2.56130700	0.03273700	-3.13321800
C	4.09802600	-1.54414200	-0.02226500
H	5.79287900	-0.33271900	-0.59283200
C	2.79467100	-1.90510500	-0.35745300
S	0.53374900	-1.68089300	-1.95304500
C	4.76407500	-2.08597100	1.21044100
H	2.21226800	-2.58313900	0.25439800
O	0.55694500	-2.55557800	-3.12553300
O	-0.06400700	-2.25184200	-0.70176700
O	-0.02803200	-0.30122500	-2.26855800
F	5.60933100	-3.09747200	0.92353500
F	3.86117800	-2.55833900	2.09886100
F	5.48963600	-1.12870700	1.83161300

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Pd	-0.49880800	-0.63167300	-1.25428400
O	1.01656000	-0.46032100	-2.56267600
C	2.24919400	-0.67501700	-2.20607500
O	2.63128100	-1.04933100	-1.08778300
Ag	1.54154500	-1.85573500	0.86991900
O	0.25431600	-3.41453400	-0.19018600
C	-0.33757300	-3.48806200	-1.29306500
O	-0.84218200	-2.50152300	-1.95314600
C	-0.49912200	-4.84117500	-1.95252300
H	-1.31509600	-4.83616900	-2.67708800
H	0.43355800	-5.07740100	-2.47804300
H	-0.65840000	-5.60861600	-1.19172500
C	3.26053000	-0.34862500	-3.28784900
H	4.15861100	-0.95340800	-3.14935200
H	2.84031800	-0.50010800	-4.28412600
H	3.53593800	0.70745900	-3.18539200
N	-2.16366700	-0.76404800	-0.02417300
C	-3.18579900	0.15144700	-0.09395000
C	-2.22589800	-1.71002500	0.90298400
C	-3.19617000	1.16731000	-1.07860900
C	-4.25652300	0.06382400	0.84896800
C	-3.30438800	-1.76476700	1.82172500
H	-1.41582200	-2.43008800	0.93234300
C	-4.23099800	2.06997600	-1.11909600
H	-2.38455400	1.21390700	-1.79582900
C	-5.30966300	1.00659700	0.79191000
N	-4.29599200	-0.90299300	1.80651100
H	-3.31579500	-2.54135500	2.58152700
C	-5.29708600	1.99526800	-0.17566700
H	-4.24963600	2.84955400	-1.87243200
H	-6.10985300	0.92685600	1.51824800
C	-6.36040400	2.95340600	-0.24373700
N	-7.21733200	3.73569400	-0.31099700
N	0.16498000	1.13902300	-0.35668100
C	0.28916800	0.90835900	0.96510800
C	1.06070000	1.94263600	-0.95937900
C	1.39527500	1.31938600	1.69122600
H	-0.47027200	0.31102700	1.45068800
C	2.12548500	2.49813900	-0.25504100
H	0.95217100	2.07569900	-2.02750300
C	2.33626500	2.13954200	1.08034100
S	1.67567900	0.41606700	3.24675900
C	3.07276400	3.42507000	-0.97110000
H	3.21975700	2.45603200	1.62437300

O	2.32419800	-0.84469400	2.68632300
O	2.60387200	1.22979200	4.03537600
O	0.31565300	0.17288100	3.76288400
F	4.29838300	3.39748500	-0.42340100
F	2.63201800	4.69814800	-0.93290200
F	3.19190200	3.08596800	-2.27802600

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C	1.67645800	-2.92183700	-1.74444900
C	1.80904900	-2.64454800	-3.10513000
C	0.66387400	-2.54732500	-3.90279000
C	-0.61854600	-2.73793900	-3.38717800
C	-0.76446200	-3.01719800	-2.02940000
H	2.78633100	-2.51230000	-3.55184100
H	-1.48770200	-2.67003200	-4.03156300
H	-1.74282900	-3.23922500	-1.61413000
C	0.37153200	-3.06251000	-1.17858800
H	0.31261400	-3.50543100	-0.18971400
Pd	-0.22490200	-0.93882700	-0.54519100
O	0.42484100	-0.02551400	-2.23848300
C	1.21584200	0.98612100	-2.38524100
O	2.12959100	1.32178300	-1.59373500
Ag	2.91321000	0.16876200	-0.00544100
O	3.93270300	-1.10592300	1.35592500
C	3.06145800	-1.68849600	2.08907500
O	1.82898400	-1.44729700	2.04262500
C	3.57927900	-2.76044200	3.03182600
H	3.46407000	-3.73726900	2.54549000
H	4.63668900	-2.61005900	3.25739100
H	2.99361000	-2.77256000	3.95444800
C	0.96519400	1.83452600	-3.60254500
H	1.91331000	2.20200100	-4.00185700
H	0.40894900	1.27996900	-4.36046500
H	0.36970700	2.70782200	-3.28756000
H	0.78589300	-2.32700300	-4.95917200
O	2.69012600	-3.09632200	-0.88381600
C	4.02948300	-2.86970900	-1.33678500
H	4.31639300	-3.62360700	-2.07839200
H	4.12613400	-1.86417000	-1.76041200
H	4.65062500	-2.93994000	-0.44677800
N	-1.40656200	-1.73268100	0.96212900
C	-2.77441700	-1.62795500	0.82823600
C	-0.91325200	-2.28787800	2.05852900

C	-3.36719900	-1.01860900	-0.30328700
C	-3.60750500	-2.14201100	1.86975900
C	-1.77943400	-2.78847800	3.06667900
H	0.17180100	-2.29788700	2.16862500
C	-4.73539000	-0.92010800	-0.39590400
H	-2.73417100	-0.62235300	-1.08936800
C	-5.01281700	-2.04073000	1.74983400
N	-3.08840100	-2.72875600	2.98424400
H	-1.34748000	-3.24240300	3.95475900
C	-5.57014100	-1.43944200	0.63495100
H	-5.19081800	-0.43828500	-1.25382500
H	-5.62533300	-2.44000300	2.54964400
C	-6.99402200	-1.34225400	0.50694700
N	-8.14855900	-1.27193800	0.39443700
N	-0.46303300	0.92472800	0.25769600
C	-1.07945000	1.87131400	-0.47010400
C	0.28592200	1.25812500	1.32516600
C	-0.93408800	3.21936600	-0.18135500
H	-1.67561100	1.55818600	-1.31757300
C	0.46278400	2.59581200	1.66559200
H	0.76809500	0.44670500	1.86284400
C	-0.14081200	3.59500000	0.90073800
S	-1.66022400	4.40381100	-1.36568200
C	1.41286100	2.90186300	2.79211700
H	-0.00967800	4.64860400	1.12362100
O	-2.92014400	3.72588600	-1.74840900
O	-1.77950600	5.64771400	-0.58442800
O	-0.61318600	4.40500000	-2.42235600
F	1.33847900	4.18224600	3.18411500
F	2.69278800	2.66031100	2.41009900
F	1.17351400	2.11548900	3.86389500

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C	-2.49564300	-2.08924500	-1.82958300
C	-3.25303000	-2.28727300	-2.98807900
C	-4.02839200	-1.23975200	-3.48335700
C	-4.08592700	-0.00502000	-2.82772700
C	-3.32508500	0.17909100	-1.68125300
H	-3.24865700	-3.23948500	-3.50441900
H	-4.71228000	0.79286800	-3.21361700
H	-3.37629300	1.13403700	-1.16641800
C	-2.49200500	-0.83739900	-1.14754600
H	-2.81420400	-1.11992500	0.16913300

Pd	-0.62884400	-0.06721100	-0.51454700
O	0.31601300	-1.20746400	-1.91723100
C	1.17617700	-2.12237200	-1.63389300
O	1.29924300	-2.68727500	-0.51125600
Ag	-0.22291200	-2.49462500	0.97535100
O	-1.80622100	-2.35296200	2.41135100
C	-3.01873800	-2.06636400	2.20268300
O	-3.48251200	-1.40367900	1.21180500
C	-4.03624200	-2.52991500	3.22253400
H	-4.89346600	-1.85439300	3.25046600
H	-4.39498500	-3.52233000	2.92416300
H	-3.57380200	-2.61894900	4.20750900
C	2.12195300	-2.49487500	-2.74277400
H	2.45366800	-3.52843200	-2.62454800
H	1.65333100	-2.34155800	-3.71742000
H	3.00571900	-1.83763100	-2.68300800
H	-4.60849800	-1.39846500	-4.38813700
O	-1.77346300	-3.07669000	-1.24816700
C	-1.56192200	-4.30055100	-1.95108700
H	-2.49890300	-4.85612800	-2.06779800
H	-1.11435700	-4.10735800	-2.93161200
H	-0.86640200	-4.87302400	-1.33763100
N	-1.44373600	1.32735800	0.76807900
C	-1.59342000	2.63152200	0.35983300
C	-1.72232800	1.02716700	2.02664800
C	-1.27386600	3.02703400	-0.96062300
C	-2.07230200	3.59868400	1.29699600
C	-2.19060000	2.01305400	2.93039800
H	-1.57760900	0.00089500	2.34051900
C	-1.43128600	4.33867900	-1.33871100
H	-0.90234800	2.28459400	-1.65944600
C	-2.23488000	4.94178600	0.88427000
N	-2.37202400	3.26715500	2.58321500
H	-2.41507600	1.73191100	3.95603000
C	-1.92092600	5.30631700	-0.41310900
H	-1.18081200	4.65140400	-2.34617600
H	-2.60217800	5.66094000	1.60686800
C	-2.09034000	6.66405700	-0.83882600
N	-2.23355300	7.76177200	-1.19259000
N	1.29373300	0.56225000	0.04532800
C	2.21696100	0.77149800	-0.90990900
C	1.68813700	0.38427700	1.31747300
C	3.57806900	0.76447300	-0.63210000
H	1.86730500	0.91396400	-1.92481200

C	3.03233200	0.38450100	1.66985300
H	0.91445800	0.22404700	2.05823200
C	3.99933900	0.56437500	0.68027900
S	4.73899300	0.83972600	-2.03631600
C	3.37981200	0.08642100	3.10189500
H	5.06136600	0.55461400	0.90159500
O	4.06994500	1.78671400	-2.95520100
O	6.00148600	1.28609400	-1.41811900
O	4.71262700	-0.58134400	-2.47807300
F	4.65966700	0.36537200	3.38476300
F	3.16670600	-1.22135500	3.38486400
F	2.59594400	0.79530700	3.95087300

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C	-1.99421000	-2.38419700	-1.89165700
C	-3.02423800	-3.05035500	-2.56762100
C	-4.23524900	-2.40277100	-2.80606900
C	-4.42748000	-1.09784600	-2.35724900
C	-3.39254700	-0.44270600	-1.68562600
H	-2.88503800	-4.07340800	-2.89953300
H	-5.36861100	-0.58631700	-2.53619700
H	-3.55428400	0.58200400	-1.36462700
C	-2.15142700	-1.05453300	-1.44791900
H	-2.44438100	-2.39085300	0.33337500
Pd	-0.62915700	0.03736400	-0.69388400
O	0.59112600	-0.58856300	-2.20491000
C	1.67590600	-1.26037200	-2.05818700
O	2.01547500	-1.89820000	-1.02110500
Ag	0.59677400	-2.27084800	0.54664100
O	-0.86452800	-2.89500300	2.09584600
C	-2.05405500	-3.22439200	2.04092800
O	-2.88036000	-2.89535000	1.06378300
C	-2.70383300	-4.05194600	3.11156300
H	-3.70949600	-3.68253000	3.32681700
H	-2.80122300	-5.08098000	2.74580800
H	-2.08453600	-4.05133200	4.00866300
C	2.62914100	-1.23696000	-3.22279800
H	3.12650800	-2.20540800	-3.31698000
H	2.11088700	-0.97133600	-4.14588500
H	3.40248000	-0.48027000	-3.01277900
H	-5.02709300	-2.92618000	-3.33348700
O	-0.81828400	-3.02780900	-1.57159500
C	-0.35139000	-4.06647100	-2.43063900

H	-0.90888100	-4.99818700	-2.27734900
H	-0.42663100	-3.75761900	-3.47851400
H	0.69574700	-4.21931700	-2.16579500
N	-1.83594100	0.95016300	0.71376900
C	-2.31399300	2.21611700	0.47422500
C	-2.08216300	0.40718400	1.89568900
C	-2.06808000	2.86652900	-0.75851800
C	-3.06653100	2.88027200	1.49232900
C	-2.82658100	1.09343200	2.88553200
H	-1.68160200	-0.58081800	2.08263800
C	-2.55596800	4.13276300	-0.97274700
H	-1.49042200	2.35151900	-1.51990000
C	-3.56373600	4.18203700	1.24895200
N	-3.31699200	2.29809800	2.69729000
H	-3.00874800	0.61603200	3.84512900
C	-3.31356600	4.79824200	0.03578300
H	-2.36734900	4.64047100	-1.91196000
H	-4.13277400	4.67030800	2.03125300
C	-3.82053100	6.11417000	-0.21869800
N	-4.23540200	7.17837200	-0.43318900
N	1.09669700	1.04429200	0.13522300
C	2.04490100	1.53610400	-0.68194600
C	1.45345400	0.62204500	1.36008300
C	3.38722900	1.58487100	-0.32040500
H	1.73401400	1.87386700	-1.66336500
C	2.77723700	0.61865100	1.78464900
H	0.66119700	0.26823300	2.01048300
C	3.76786100	1.09961400	0.92911700
S	4.61245500	2.12947000	-1.55593000
C	3.07912300	-0.02765600	3.10508000
H	4.81621600	1.11242200	1.20787100
O	3.86487200	3.15309900	-2.31884000
O	5.73946300	2.60348400	-0.72961300
O	4.85677400	0.85821900	-2.28945600
F	4.33168700	0.19730800	3.51925800
F	2.90870000	-1.37808600	3.02162200
F	2.22929000	0.39664500	4.07113900

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Pd	-0.67826100	-0.81493000	0.63526700
O	-2.04315100	-0.40079300	2.09374200
C	-2.94716100	0.51348100	2.01781500
O	-3.32138700	1.09317000	0.96311900

Ag	-3.08132400	-0.05888000	-0.84297500
O	-2.56789100	-1.97496400	-1.70875400
C	-2.16397900	-2.85488700	-0.88994700
O	-1.49294400	-2.62475200	0.17876600
C	-2.49131900	-4.30009600	-1.17122700
H	-1.89722200	-4.97070100	-0.55002100
H	-3.55454800	-4.46173100	-0.96018200
H	-2.33376500	-4.51143900	-2.23211000
C	-3.61545900	0.88854600	3.31918500
H	-4.61120100	0.43152500	3.34081400
H	-3.04596800	0.53493000	4.17917100
H	-3.75165300	1.97210800	3.36066500
N	0.84639700	-1.26669500	-0.68929200
C	2.13754600	-1.44650300	-0.25713500
C	0.60023200	-1.32398000	-1.99195100
C	2.45976000	-1.50566600	1.11856300
C	3.17433000	-1.59517800	-1.23411800
C	1.64777700	-1.50333400	-2.92740700
H	-0.43170900	-1.23174500	-2.31084200
C	3.76716300	-1.66462800	1.51034600
H	1.66377000	-1.46219700	1.85279800
C	4.51612200	-1.74140800	-0.80800300
N	2.90729000	-1.61014700	-2.56642600
H	1.41708700	-1.53973300	-3.98876600
C	4.81042500	-1.76786300	0.54321000
H	4.02130800	-1.72508800	2.56280000
H	5.28672400	-1.84149400	-1.56346300
C	6.16334200	-1.91314500	0.98991500
N	7.25604000	-2.02416000	1.36909100
N	0.20753700	0.95903100	1.20597000
C	0.47588400	1.99121100	0.34272200
C	0.53842400	1.09569900	2.48338600
C	0.07885800	1.95308800	-1.01371800
C	1.16058400	3.14439200	0.84595800
C	1.20265200	2.25567100	2.94821600
H	0.27746700	0.28661000	3.15553600
C	0.37237500	3.00577800	-1.84605900
H	-0.47845200	1.09938500	-1.37826700
C	1.46266400	4.21341100	-0.03177200
N	1.52333300	3.25083300	2.15085000
H	1.47187600	2.33647500	3.99789600
C	1.07974800	4.14470200	-1.35882900
H	0.06203500	2.98759400	-2.88502000
H	1.98702000	5.07323000	0.36862200

C	1.37825000	5.21732500	-2.25948400
N	1.61557000	6.07620000	-3.00520100
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-1 1			
C	0.86007600	1.77436200	-0.03669100
C	0.97326500	0.38055900	-0.02544300
C	-0.19408600	-0.37347500	0.00047900
C	-1.41863500	0.29751200	0.03419500
C	-1.42349400	1.69463800	0.03790600
N	-0.30822900	2.43216900	-0.00121800
H	-0.12562500	-1.45594200	-0.01325600
H	1.76375300	2.37541300	-0.09120900
H	-2.36490300	2.23842500	0.07543200
S	2.60338900	-0.42611400	0.00314700
O	2.97014300	-0.39243300	1.44114800
O	2.32361200	-1.78136200	-0.53693600
O	3.43028500	0.44516100	-0.86929200
C	-2.70711800	-0.46102100	0.00265400
F	-2.61823200	-1.65296100	0.63586000
F	-3.11556900	-0.73020300	-1.26480700
F	-3.72200100	0.22631500	0.58775100
Pre_TS3°			
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C	2.82189700	-0.48177500	2.11541400
C	3.29011400	-1.78687400	2.33965800
C	2.50729200	-2.66623200	3.07818900
C	1.25219200	-2.30365300	3.60877800
C	0.77685600	-1.02834500	3.39012700
H	4.26050300	-2.09697500	1.97452300
H	0.68770000	-3.01534100	4.20053400
H	-0.15640000	-0.69563700	3.83452100
C	1.51527800	-0.10869000	2.58151900
H	1.34069600	0.95384000	2.71483300
Pd	0.31719800	-0.37704200	0.69411700
O	0.64567400	-2.37809100	0.58216200
C	1.60386200	-2.91946600	-0.08488000
O	2.45357300	-2.31807800	-0.78537500
Ag	2.34922700	-0.33519500	-1.55912200
O	1.89385100	1.49713400	-2.54392100
C	2.76161200	2.37583000	-2.13802400
O	3.54744600	2.16827400	-1.19605500
C	2.74342700	3.69763300	-2.88050900

H	3.41680400	4.41571900	-2.41009400
H	3.05774500	3.53402800	-3.91678500
H	1.72521700	4.09917300	-2.91553900
C	1.69182800	-4.42427200	0.00976400
H	2.72212200	-4.70991200	0.24019200
H	1.00988700	-4.81925100	0.76302200
H	1.44681100	-4.85514700	-0.96697000
H	2.88962800	-3.66550500	3.26642300
O	3.50415200	0.48841000	1.51452100
C	4.79677700	0.21254800	0.93429500
H	5.51853600	-0.00311800	1.72743300
H	4.72474600	-0.62750100	0.23743200
H	5.05499800	1.11712900	0.39071000
N	-0.02483300	1.64809200	0.76614300
C	-1.26982000	2.19515700	0.96554300
C	0.98915400	2.44703300	0.46355100
C	-2.37722600	1.40294600	1.34341700
C	-1.43152600	3.60490000	0.78320900
C	0.78843100	3.84225400	0.30358300
H	1.97338900	2.01302100	0.31535100
C	-3.61006700	1.98694000	1.51449800
H	-2.24234000	0.33947700	1.50257600
C	-2.71046800	4.18365500	0.95886400
N	-0.38778800	4.41018800	0.44385100
H	1.63664100	4.46711300	0.03940500
C	-3.78523800	3.38731400	1.31458700
H	-4.46504000	1.38786500	1.80789500
H	-2.81534600	5.25223400	0.81137100
C	-5.08601500	3.95992100	1.49239400
N	-6.14817000	4.40804800	1.63779200
N	-1.03648300	-0.49966000	-0.92858400
C	-2.11716300	-1.34816700	-0.87811100
C	-0.88705300	0.27958200	-1.99133500
C	-2.36094500	-2.18312900	0.23848700
C	-3.03329200	-1.35746700	-1.97901900
C	-1.81147400	0.23166900	-3.06602900
H	-0.03054000	0.94699400	-2.03760200
C	-3.47067000	-2.99381700	0.25863200
H	-1.65578400	-2.19656100	1.05967300
C	-4.16557900	-2.20532800	-1.93827900
N	-2.85828300	-0.56160000	-3.06784500
H	-1.65285100	0.87276600	-3.92890800
C	-4.38412700	-3.01079700	-0.83548500
H	-3.66251200	-3.63690000	1.11050100

H	-4.84383900	-2.19502100	-2.78350800
C	-5.52883200	-3.86970700	-0.77654100
N	-6.45279600	-4.57128900	-0.71079800
TS3°			
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C	2.61650100	-0.28707700	2.17778900
C	2.92387000	-0.18872000	3.53819500
C	2.31714800	0.80186200	4.30725100
C	1.42852100	1.72500000	3.73959400
C	1.13139800	1.62295300	2.39136100
H	3.62614000	-0.86887600	4.00380400
H	0.98977800	2.50886100	4.34794600
H	0.46477700	2.35433400	1.94666900
C	1.70112500	0.62044600	1.55292100
H	2.41707000	1.21792300	0.58835000
Pd	0.27151600	-0.14165300	0.22035900
O	0.46968500	-2.00411800	1.03918200
C	0.95427400	-2.98870500	0.37384500
O	1.58755100	-2.90654500	-0.71133300
Ag	2.58712800	-1.08973700	-1.27061100
O	3.58524700	0.68851000	-1.87019900
C	3.84157900	1.69370100	-1.13981600
O	3.24625200	1.99932300	-0.05356000
C	4.93913700	2.62635600	-1.59718100
H	4.78799200	3.63072500	-1.19800600
H	5.89476200	2.24631200	-1.21637200
H	4.99649300	2.64062000	-2.68751400
C	0.69813300	-4.35402200	0.97026600
H	1.28029900	-5.11587500	0.45126900
H	0.94032400	-4.34835600	2.03675300
H	-0.36841300	-4.58892700	0.88113800
H	2.55706500	0.86474500	5.36470600
O	3.20883200	-1.18266500	1.35897400
C	4.16652000	-2.10750800	1.88676000
H	5.02945000	-1.57903600	2.30352200
H	3.70728900	-2.74284700	2.65070300
H	4.47823400	-2.71696400	1.03903800
N	-0.13889500	1.71669900	-0.59006000
C	-1.23873100	2.43783100	-0.18807700
C	0.58169600	2.18032200	-1.60063600
C	-2.06010900	1.99734400	0.87557300
C	-1.55426200	3.65532200	-0.86949900
C	0.24314400	3.39429400	-2.24879600

H	1.43985600	1.59961100	-1.91583900
C	-3.15932400	2.73498000	1.24467200
H	-1.80588500	1.07962800	1.39346000
C	-2.68950900	4.40078000	-0.47207300
N	-0.79558100	4.11876900	-1.89938000
H	0.85956400	3.75093600	-3.06979200
C	-3.48218200	3.94744100	0.56747800
H	-3.79406400	2.40389600	2.05912800
H	-2.91191400	5.31980900	-1.00166400
C	-4.63596900	4.69032400	0.97801900
N	-5.57567900	5.28065000	1.32246300
N	-1.22893700	-0.97174100	-1.06869300
C	-2.35658500	-1.58620900	-0.58723000
C	-1.05772700	-0.91660000	-2.37972700
C	-2.59511900	-1.70558700	0.80358100
C	-3.30850300	-2.11399500	-1.51776700
C	-2.01017900	-1.45901400	-3.27663300
H	-0.15481700	-0.44161900	-2.74754300
C	-3.74365900	-2.31326500	1.24925800
H	-1.85045500	-1.34619800	1.50276200
C	-4.48678500	-2.73224300	-1.03539700
N	-3.11475600	-2.03861200	-2.86172800
H	-1.83743900	-1.40099500	-4.34811400
C	-4.70306600	-2.82807900	0.32723100
H	-3.93283100	-2.41508900	2.31223600
H	-5.19632500	-3.12119400	-1.75635100
C	-5.89003000	-3.45141400	0.83164300
N	-6.84758800	-3.95332800	1.25765000

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C	2.73759300	-0.31045500	2.00577300
C	3.57766300	0.13873100	3.03280100
C	3.32854600	1.35860000	3.66051000
C	2.25050100	2.14242100	3.25947900
C	1.41701600	1.68797000	2.23478500
H	4.42913200	-0.45498700	3.34304900
H	2.05098200	3.09566900	3.73859800
H	0.57497100	2.30862300	1.94845500
C	1.62628800	0.45820700	1.58795100
H	3.25719000	1.18021200	0.32887200
Pd	0.19306800	-0.19100600	0.31737400
O	0.21562400	-2.06121900	1.14201600
C	0.58997400	-3.08512800	0.47130600

O	1.19971600	-3.06581700	-0.63304400
Ag	2.39305900	-1.33734700	-1.16003400
O	3.68275800	0.29426300	-1.87448800
C	4.26662600	1.23874800	-1.32369600
O	3.97195700	1.69576500	-0.12197300
C	5.39301600	1.97354700	-1.98538600
H	5.30881400	3.04823800	-1.80597600
H	6.33721300	1.63955600	-1.53859800
H	5.40878400	1.75281500	-3.05267300
C	0.25472800	-4.42167500	1.09481100
H	0.50220900	-5.23696900	0.41465800
H	0.82266800	-4.53473700	2.02461700
H	-0.80663800	-4.45514400	1.35721400
H	3.98798200	1.69317700	4.45501400
O	2.99326300	-1.47904100	1.32564900
C	3.93781900	-2.40637100	1.86185400
H	4.95950600	-2.01364000	1.80989600
H	3.68765300	-2.65473000	2.89840100
H	3.85776200	-3.29726300	1.23783800
N	-0.03699100	1.69309900	-0.52026700
C	-1.10131200	2.48621200	-0.16397900
C	0.74496000	2.10776400	-1.50693700
C	-1.97118100	2.11489800	0.88796000
C	-1.32749800	3.70810900	-0.87335800
C	0.49888200	3.32684000	-2.18385400
H	1.57739500	1.47361900	-1.78507700
C	-3.03582400	2.91985500	1.21372400
H	-1.77770000	1.19714100	1.43218400
C	-2.43089900	4.52197600	-0.52284100
N	-0.51180000	4.11195600	-1.88419900
H	1.16097400	3.63717000	-2.98826600
C	-3.27444700	4.13305300	0.50248000
H	-3.70638700	2.64358400	2.01982000
H	-2.58801400	5.44151900	-1.07444000
C	-4.39633700	4.94621100	0.86547300
N	-5.31109700	5.59492900	1.16972500
N	-1.41915600	-0.90010100	-0.98896000
C	-2.58920400	-1.42350300	-0.50269300
C	-1.26140700	-0.85116600	-2.30086400
C	-2.82153800	-1.53077400	0.89080600
C	-3.59205100	-1.86569300	-1.42370800
C	-2.26331100	-1.30718400	-3.19232300
H	-0.32714200	-0.44680200	-2.67658400
C	-4.01105700	-2.04420200	1.34734900

H	-2.04168100	-1.23807400	1.58281000
C	-4.81163300	-2.38795200	-0.93094900
N	-3.40764200	-1.79755100	-2.76994600
H	-2.09829900	-1.25569100	-4.26550900
C	-5.01959400	-2.47319900	0.43377700
H	-4.19624800	-2.13604400	2.41196200
H	-5.55911800	-2.71348600	-1.64495300
C	-6.24864400	-2.99938400	0.94826600
N	-7.24038800	-3.42269200	1.38146000

Pd₃(OAc)₆

0 1

Pd	0.00000000	1.83699200	0.00000000
C	2.27374300	1.24863400	1.86564600
O	1.60141200	2.11330500	1.23022300
O	2.29462200	-0.00437400	1.66782100
C	0.05552200	-2.59343600	-1.86564600
O	-1.02947000	-2.44351600	-1.23022300
O	1.15109900	-1.98501400	-1.66782100
C	0.05889200	-3.63939500	-2.95803600
H	0.79532500	-3.38371500	-3.72235600
H	0.34390200	-4.60131700	-2.51622700
H	-0.93684800	-3.73811500	-3.39383400
C	3.18125500	1.76869500	2.95803600
H	2.76887900	2.68039100	3.39383400
H	3.32804600	1.00308600	3.72235600
H	4.15680800	2.00283100	2.51622700
Pd	-1.59088200	-0.91849600	0.00000000
C	-0.05552200	-2.59343600	1.86564600
O	1.02947000	-2.44351600	1.23022300
O	-1.15109900	-1.98501400	1.66782100
C	2.21822000	1.34480200	-1.86564600
O	1.14352300	1.98938800	-1.66782100
O	2.63088200	0.33021100	-1.23022300
C	3.12236300	1.87070000	-2.95803600
H	3.70572600	1.05772400	-3.39383400
H	2.53272100	2.38062900	-3.72235600
H	3.81290600	2.59848600	-2.51622700
C	-0.05889200	-3.63939500	2.95803600
H	0.93684800	-3.73811500	3.39383400
H	-0.79532500	-3.38371500	3.72235600
H	-0.34390200	-4.60131700	2.51622700
Pd	1.59088200	-0.91849600	0.00000000
C	-2.27374300	1.24863400	-1.86564600

O	-1.60141200	2.11330500	-1.23022300
O	-2.29462200	-0.00437400	-1.66782100
C	-3.18125500	1.76869500	-2.95803600
H	-2.76887900	2.68039100	-3.39383400
H	-3.32804600	1.00308600	-3.72235600
H	-4.15680800	2.00283100	-2.51622700
C	-2.21822000	1.34480200	1.86564600
O	-1.14352300	1.98938800	1.66782100
O	-2.63088200	0.33021100	1.23022300
C	-3.12236300	1.87070000	2.95803600
H	-3.81290600	2.59848600	2.51622700
H	-3.70572600	1.05772400	3.39383400
H	-2.53272100	2.38062900	3.72235600

Ag₂(OAc)₄

0 1

C	-2.67638300	-0.00002500	-0.00461700
O	-2.11179300	1.13864700	-0.00663400
O	-2.11179000	-1.13869200	-0.00664400
O	2.11179000	1.13869200	-0.00662400
O	2.11179300	-1.13864700	-0.00663200
C	2.67638300	0.00002500	-0.00460300
C	4.19247000	-0.00000400	0.03964600
H	4.50889400	-0.00079900	1.08940200
H	4.58956700	-0.89834700	-0.43664200
H	4.58961400	0.89898100	-0.43537800
C	-4.19247000	0.00000300	0.03962600
H	-4.58956600	0.89835500	-0.43664900
H	-4.58961200	-0.89897300	-0.43541500
H	-4.50889900	0.00078000	1.08938100
Ag	0.00000600	-1.38713200	-0.00684300
Ag	-0.00000600	1.38713200	-0.00683200

(HOAc)₂

0 1

C	-1.92185400	0.05576800	0.00001700
O	-1.24565900	1.08404800	-0.00000300
O	-1.41970000	-1.16630100	0.00017500
H	-0.41469500	-1.12640100	0.00032600
H	0.41469800	1.12636300	0.00015000
O	1.24567600	-1.08406600	0.00005900
C	1.92184700	-0.05576900	0.00007000
O	1.41969700	1.16629600	0.00008000
C	3.42847000	-0.07504500	-0.00001700

H	3.80384000	0.45453700	0.88164200
H	3.78729600	-1.10427400	-0.00017200
H	3.80378300	0.45480900	-0.88153200
C	-3.42847700	0.07507000	-0.00034100
H	-3.80362400	-0.45485000	-0.88189200
H	-3.80402200	-0.45444300	0.88128100
H	-3.78729900	1.10430100	-0.00066300

L7

01

C	0.14765800	-1.99275100	0.00000000
C	-1.08578300	-1.38988800	0.00000000
C	-1.18897400	0.02421900	0.00000000
C	0.00000000	0.81668400	0.00000000
C	1.26264300	0.18158200	0.00000000
C	1.33422300	-1.20134700	0.00000000
H	0.23836200	-3.07350800	0.00000000
H	-2.00386500	-1.96765500	0.00000000
H	2.15491400	0.79730300	0.00000000
C	-1.26037800	2.71006500	0.00000000
C	-2.44543500	1.92084600	0.00000000
H	-1.33000500	3.79634800	0.00000000
H	-3.42061000	2.40466500	0.00000000
N	-0.05701400	2.18111600	0.00000000
N	-2.42340600	0.60577600	0.00000000
C	2.61028400	-1.85368300	0.00000000
N	3.63981600	-2.39425000	0.00000000

L8

01

C	0.91391100	1.72726600	-0.02316100
C	0.98291300	0.34383800	-0.02223900
C	-0.20633400	-0.38521200	-0.01989800
C	-1.43641300	0.28235600	0.00425100
C	-1.46471900	1.66478300	0.01655000
N	-0.29167100	2.33886000	-0.00026800
H	-0.15418500	-1.46989500	-0.05355000
H	1.80858500	2.33871300	-0.05853800
H	-2.37543800	2.24691300	0.03160200
H	-0.32033200	3.35437100	-0.00361200
S	2.63289600	-0.46335000	0.00337000
O	2.76953600	-0.74832300	1.44508200
O	2.40680500	-1.62605500	-0.87439100
O	3.48793300	0.61915300	-0.52944700

C	-2.72939900	-0.49909400	0.00069400
F	-2.77877600	-1.33808800	1.04684600
F	-2.83717300	-1.22976100	-1.12042700
F	-3.79707500	0.32447900	0.06968500

Anisole

0 1

C	0.03608700	1.06137600	-0.00022600
C	-1.33154500	1.35203900	-0.00001900
C	-2.28032800	0.33321600	0.00013600
C	-1.85147600	-0.99839500	0.00016200
C	-0.49597200	-1.30398000	-0.00004600
C	0.45483300	-0.27362100	-0.00023500
H	0.75516300	1.87195400	-0.00039900
H	-1.64886800	2.39136100	-0.00003900
H	-3.34007700	0.56920000	0.00024500
H	-2.57934200	-1.80515100	0.00029400
H	-0.14478500	-2.33085400	-0.00004000
O	1.76036700	-0.67517000	-0.00028700
C	2.76201300	0.32686900	0.00035200
H	2.69838500	0.96064600	0.89492600
H	3.71645900	-0.20237800	0.00014700
H	2.69846000	0.96155600	-0.89359000

Pre_TS1^m

0 1

C	-3.76223000	0.39351800	1.45756400
C	-4.47940300	1.53980600	1.11695700
C	-3.92404700	2.83013300	1.33096600
C	-2.63763700	2.96305500	1.78972900
C	-1.84229800	1.80702800	2.04215500
H	-0.91168200	1.91503300	2.59095600
C	-2.44552200	0.52506000	1.92320000
H	-1.93205800	-0.37598700	2.24700300
Pd	-0.94595200	1.11914800	0.02365800
O	-2.44851100	1.92524400	-1.03197600
C	-3.12356600	1.24368500	-1.90222500
O	-3.07819600	0.01311400	-2.07223700
Ag	-2.33404000	-1.61156900	-0.67334400
O	-3.29463300	-2.93764400	0.76260900
C	-2.59300000	-3.09927200	1.82213500
O	-1.52122800	-2.50116200	2.07807500
C	-3.13440700	-4.11752000	2.81775400
H	-2.64908200	-4.00866600	3.78974800

H	-4.21861600	-4.01450300	2.91937100
H	-2.93818400	-5.12588300	2.43510200
C	-4.08702000	2.08764700	-2.71233300
H	-4.46925100	1.51096200	-3.55582500
H	-4.92111800	2.38215800	-2.06489800
H	-3.59599000	2.99876600	-3.06320600
H	-4.53498700	3.69319600	1.08962300
N	0.73284700	0.45717200	1.01658200
C	1.86287800	1.24000900	1.06038800
C	0.78390200	-0.77032300	1.51045600
C	1.88072300	2.54235800	0.50862000
C	3.04395900	0.70598100	1.65857100
C	1.97804800	-1.25746000	2.10689300
H	-0.10685600	-1.39640600	1.46449100
C	3.03908700	3.28126100	0.53821200
H	0.98347100	2.93036700	0.03876000
C	4.22318200	1.48473300	1.68154300
N	3.07971500	-0.54820800	2.18844200
H	1.98981700	-2.26735700	2.50573800
C	4.22340100	2.75137400	1.12566400
H	3.06761600	4.27281300	0.10079000
H	5.11284100	1.05000700	2.12169400
C	5.42101500	3.53721700	1.12613000
N	6.38788400	4.18229100	1.12688800
N	4.34410600	0.85616100	-1.80592500
C	3.06004700	0.73902900	-2.15434800
C	4.89935300	-0.15884900	-1.13380100
C	2.29052700	-0.38622500	-1.84186900
H	2.61455000	1.57729400	-2.68240000
C	4.20843800	-1.32264800	-0.78792700
H	5.93777500	-0.03103100	-0.83976700
C	2.87027600	-1.44697800	-1.15752400
S	0.55214500	-0.43286300	-2.28647000
C	4.90375800	-2.40652900	-0.01203800
H	2.28167100	-2.31826800	-0.89614200
O	0.44969300	-0.51002200	-3.74087300
O	-0.01246900	-1.54723800	-1.47775600
O	0.05410000	0.94336200	-1.78353600
F	5.63619300	-3.20527500	-0.81449700
F	4.01971100	-3.19411300	0.63983300
F	5.74510500	-1.88308200	0.90531900
H	-4.17436100	-0.60049800	1.34240900
H	-2.21112000	3.94935700	1.94241600
O	-5.70481900	1.52752100	0.56160700

C	-6.26754100	0.25926500	0.20353900
H	-6.45656900	-0.35048800	1.09358900
H	-7.21037400	0.48886700	-0.29233600
H	-5.60214700	-0.27823200	-0.48028800

TS1^m

0 1

C	-3.78084000	1.29426200	0.44972300
C	-4.65788400	2.37089300	0.53388700
C	-4.15572500	3.64734000	0.84643300
C	-2.79731800	3.83794700	1.08226700
C	-1.91678900	2.76042600	0.99698900
H	-0.86183900	2.91293000	1.20206400
C	-2.39063700	1.46632800	0.67926300
H	-2.03474800	0.60612700	1.61826200
Pd	-1.12632900	0.41162300	-0.62168300
O	-2.63666500	0.28379900	-1.97768200
C	-3.16974500	-0.83314600	-2.31283300
O	-3.12405500	-1.91048500	-1.66806700
Ag	-2.16502400	-2.13277800	0.26547700
O	-1.92458400	-2.09170400	2.41770100
C	-1.95461100	-1.10104000	3.19876800
O	-1.87239100	0.12926600	2.86675100
C	-2.08929300	-1.37843500	4.68378500
H	-1.51411500	-0.65223900	5.26306600
H	-3.14349100	-1.26811200	4.96425000
H	-1.77340700	-2.39766900	4.91325900
C	-3.91162700	-0.81781100	-3.63205400
H	-4.68790300	-1.58525500	-3.64155100
H	-4.33538300	0.16925800	-3.82961000
H	-3.19016300	-1.04383600	-4.42586700
H	-4.85836300	4.47277600	0.90577200
N	0.54900100	0.62367100	0.56208500
C	1.50480100	1.56161900	0.25471100
C	0.79372700	-0.22289600	1.54831700
C	1.33544500	2.44971400	-0.83308300
C	2.70159700	1.60944300	1.03252700
C	1.98362000	-0.13090800	2.31370700
H	0.06823700	-0.99935700	1.73677800
C	2.33331300	3.33953100	-1.14919500
H	0.42479100	2.39333100	-1.42038900
C	3.71173000	2.53876400	0.69500700
N	2.91555900	0.76278900	2.07685500
H	2.15161300	-0.83598000	3.12263100

C	3.53417700	3.38610200	-0.38368200
H	2.22207400	4.00992600	-1.99388600
H	4.61975200	2.54382100	1.28633900
C	4.56317800	4.31494400	-0.74500500
N	5.39189700	5.07439200	-1.04079200
N	4.16089100	0.31929500	-2.05156000
C	2.96133900	-0.22849200	-2.26750900
C	4.86245200	-0.11965900	-1.00038900
C	2.42343300	-1.22751300	-1.44878200
H	2.38851000	0.15437300	-3.10689500
C	4.40710300	-1.11676400	-0.13449000
H	5.82256500	0.35908200	-0.82729800
C	3.16063600	-1.69542100	-0.36893400
S	0.76952000	-1.85535000	-1.77141200
C	5.24409100	-1.53408300	1.04164400
H	2.75172300	-2.45612300	0.28552400
O	0.83583600	-2.74787800	-2.92740900
O	0.31792900	-2.43669800	-0.47578600
O	0.00712300	-0.56379600	-2.10966700
F	6.16188700	-2.46226000	0.70287700
F	4.48272400	-2.06652900	2.02576800
F	5.91228600	-0.48316300	1.56288300
H	-4.14564800	0.30184800	0.21854000
H	-2.43134700	4.82967100	1.33189000
O	-6.00034800	2.29837600	0.32968500
C	-6.54207800	1.03964200	-0.04741500
H	-6.39547100	0.28871500	0.73980900
H	-7.60974100	1.20614200	-0.19512500
H	-6.09355600	0.67684100	-0.98099200

Pro 1^m

0 1

C	-3.55251500	1.36603300	0.37411400
C	-4.41493600	2.06625100	1.23464400
C	-3.92414000	3.12587500	2.00956100
C	-2.58476600	3.47978300	1.90686100
C	-1.71411500	2.79056900	1.05134600
H	-0.67557000	3.09944700	0.99162800
C	-2.19432000	1.73297700	0.27175900
H	-2.91009500	0.20016800	2.05100700
Pd	-1.01776100	0.70550600	-0.95491400
O	-2.45378100	0.70454400	-2.40476400
C	-3.30953300	-0.22142100	-2.60640400
O	-3.52939600	-1.22075700	-1.86909300

Ag	-2.14422700	-1.84123900	-0.27078200
O	-2.17436900	-2.08579500	2.05985100
C	-2.52787400	-1.42114100	3.03254700
O	-2.89478800	-0.14894400	2.97778600
C	-2.58160800	-1.98129500	4.42748400
H	-2.05304200	-1.31914400	5.11961500
H	-3.62566500	-2.02831700	4.75590000
H	-2.14646600	-2.98038100	4.44310200
C	-4.12595800	-0.08190200	-3.87532600
H	-5.09073100	-0.58078300	-3.76415600
H	-4.25929000	0.96955500	-4.13785100
H	-3.57760700	-0.57046600	-4.68920000
H	-4.60485300	3.64967600	2.67193000
N	0.54551800	0.80045000	0.39242100
C	1.64483200	1.58118600	0.13582800
C	0.55786900	0.04422600	1.47808700
C	1.70876000	2.38984000	-1.02353600
C	2.74217700	1.55917900	1.05002800
C	1.65971500	0.04992100	2.36745600
H	-0.29651100	-0.59409100	1.65100600
C	2.83562900	3.13349700	-1.27490600
H	0.86596700	2.39071500	-1.70762600
C	3.89145600	2.33484100	0.77340400
N	2.72753300	0.79035500	2.17266200
H	1.64321700	-0.59058400	3.24492200
C	3.94012900	3.10506500	-0.37399200
H	2.90204400	3.74365600	-2.16849500
H	4.72190200	2.28393800	1.46758300
C	5.11057100	3.87569500	-0.67112900
N	6.05651200	4.50556800	-0.91502900
N	4.41676200	-0.05290000	-1.78372700
C	3.19745600	-0.48860200	-2.11461200
C	4.93361400	-0.47730000	-0.62537400
C	2.45751400	-1.35985800	-1.30849700
H	2.77572700	-0.11523900	-3.04324300
C	4.26714700	-1.34766100	0.24077200
H	5.91456500	-0.08918100	-0.36410900
C	3.00171000	-1.81231400	-0.11319700
S	0.80290600	-1.84728700	-1.81065100
C	4.90389700	-1.74933800	1.54097800
H	2.43418400	-2.47286800	0.53098800
O	0.92033100	-2.85032400	-2.86869900
O	0.16630200	-2.31396100	-0.52808600
O	0.19765600	-0.54222000	-2.29842700

F	5.76574700	-2.77499100	1.38523000
F	3.97725700	-2.14107800	2.44642400
F	5.59782200	-0.72454200	2.08163000
H	-3.93963700	0.56882900	-0.24431200
H	-2.20548400	4.30594600	2.50281800
O	-5.73342300	1.76807700	1.38971400
C	-6.27419600	0.71065200	0.61040200
H	-5.78639100	-0.24659600	0.83749700
H	-7.33012000	0.65264600	0.87802500
H	-6.17801400	0.91226700	-0.46370600

Pre_TS1P

0 1

C	-3.54469400	0.00035700	1.65438000
C	-4.62505500	0.71780900	1.20592300
C	-4.52478900	2.12203700	1.03848000
C	-3.35812900	2.80775200	1.40293000
C	-2.26308700	2.07950600	1.86683600
H	-5.56274800	0.23816200	0.94643500
H	-3.28597700	3.88304100	1.30428700
H	-1.37732300	2.60709900	2.20915100
C	-2.31117100	0.66005600	1.94827800
H	-1.58482900	0.10567200	2.53008700
Pd	-1.17655500	0.70537200	-0.00783000
O	-2.78180400	1.21369300	-1.10340100
C	-3.35664700	0.38481600	-1.91004700
O	-3.14927300	-0.84092200	-1.97978600
Ag	-2.18108400	-2.20480700	-0.56069200
O	-2.02955300	-3.85815200	0.80425900
C	-1.75824400	-3.49060600	1.99765400
O	-1.55431300	-2.30375100	2.35735400
C	-1.65978600	-4.61434700	3.02170100
H	-1.63462500	-4.21553100	4.03778800
H	-2.49937400	-5.30577200	2.90659500
H	-0.74268400	-5.18670400	2.83864600
C	-4.38622300	1.03016800	-2.81340100
H	-4.89226900	0.27116300	-3.41103100
H	-5.11343900	1.57666300	-2.20367000
H	-3.89148900	1.75137300	-3.47183700
N	0.58559800	0.40817500	1.01342800
C	1.57780300	1.35920400	0.97456300
C	0.83178300	-0.75349300	1.59890000
C	1.38322900	2.60619400	0.33470700
C	2.83368600	1.06368800	1.58545000

C	2.09825400	-1.00700900	2.18965400
H	0.02010500	-1.48025900	1.64937100
C	2.40636600	3.52258400	0.29918200
H	0.43551400	2.80807700	-0.15169200
C	3.87204200	2.02171100	1.53806400
N	3.07563100	-0.13041200	2.19351300
H	2.27954100	-1.97089100	2.65628600
C	3.66361000	3.23223000	0.90263800
H	2.27295500	4.47336900	-0.20440900
H	4.82354200	1.76462700	1.98827700
C	4.71736800	4.19984700	0.83284600
N	5.56546200	4.99268400	0.77665700
N	4.14393100	1.26846000	-1.91353200
C	2.89237100	0.93154900	-2.23702100
C	4.85101700	0.39822100	-1.18345200
C	2.30614600	-0.27465400	-1.84163300
H	2.32184300	1.65345700	-2.81453400
C	4.34902500	-0.83235200	-0.75325600
H	5.85811300	0.70390100	-0.91197700
C	3.04531800	-1.18524800	-1.09717200
S	0.59433600	-0.62682100	-2.25649000
C	5.20554500	-1.73876500	0.08584000
H	2.59831400	-2.11806300	-0.77480200
O	0.49845600	-0.76424100	-3.70800000
O	0.22610400	-1.78184700	-1.40275300
O	-0.12132700	0.66934600	-1.79622300
F	6.07493000	-2.44471800	-0.66541700
F	4.45887600	-2.62750500	0.77820600
F	5.93363100	-1.02992600	0.97629600
O	-5.61995800	2.70984100	0.52445300
C	-5.58927200	4.11272600	0.26672500
H	-4.78198100	4.36121600	-0.43137500
H	-6.55343800	4.35035600	-0.18250700
H	-5.46709200	4.68109100	1.19586800
H	-3.58628000	-1.07275100	1.79950200

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C	-3.98267700	0.66884000	0.14476000
C	-4.98152000	1.61759900	0.15887400
C	-4.65754500	2.97301000	0.37349300
C	-3.32245100	3.35442600	0.59824900
C	-2.33497300	2.38004300	0.59438500
H	-6.02336100	1.35644900	0.00436500

H	-3.06123700	4.39034600	0.77802300
H	-1.31204100	2.68797100	0.79185900
C	-2.61528100	1.00395700	0.38228500
H	-2.25177800	0.33582200	1.48559900
Pd	-1.19036500	0.00472200	-0.74939000
O	-2.61699600	-0.50496600	-2.10606800
C	-2.95264400	-1.72550500	-2.31712900
O	-2.77088400	-2.69797000	-1.54332000
Ag	-1.89478400	-2.52595400	0.43607000
O	-1.76869000	-2.19082100	2.57793600
C	-1.99552200	-1.14115500	3.23749000
O	-2.09921500	0.04362100	2.76783100
C	-2.15500100	-1.27099300	4.74008200
H	-1.74056600	-0.39654000	5.24738100
H	-3.22534100	-1.31628800	4.97359200
H	-1.68317400	-2.18826100	5.09688900
C	-3.61800700	-1.98575500	-3.65125800
H	-4.26881200	-2.85979100	-3.58781600
H	-4.17502600	-1.10841400	-3.98676300
H	-2.82961400	-2.19173800	-4.38462700
N	0.38435200	0.59683000	0.44765400
C	1.22598000	1.60618600	0.04636000
C	0.68833500	-0.07161800	1.54790500
C	0.99506900	2.31436600	-1.15622500
C	2.36639700	1.91734200	0.84725600
C	1.81935100	0.27720900	2.32867300
H	0.05827500	-0.90441100	1.82096200
C	1.88035000	3.28526300	-1.55740500
H	0.13056400	2.05492000	-1.75880500
C	3.26023200	2.92554100	0.41988400
N	2.63835400	1.25006600	2.00248400
H	2.03807300	-0.28792200	3.23014700
C	3.02482600	3.59533100	-0.76719900
H	1.72404300	3.81878900	-2.48813800
H	4.13007200	3.13063400	1.03270900
C	3.93679300	4.60478000	-1.21605300
N	4.66860100	5.42985300	-1.58323000
N	4.13001200	0.47141600	-2.00414400
C	3.02724100	-0.26346200	-2.17745000
C	4.83519200	0.27551500	-0.88428000
C	2.59233700	-1.21386100	-1.24743200
H	2.44682000	-0.07706300	-3.07614500
C	4.47922300	-0.65444600	0.09539700
H	5.71258900	0.90274000	-0.75073400

C	3.33517400	-1.42830600	-0.09383400
S	1.05654700	-2.10741900	-1.52948800
C	5.30912600	-0.79290800	1.34012500
H	3.00281600	-2.14732700	0.64555800
O	1.30584600	-3.13120400	-2.54348100
O	0.63076000	-2.56933500	-0.17723200
O	0.14311700	-0.99693700	-2.06447400
F	6.36251900	-1.61471500	1.15518100
F	4.58396200	-1.29858800	2.36469000
F	5.79996500	0.40149800	1.73538700
O	-5.69869300	3.82717600	0.35874700
C	-5.45265300	5.21636900	0.55894100
H	-4.79306600	5.61684000	-0.21964100
H	-6.42765600	5.70008900	0.49684400
H	-5.01269400	5.40138600	1.54589900
H	-4.24533200	-0.37093800	-0.02026100

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C	-3.78857700	0.77156200	-0.55040000
C	-4.77701400	1.67037000	-0.14936500
C	-4.45039900	3.00174500	0.13932500
C	-3.12016700	3.41907300	0.02011900
C	-2.13523600	2.50608300	-0.37369600
H	-5.81213800	1.35668300	-0.05584700
H	-2.83598800	4.44410600	0.22879900
H	-1.11551400	2.86863500	-0.46032300
C	-2.43895400	1.16928500	-0.66541600
H	-3.18336900	0.60890100	1.57207900
Pd	-1.04778300	-0.14144000	-1.21485600
O	-2.33891600	-1.04435500	-2.50688700
C	-2.99371000	-2.11544800	-2.26351900
O	-3.13324400	-2.67745300	-1.14533900
Ag	-1.97419500	-2.11741500	0.63382100
O	-2.12568500	-1.19007200	2.75590600
C	-2.70134100	-0.21945200	3.24706400
O	-3.25031500	0.76088800	2.54605600
C	-2.85088300	-0.02820500	4.73113700
H	-2.56435600	0.98900100	5.01292900
H	-3.90430700	-0.15838300	5.00305000
H	-2.24460100	-0.76175800	5.26231400
C	-3.65200100	-2.75634300	-3.46823800
H	-4.53136700	-3.32637700	-3.16227000
H	-3.91647700	-2.00322600	-4.21322300

H	-2.93218500	-3.44824300	-3.92094100
N	0.38913000	0.79648300	-0.06367500
C	1.42385500	1.47715500	-0.65611200
C	0.39959100	0.67085800	1.25369900
C	1.49055200	1.61997600	-2.06232600
C	2.45108400	2.03418400	0.16547200
C	1.43140600	1.23906700	2.03975900
H	-0.39922100	0.10187100	1.70732000
C	2.55454600	2.27583900	-2.63142500
H	0.70252100	1.18612900	-2.66966200
C	3.53549200	2.70877800	-0.44102300
N	2.43287600	1.91312100	1.52084300
H	1.41685900	1.10799900	3.11825300
C	3.58977900	2.82261400	-1.81802500
H	2.62437600	2.37607000	-3.70860200
H	4.31572000	3.10225700	0.19971900
C	4.69680600	3.48636800	-2.43929400
N	5.59057300	4.02824400	-2.94782800
N	4.51371800	-0.51648900	-1.46466400
C	3.37057000	-1.20142900	-1.56508400
C	4.97686000	-0.25987500	-0.23620300
C	2.65536600	-1.65382200	-0.45129100
H	2.98900900	-1.37958600	-2.56622400
C	4.33057400	-0.67407100	0.93091900
H	5.89341800	0.32128300	-0.17813100
C	3.14572700	-1.40028500	0.82329900
S	1.09605000	-2.51737600	-0.68191400
C	4.89888400	-0.31471000	2.27430800
H	2.59400400	-1.72787800	1.69607000
O	1.38976600	-3.88232100	-1.11829600
O	0.41425100	-2.38100400	0.65136200
O	0.40963500	-1.69051100	-1.75719300
F	5.86044600	-1.17698300	2.66315900
F	3.94483400	-0.32249100	3.23453500
F	5.45233900	0.91723400	2.25676400
O	-5.48444100	3.80011200	0.52639400
C	-5.20399500	5.16153000	0.80538400
H	-4.79843400	5.67715400	-0.07498200
H	-6.15758300	5.61393700	1.08190400
H	-4.49748600	5.26411900	1.63984000
H	-4.07846100	-0.24663000	-0.78092500

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C	-2.78080100	-2.91523200	1.49084300
C	-1.62378900	-2.19022500	1.10624500
C	-2.97820000	-0.56955600	0.14753400
C	-4.11965800	-1.33395500	0.54442200
C	-5.41420200	-0.86242400	0.22640000
H	-6.26730400	-1.45584100	0.53355500
C	-5.56192500	0.32998900	-0.46002100
C	-4.41851400	1.08773400	-0.84632100
C	-3.15037400	0.64710400	-0.55285900
H	-4.55991000	2.02485700	-1.37307300
H	-2.28175400	1.24257200	-0.81407000
H	-0.62162400	-2.56055100	1.28675300
H	-2.66487000	-3.85237000	2.02931900
N	-1.72611700	-1.04364900	0.45317200
N	-4.00118300	-2.50939300	1.22317700
Pd	0.00004100	-0.00001000	0.00001400
O	1.05711200	-2.87003200	-0.01052700
C	0.88107200	-2.47445300	-1.17025200
O	0.44417900	-1.29075800	-1.50184500
C	1.20174000	-3.35378400	-2.36724600
H	2.11855700	-2.98983000	-2.84526000
H	1.35328800	-4.38530800	-2.04470200
H	0.40174900	-3.29970800	-3.11095800
O	-1.05740400	2.86985200	0.01042300
C	-0.88131900	2.47435900	1.17016700
O	-0.44416100	1.29077200	1.50182500
C	-1.20222600	3.35364300	2.36713000
H	-0.40187400	3.30031600	3.11051400
H	-1.35468300	4.38499800	2.04447700
H	-2.11854000	2.98904300	2.84560800
C	-6.87081600	0.81522200	-0.78474600
N	-7.92830700	1.21692100	-1.05269300
C	2.78081000	2.91565000	-1.49011800
C	1.62382000	2.19047700	-1.10576400
C	2.97827900	0.56955000	-0.14755400
C	4.11971000	1.33414000	-0.54415100
C	5.41426900	0.86256000	-0.22626200
H	6.26734800	1.45612500	-0.53319600
C	5.56203400	-0.33008300	0.45975100
C	4.41864800	-1.08801000	0.84576400
C	3.15049200	-0.64734100	0.55242300
H	4.56007100	-2.02530700	1.37220000
H	2.28190100	-1.24294500	0.81343500
H	0.62164200	2.56083000	-1.28616300

H	2.66484800	3.85298300	-2.02824700
N	1.72617900	1.04369600	-0.45305600
N	4.00120300	2.50979500	-1.22252600
C	6.87094000	-0.81536300	0.78434600
N	7.92844500	-1.21710200	1.05218000

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C	1.96315600	-2.19246100	2.53459400
C	0.82746900	-1.53805500	1.99724100
C	2.18561800	-0.43479000	0.48042000
C	3.31129200	-1.11023600	1.04894600
C	4.60103500	-0.87108500	0.52019500
H	5.44387400	-1.38887100	0.96250800
C	4.75418300	0.00464600	-0.53954400
C	3.62344000	0.66391200	-1.10588400
C	2.36112800	0.44685500	-0.61111500
H	3.77022200	1.34053100	-1.94020700
H	1.50212000	0.94965000	-1.04084700
H	-0.16955900	-1.72950800	2.37591500
H	1.83875000	-2.89368600	3.35622100
N	0.94322400	-0.67333100	1.00537800
N	3.18035800	-1.98615800	2.08362400
Pd	-0.78079500	0.22909700	0.26964600
O	0.36376600	2.85448000	-1.00138100
C	0.28600900	2.94278800	0.22679900
O	-0.16312500	2.01001500	1.02605600
C	0.75683000	4.18382800	0.97026600
H	0.03362300	4.47415900	1.73761700
H	1.70232200	3.96066300	1.47815200
H	0.91457400	5.00269100	0.26616600
C	-4.30505000	-0.54102100	-0.75281500
C	-3.74838600	-0.59244100	-2.04181200
C	-2.72627600	0.25981100	-2.43496400
C	-2.24153700	1.21288400	-1.52564500
C	-2.76608800	1.26777100	-0.21043700
C	-3.82279400	0.38587100	0.16208400
H	-5.10008500	-1.22718300	-0.48903200
H	-4.13769800	-1.32486200	-2.74400300
H	-2.30136000	0.19659300	-3.43021700
H	-1.48613100	1.93488600	-1.81781400
H	-2.56259600	2.11291700	0.43858200
O	-4.28661700	0.55153800	1.42262300
C	-5.28577200	-0.34598600	1.88996600

H	-5.48495300	-0.05819300	2.92259500
H	-6.20685900	-0.25622900	1.30072800
H	-4.92878200	-1.38248000	1.85643400
C	6.05838700	0.25421600	-1.07913500
N	7.11351600	0.46363800	-1.52015100
O	-1.43731900	-1.61775700	-0.18854900
C	-0.79612500	-2.17819000	-1.18887100
O	0.15252700	-1.67579000	-1.78631900
C	-1.37266400	-3.53280200	-1.57131100
H	-1.59459400	-4.13044900	-0.68233100
H	-2.31624300	-3.37647200	-2.10676300
H	-0.67674000	-4.06461200	-2.22271000

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C	-2.57186000	-2.55128700	1.91946900
C	-1.35231400	-2.03826800	1.41182000
C	-2.51510600	-0.39742900	0.27732500
C	-3.73127600	-0.94109300	0.80042600
C	-4.96415900	-0.34535300	0.44787500
H	-5.87628100	-0.76948800	0.85098800
C	-4.97831100	0.75183000	-0.39547500
C	-3.76109600	1.28716800	-0.90988700
C	-2.55026300	0.72448800	-0.58446900
H	-3.79931500	2.15292100	-1.56178000
H	-1.61967900	1.15218900	-0.95133900
H	-0.40152100	-2.49873400	1.65578800
H	-2.55794800	-3.41665400	2.57794800
N	-1.32406400	-0.98499800	0.61497300
N	-3.73996600	-2.02348400	1.62807500
Pd	0.59497500	-0.35102400	-0.05934700
O	2.74037800	-1.96223900	-1.80204800
C	1.68493500	-2.63556800	-1.59607900
O	0.68085100	-2.22289800	-0.93774500
C	1.62862500	-4.04142500	-2.14843500
H	2.18235500	-4.70495600	-1.47415700
H	0.59605000	-4.38719200	-2.21627100
H	2.11332700	-4.07881800	-3.12656900
C	4.35337200	1.39451600	0.68686900
C	4.38827300	2.41548800	-0.26588700
C	3.52404700	2.41899700	-1.36386900
C	2.60058100	1.38764100	-1.49676200
C	2.52205000	0.33372700	-0.55883600
C	3.41824800	0.36549600	0.54398300

H	5.03894400	1.42357900	1.52532400
H	5.11124700	3.21829400	-0.14547800
H	3.56790800	3.21977000	-2.09509300
H	1.91512100	1.38353800	-2.33718200
H	2.60784600	-0.84225000	-1.19501500
O	3.30047500	-0.66793400	1.41792800
C	4.17092600	-0.71145100	2.53949400
H	3.90397300	-1.61534700	3.08841400
H	5.22133800	-0.76989400	2.22806500
H	4.02847000	0.16378800	3.18479600
C	-6.22462200	1.36047700	-0.75731300
N	-7.23144800	1.85930300	-1.05596500
O	0.45682500	1.37598900	0.98506600
C	0.24282900	2.47778900	0.31628800
O	-0.09607000	2.54413500	-0.86838700
C	0.49410800	3.73069600	1.14068000
H	0.19544600	3.58764400	2.18240900
H	1.57117700	3.93663300	1.12445400
H	-0.03255400	4.58129500	0.70324300

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C	2.53734200	2.57103800	1.98747000
C	1.33948800	1.91466900	1.60623900
C	2.55486100	0.44368300	0.31514300
C	3.74870900	1.12826500	0.70593600
C	4.99517800	0.68940800	0.20326800
H	5.89077200	1.21959000	0.50547400
C	5.04307400	-0.39686000	-0.65341100
C	3.84889300	-1.07995900	-1.02899100
C	2.62498500	-0.66922600	-0.55768800
H	3.91777300	-1.93738000	-1.68938800
H	1.71518000	-1.20945200	-0.81191200
H	0.37336200	2.24924000	1.97118700
H	2.49470800	3.42042200	2.66553700
N	1.34609200	0.87802600	0.78924400
N	3.71996700	2.19834500	1.55016700
Pd	-0.62703800	0.03565800	0.24536900
O	-2.36798200	1.21753500	-2.36864100
C	-1.57597000	2.10151100	-1.80358100
O	-0.89480900	1.88679400	-0.79202400
C	-1.55878600	3.43494600	-2.49291900
H	-2.54858700	3.89653800	-2.41078800
H	-0.80902400	4.08195600	-2.03809100

H	-1.34823600	3.29781700	-3.55780400
C	-4.87597800	-0.47988900	0.17056000
C	-5.06278200	-1.62961600	-0.60453900
C	-3.97263400	-2.29602500	-1.15298000
C	-2.67727700	-1.81449900	-0.91609300
C	-2.46091200	-0.66199500	-0.15057300
C	-3.58255100	0.00097500	0.39541600
H	-5.73888400	0.02386400	0.59102400
H	-6.07203600	-1.99457400	-0.77419800
H	-4.11696400	-3.18966400	-1.75326200
H	-1.81709000	-2.34513400	-1.31146900
H	-2.39614300	0.39168900	-1.80789400
O	-3.31453000	1.13724400	1.11906900
C	-4.40325600	1.81987400	1.71507300
H	-3.97000300	2.66670000	2.25012400
H	-5.11125300	2.19001600	0.96104700
H	-4.93986300	1.17752000	2.42513800
C	6.30306100	-0.84616900	-1.16852200
N	7.32096300	-1.21492400	-1.59244400
O	-0.29171800	-1.64376800	1.33375600
C	0.08381300	-2.70766700	0.68106700
O	0.35028000	-2.75566400	-0.52593900
C	0.14644800	-3.95148000	1.55482400
H	0.53228400	-3.71288400	2.54952400
H	-0.86955200	-4.34466900	1.67849500
H	0.76397600	-4.71499200	1.07753300

Int Pd2

0 1

Pd	1.45202400	-0.36506100	0.92865900
C	2.13775200	-2.99270100	0.00747500
O	1.34622400	-1.97690600	-0.27738900
O	3.06978600	-2.95757400	0.80236700
C	1.77049300	-4.24799300	-0.76924900
H	1.66557700	-4.02191400	-1.83531000
H	2.53388800	-5.01378200	-0.62385200
H	0.80578000	-4.62839900	-0.41367400
Pd	-1.45195200	0.36018900	0.93071100
C	-2.13785600	2.99218900	0.02219500
O	-3.06952200	2.95347000	0.81734300
O	-1.34676200	1.97754500	-0.26799500
C	-1.77043100	4.25121800	-0.74836800
H	-1.66364700	4.03012000	-1.81527600
H	-2.53458500	5.01580000	-0.60059800

H	-0.80658800	4.63073600	-0.38947200
C	0.49604900	1.77492700	2.70128900
O	1.52180300	1.29812800	2.11906900
O	-0.71492000	1.47849700	2.47980600
C	0.75561300	2.78399000	3.79688000
H	-0.11009700	3.43507400	3.92838500
H	0.93266200	2.24130700	4.73268900
H	1.65136800	3.36623600	3.57049300
C	-0.49526700	-1.78798300	2.69322500
O	0.71565000	-1.49046400	2.47290600
O	-1.52115100	-1.30851200	2.11343700
C	-0.75462200	-2.80223700	3.78404800
H	-0.93171600	-2.26400500	4.72241600
H	-1.65032300	-3.38350700	3.55496300
H	0.11116700	-3.45384600	3.91244700
C	2.16595800	2.49797500	-2.16834000
C	1.59553500	1.68333700	-1.15715500
C	3.62045200	0.56378700	-0.94718600
C	4.15752800	1.41228600	-1.96639700
C	5.50569100	1.25231000	-2.36113800
H	5.89614300	1.90470500	-3.13327300
C	6.28675600	0.28043300	-1.76093500
C	5.74121900	-0.56229400	-0.74963000
C	4.43435700	-0.42477300	-0.34611300
H	6.36975500	-1.32289400	-0.29997900
H	4.01329400	-1.09124600	0.40178100
H	0.56290900	1.82061200	-0.84475500
H	1.55201000	3.26250800	-2.63807900
N	2.31123000	0.73864100	-0.56714200
N	3.41056000	2.37793600	-2.57104800
C	7.65371600	0.11222500	-2.15768300
N	8.76297100	-0.03106900	-2.47455600
C	-2.16683500	-2.48800200	-2.17967300
C	-1.59628700	-1.67857100	-1.16438700
C	-3.62079600	-0.55924600	-0.94932200
C	-4.15799700	-1.40249000	-1.97282000
C	-5.50601000	-1.24002000	-2.36705400
H	-5.89655500	-1.88842200	-3.14249800
C	-6.28682400	-0.27082900	-1.76220100
C	-5.74118700	0.56662400	-0.74657700
C	-4.43446500	0.42659100	-0.34347600
H	-6.36953300	1.32519800	-0.29325500
H	-4.01332700	1.08914400	0.40784400
H	-0.56375900	-1.81774000	-0.85250300

H	-1.55312800	-3.25052700	-2.65297700
N	-2.31170200	-0.73645100	-0.56992700
N	-3.41129200	-2.36544700	-2.58207200
C	-7.65363000	-0.10010500	-2.15840500
N	-8.76275800	0.04518800	-2.47481600

Pre_TS^{Pd2}

0 1

Pd	-0.66778100	0.89125700	0.20845400
C	-1.45515600	2.44727300	-2.01874300
O	-0.42746800	1.74550600	-1.59628900
O	-2.52037700	2.57204600	-1.42039500
C	-1.18810700	3.12352400	-3.35583400
H	-0.78405400	2.40613000	-4.07689100
H	-2.10912900	3.56458800	-3.74051300
H	-0.43936400	3.91237300	-3.22125000
Pd	1.81722400	-0.69175200	0.27008000
C	-0.27318500	-1.03245200	2.40985400
O	-0.93599500	-0.01130600	2.03759500
O	0.71450000	-1.55539900	1.81905300
C	-0.69931000	-1.67220200	3.71394000
H	-0.50540300	-2.74634000	3.68683600
H	-0.09940600	-1.24010300	4.52317900
H	-1.75302500	-1.47195400	3.91651300
C	1.74938100	1.92183900	1.60164900
O	0.64496700	2.21850300	1.05876300
O	2.37298500	0.81545100	1.52790200
C	2.42370300	3.01496400	2.39932700
H	3.13795100	2.58926300	3.10617000
H	2.96620300	3.66247000	1.70134800
H	1.67799100	3.62103600	2.91804200
C	-2.69847900	-2.19761600	-1.93950300
C	-1.73202200	-1.30443200	-1.41128500
C	-3.40608200	-0.23756800	-0.20735100
C	-4.34686400	-1.16261900	-0.75475200
C	-5.70891100	-1.06538900	-0.38540500
H	-6.40939000	-1.77507100	-0.80944300
C	-6.11116200	-0.07912900	0.49680100
C	-5.16553900	0.84432000	1.03235600
C	-3.83967500	0.76932600	0.68583700
H	-5.51082800	1.61584500	1.71121900
H	-3.11697200	1.47996800	1.06515200
H	-0.67791000	-1.41227800	-1.63961800
H	-2.37926800	-2.97510000	-2.62912600

N	-2.08643100	-0.35137100	-0.56597200
N	-3.97319100	-2.14114800	-1.62634300
C	-7.48828500	0.02372300	0.87989700
N	-8.60251000	0.11251500	1.19965200
O	2.80398800	-3.50025000	-0.22850000
C	1.78056400	-3.29850500	-0.86617100
O	1.17542400	-2.12734300	-0.96796800
C	1.05207400	-4.38926400	-1.63689600
H	0.82647500	-4.05833100	-2.65594800
H	1.66120900	-5.29410700	-1.66528500
H	0.10058300	-4.60949600	-1.13922700
C	4.79329800	1.54719400	-0.38802200
C	3.77851200	2.37236000	-0.91441000
C	2.66997300	1.85002400	-1.55411100
C	2.56417400	0.44975700	-1.70578400
C	3.56997700	-0.40158300	-1.18681500
C	4.69376600	0.16960200	-0.51815900
H	5.64282200	2.00005900	0.10837800
H	3.87861000	3.44917400	-0.80614000
H	1.87144700	2.47998000	-1.92244600
H	1.77211400	0.03629000	-2.31941500
H	3.62855700	-1.45329500	-1.44263800
O	5.60441100	-0.72589800	-0.07949000
C	6.69910100	-0.24640800	0.68961300
H	7.26691200	-1.13032800	0.98027400
H	7.33770700	0.42295500	0.09916200
H	6.34677800	0.27814700	1.58615900

TS^{Pd2}

0 1

Pd	0.73195300	-0.65562300	0.53916900
C	1.27060600	-2.73518700	-1.31932700
O	0.71748100	-1.54426700	-1.26685400
O	1.95851500	-3.23874200	-0.43437500
C	0.95535900	-3.46670000	-2.61537600
H	1.04565400	-2.79514800	-3.47401200
H	1.61983900	-4.32471200	-2.73158200
H	-0.08167700	-3.82132600	-2.58088700
Pd	-1.83261000	0.85986200	0.38492500
C	0.10494200	1.31113800	2.64990000
O	0.78136800	0.26631600	2.37394100
O	-0.77093400	1.85673600	1.92115400
C	0.37512900	1.94469200	3.99797100
H	0.31222200	3.03265800	3.91915700

H	-0.40303900	1.61500200	4.69605100
H	1.34852600	1.64041500	4.38624700
C	-1.74702100	-1.76399000	1.70956000
O	-0.60842500	-2.03952700	1.22907900
O	-2.34010600	-0.63914300	1.68525900
C	-2.50847400	-2.90448500	2.34500100
H	-3.11106900	-2.53872000	3.17945900
H	-3.18785500	-3.31227600	1.58723900
H	-1.82692900	-3.69104200	2.67223100
C	2.73642700	2.89817500	-0.76389100
C	1.77829900	1.91823900	-0.40226800
C	3.48440500	0.36480200	-0.15910000
C	4.42088600	1.38584500	-0.51673900
C	5.79973600	1.07594300	-0.55773800
H	6.49630200	1.86145400	-0.82613000
C	6.22379800	-0.20706900	-0.25937000
C	5.28132900	-1.22043100	0.08178700
C	3.93599600	-0.94361000	0.13420700
H	5.63730100	-2.22227400	0.29471000
H	3.21239300	-1.72616400	0.35030000
H	0.72203500	2.15751700	-0.35879500
H	2.39966600	3.90406200	-1.00301100
N	2.14934600	0.68306600	-0.10401500
N	4.02658400	2.65466300	-0.81814100
C	7.62040800	-0.52711600	-0.29946800
N	8.75159600	-0.79365200	-0.32965700
O	-2.50148400	1.74826500	-2.61866100
C	-1.73051300	2.56154800	-2.02803900
O	-1.33208300	2.44083000	-0.82652900
C	-1.20719000	3.74865600	-2.80305900
H	-0.18057600	3.53234900	-3.12187100
H	-1.81831900	3.93009900	-3.68796000
H	-1.18380700	4.63308000	-2.16196300
C	-5.20229200	-1.34029400	-0.78938700
C	-4.61296700	-2.50462200	-1.28637300
C	-3.25809200	-2.54696600	-1.63097900
C	-2.48012100	-1.40642000	-1.46197200
C	-3.03143000	-0.20560400	-0.95709500
C	-4.41198600	-0.19920100	-0.61489600
H	-6.25500900	-1.34150200	-0.53289400
H	-5.23001700	-3.39103200	-1.41008300
H	-2.82028600	-3.46035900	-2.02218000
H	-1.42303100	-1.42791700	-1.70992800
H	-2.75790300	0.80147200	-1.79853700

O	-4.88290600	0.97423800	-0.12838700
C	-6.25464800	1.06549900	0.23287600
H	-6.39861600	2.08545400	0.59008000
H	-6.90656400	0.88249100	-0.63018600
H	-6.49865600	0.35819500	1.03452700

Pro^{Pd2}

0 1

Pd	-0.59134400	-1.20136100	0.58428900
C	-0.99984800	0.95870500	2.54834400
O	-0.57655800	0.68659200	1.32222800
O	-1.59530100	0.15896100	3.25494100
C	-0.69041200	2.38403700	2.96698300
H	-1.20133900	3.08488400	2.29694000
H	-1.02297800	2.55053000	3.99255800
H	0.38359000	2.57597400	2.87989100
Pd	1.93329100	-0.50497700	-0.63170400
C	0.36019300	-3.11264400	-1.33543100
O	-0.44595400	-3.01265000	-0.33966500
O	1.06309600	-2.18335700	-1.81037500
C	0.45125200	-4.48486800	-1.96540300
H	0.55086900	-4.39091700	-3.04957000
H	1.35808400	-4.97308900	-1.58977800
H	-0.41279200	-5.09944600	-1.70720900
C	1.93691700	-2.18314900	1.76110500
O	0.72373000	-1.87536000	1.99662200
O	2.61188100	-1.89378300	0.72898100
C	2.65518400	-2.93226200	2.86002500
H	3.47609500	-3.51884900	2.44328600
H	3.07710400	-2.19608000	3.55438400
H	1.96002000	-3.56802600	3.41134000
C	-2.50886200	0.03613600	-3.04050300
C	-1.64093100	-0.52690600	-2.07307000
C	-3.21010900	-0.07752400	-0.42422100
C	-4.05561200	0.48837800	-1.43036700
C	-5.31909300	1.00602800	-1.06224500
H	-5.94574300	1.43269300	-1.83652200
C	-5.72401000	0.95395600	0.25975300
C	-4.87836300	0.38004700	1.25340100
C	-3.64619300	-0.12915500	0.92038200
H	-5.21577500	0.35148000	2.28342700
H	-2.99562900	-0.54234200	1.68465700
H	-0.66848700	-0.92133200	-2.34290400
H	-2.19557300	0.06350700	-4.08128900

N	-1.98009700	-0.56631100	-0.79264400
N	-3.68313400	0.54499300	-2.73932800
C	-7.00267500	1.47880000	0.63895000
N	-8.03799000	1.90371500	0.95343600
O	0.03523500	2.32927000	-0.59912600
C	0.58670800	1.98354700	-1.73298300
O	1.19972100	0.93074700	-1.96880600
C	0.38796800	2.99693500	-2.82678000
H	-0.67519700	3.04685400	-3.08749600
H	0.68331600	3.98730000	-2.46820700
H	0.97311400	2.72030500	-3.70350600
C	4.40275600	2.77123400	0.51242300
C	4.11465800	2.94540000	1.86918900
C	3.20575100	2.10673100	2.50614800
C	2.57147500	1.09310000	1.77456800
C	2.83232500	0.91269400	0.41786000
C	3.77077100	1.75246500	-0.21122400
H	5.12469800	3.42304700	0.03339500
H	4.61412900	3.73673700	2.42119100
H	2.98782900	2.22838500	3.56377700
H	1.85571900	0.44816800	2.27081100
H	0.02952100	1.63699000	0.14193300
O	4.01342100	1.50674500	-1.53915100
C	4.98372800	2.29600100	-2.19963100
H	5.03196700	1.91712700	-3.22190100
H	4.69971400	3.35759600	-2.21829600
H	5.97109200	2.19988600	-1.72887600

Int 4

0 1

Pd	0.03442800	0.12042100	0.80754100
O	-1.61238200	0.90885600	1.67919000
C	-2.79298500	0.97301500	1.16855300
O	-3.14460100	0.62661500	0.02171600
Ag	-1.56185700	-0.12232600	-1.48054400
O	-1.26652700	-2.30310900	-0.69429300
C	-1.08548900	-2.53671400	0.52669100
O	-0.55970100	-1.74426500	1.39250900
C	-1.53549200	-3.87549300	1.08238100
H	-1.02568600	-4.10863600	2.01900100
H	-2.61362800	-3.82285500	1.27424400
H	-1.36611700	-4.66246200	0.34343000
C	-3.83661700	1.52404800	2.12767000
H	-4.75874300	1.75475500	1.59185800

H	-4.04378400	0.77318400	2.89828800
H	-3.45408100	2.41592300	2.63141500
O	0.59412900	1.97189200	0.13552000
C	0.41794400	2.27706700	-1.10127200
O	-0.12139900	1.57326300	-1.98840600
C	0.90925900	3.66203800	-1.48783700
H	1.65369200	4.03244200	-0.78034800
H	1.31625600	3.64304800	-2.50174700
H	0.05331600	4.34680900	-1.48313100
N	1.80274800	-0.61970700	0.04006400
C	1.81867500	-1.44378200	-1.02517700
C	2.96359300	-0.15470900	0.54180600
C	2.99825600	-1.81244500	-1.65584100
H	0.84850400	-1.80206500	-1.34734800
C	4.19376500	-0.47270600	-0.04814200
O	2.80820300	0.60084500	1.63520000
C	4.20050300	-1.30664400	-1.16056000
H	2.96679200	-2.47325800	-2.51400500
H	5.11731300	-0.08539400	0.36156000
C	3.94062600	1.27636100	2.17591300
H	5.14424800	-1.56533200	-1.63122700
H	3.55239600	1.87176200	3.00118100
H	4.68363400	0.56322000	2.55145100
H	4.39624700	1.93374300	1.42701600

Pre_TS4°

0 1

C	-2.03132000	1.16208800	1.51434400
C	-2.30604500	2.52668500	1.50081300
C	-1.31429200	3.43640100	1.89643900
C	-0.06052400	3.01462100	2.32109300
C	0.22789000	1.64092700	2.33740700
H	-3.28230400	2.88845100	1.20055400
H	0.68824100	3.73239800	2.63805700
H	1.16407300	1.28750500	2.75695800
C	-0.73352600	0.69747500	1.89594200
H	-0.64114800	-0.37242800	2.07123600
Pd	0.66594300	0.77888000	0.04534100
O	-0.33633400	2.27476800	-0.83367600
C	-1.34874200	2.05263800	-1.61264400
O	-1.86353600	0.95281700	-1.85426400
Ag	-1.10775800	-1.35848100	-1.21856700
O	-2.70836900	-2.38541400	-0.18249100
C	-2.36883200	-2.64331100	1.02393400

O	-1.22769800	-2.47730600	1.51401300
C	-3.48731000	-3.14251700	1.93143200
H	-3.09213500	-3.81291400	2.69894500
H	-3.92508900	-2.27247300	2.43658600
H	-4.27294800	-3.64039200	1.35799600
C	-1.93022300	3.32759300	-2.20339600
H	-2.48415200	3.85834900	-1.42030200
H	-1.13337100	3.99039300	-2.55119000
H	-2.60995800	3.08532500	-3.02217300
H	-1.54507100	4.49800800	1.87902200
O	-2.91080900	0.19496900	1.22464300
C	-4.10214100	0.51491600	0.50634300
H	-4.79548000	1.09009300	1.13264600
H	-3.85130300	1.06252000	-0.40629500
H	-4.53294100	-0.44969500	0.24227700
O	1.80287900	0.63905800	-1.66726300
C	1.60036300	-0.30314800	-2.51865600
O	0.73955800	-1.20437700	-2.45419600
C	2.51492800	-0.26452500	-3.73204300
H	2.74261300	-1.28255300	-4.05636900
H	1.98297900	0.23833600	-4.54779600
H	3.43280500	0.28855100	-3.52346800
N	1.96379500	-0.61333400	0.86465600
C	1.63562300	-1.91090500	1.02691000
C	3.24764500	-0.22146900	1.00111800
C	2.59809400	-2.87384000	1.30636900
H	0.57690100	-2.15737300	0.95063500
C	4.26839700	-1.13718600	1.26818200
C	3.92980900	-2.48022900	1.41464200
H	2.29305900	-3.90629000	1.42863200
H	5.29390300	-0.80652800	1.36850300
H	4.70797800	-3.20877500	1.62239900
O	3.41672900	1.10556100	0.87681300
C	4.74007700	1.61972800	0.74799600
H	5.30920400	1.48600100	1.67542900
H	5.26249100	1.13828000	-0.08559900
H	4.61772200	2.68241100	0.54169800

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C	-1.95860100	1.97661900	-0.02601600
C	-2.58925400	3.16524700	-0.40544800
C	-1.81103000	4.24594200	-0.82270900
C	-0.41653100	4.16719000	-0.84012300

C	0.19481400	2.97764700	-0.45573700
H	-3.66833900	3.26126200	-0.37836300
H	0.17707800	5.02212200	-1.15038400
H	1.27771900	2.91420800	-0.46473800
C	-0.54243200	1.83982200	-0.05542600
H	-0.16661000	1.35606900	1.16111800
Pd	0.27402500	0.04579100	-0.84875900
O	-1.39510700	-0.15069500	-2.00176400
C	-2.27278800	-1.07361000	-1.85548800
O	-2.39927900	-1.86100500	-0.88902400
Ag	-1.22232800	-1.53814700	0.99068100
O	-0.74437800	-0.67223800	2.96962600
C	-0.24572200	0.44556800	3.24312000
O	0.13746800	1.34857700	2.41613000
C	-0.01496200	0.79173700	4.70498100
H	1.05904700	0.91892900	4.88027300
H	-0.49593700	1.74660200	4.93855600
H	-0.40350600	0.00538000	5.35387400
C	-3.24169400	-1.19424900	-3.02060200
H	-3.53059400	-0.20340700	-3.38170100
H	-2.73764400	-1.71132000	-3.84493700
H	-4.12286600	-1.76824800	-2.72807200
H	-2.30632500	5.16566500	-1.12343800
O	-2.63562900	0.90109700	0.44336100
C	-4.05441300	0.88792800	0.39803800
H	-4.48243000	1.65388200	1.05632000
H	-4.41396800	1.04023400	-0.62669500
H	-4.34714800	-0.10353600	0.74343400
O	1.00879000	-1.68680100	-1.73654800
C	1.06621900	-2.74673600	-1.00447400
O	0.71474400	-2.83955700	0.19006900
C	1.59161700	-3.98163700	-1.72179500
H	2.10568200	-4.63645300	-1.01426000
H	0.73595100	-4.53151600	-2.13150600
H	2.25303600	-3.71187300	-2.54824600
N	2.09712900	0.19323100	0.12033200
C	2.31087500	-0.42969200	1.29410600
C	3.12902700	0.78117200	-0.51388100
C	3.56132500	-0.46804000	1.89448800
H	1.45269100	-0.91711300	1.73100300
C	4.41872700	0.79085300	0.02894100
C	4.62696000	0.15702800	1.24965100
H	3.68694600	-0.98370300	2.83911700
H	5.23399300	1.27526200	-0.49191200

H	5.62058100	0.14951600	1.68768400
O	2.78603700	1.34159400	-1.68551400
C	3.80260300	1.93216000	-2.49043700
H	4.26663400	2.78384000	-1.97908200
H	4.56778500	1.19481600	-2.75740500
H	3.29298800	2.27578900	-3.38986800

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C	-0.79587900	2.06606600	1.54474700
C	-0.90723800	3.09432600	2.48512800
C	-0.01156600	4.16148300	2.45993700
C	0.99970100	4.18802400	1.49878200
C	1.11257600	3.14287900	0.57869300
H	-1.69061300	3.05194100	3.23655600
H	1.70269500	5.01648300	1.46683400
H	1.90770600	3.16503100	-0.16138500
C	0.21888600	2.06150000	0.58092600
H	-1.44719500	-0.44617700	2.41983700
Pd	0.49213400	0.58387500	-0.71542300
O	-0.76902800	1.55337000	-2.03019900
C	-2.02392400	1.42530500	-2.20678800
O	-2.78390100	0.56673800	-1.68148300
Ag	-1.81392800	-1.12679600	-0.67672300
O	-2.87351600	-2.01939200	1.43918200
C	-1.91609700	-2.28736800	2.15609900
O	-1.18027400	-1.34944400	2.76360900
C	-1.40220500	-3.68171600	2.37964300
H	-0.70571000	-3.89217800	1.55780900
H	-0.87282000	-3.77025300	3.33071200
H	-2.22601100	-4.39520500	2.32346600
C	-2.65043900	2.45843000	-3.12737800
H	-2.79428000	3.38849900	-2.56478300
H	-1.98158300	2.67723500	-3.96325300
H	-3.61928700	2.11242100	-3.49174400
H	-0.10181000	4.96059400	3.19017200
O	-1.70483900	0.99924900	1.60238000
C	-3.08971200	1.34787200	1.42979400
H	-3.42713700	2.01927500	2.22625700
H	-3.23257200	1.80928500	0.45083300
H	-3.63833600	0.40672200	1.47323100
O	0.97765500	-1.16198200	-1.97356300
C	0.76162500	-2.32038200	-1.50390300
O	-0.17438300	-2.64188000	-0.70698200

C	1.75012900	-3.40934800	-1.88952600
H	2.61565100	-3.34135100	-1.21778500
H	1.30524400	-4.40076200	-1.78230400
H	2.10719200	-3.25771000	-2.91101200
N	1.99686300	-0.19786300	0.47674000
C	1.75698700	-1.02260900	1.51061800
C	3.26510700	0.00077100	0.06847700
C	2.77304100	-1.70194400	2.17008200
H	0.72188500	-1.13590000	1.79833100
C	4.34428800	-0.64951000	0.67879000
C	4.08510300	-1.51227400	1.73910200
H	2.53052200	-2.36061600	2.99566200
H	5.35640700	-0.48158000	0.33500700
H	4.90810200	-2.02757900	2.22528100
O	3.36905000	0.86380800	-0.95297900
C	4.64253100	1.06076000	-1.56135300
H	5.35184800	1.51102600	-0.85696800
H	5.04251000	0.11500300	-1.94344700
H	4.46242200	1.74463500	-2.38995200

L3

01

C	1.16631900	1.34704400	-0.00000200
C	2.20750300	0.42806800	-0.00000200
C	1.87846000	-0.93482100	-0.00001600
C	0.54597100	-1.31311800	0.00000400
C	-0.42322500	-0.29294600	0.00002900
N	-0.13261400	1.00387500	0.00000500
H	2.65826000	-1.69136100	-0.00002900
H	1.37035000	2.41624400	0.00000200
H	3.23957700	0.76216700	0.00001100
H	0.23344600	-2.35120700	0.00001500
O	-1.71691500	-0.68388000	0.00000200
C	-2.70166000	0.35057200	-0.00001200
H	-3.66218400	-0.16715500	-0.00000300
H	-2.60801500	0.98323500	0.88786600
H	-2.60802000	0.98320500	-0.88791300

TS1P_NHAc

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C	-3.77943500	-0.41877600	0.09236400
C	-4.96633700	0.28266500	0.06586200
C	-4.97202200	1.68313500	0.24547000
C	-3.76048000	2.36150800	0.48412600

C	-2.58269600	1.63297000	0.52435900
H	-5.90654600	-0.23895600	-0.10093700
H	-3.77087800	3.43087400	0.63441000
H	-1.66187500	2.17006400	0.73291300
C	-2.53371200	0.22426600	0.34036100
H	-2.03341400	-0.33076300	1.44814500
Pd	-0.90053300	-0.44425800	-0.75751200
O	-2.15337700	-1.30601500	-2.11000700
C	-2.18371300	-2.57502300	-2.29809900
O	-1.78958900	-3.46118300	-1.50024100
Ag	-0.99644600	-3.04850000	0.47937200
O	-0.97298700	-2.64898300	2.61248800
C	-1.45063900	-1.66765000	3.24341100
O	-1.83486200	-0.55632200	2.74262800
C	-1.58275700	-1.79307400	4.74923000
H	-1.39781700	-0.83078700	5.23240600
H	-2.61080000	-2.09287500	4.98473900
H	-0.90308100	-2.55744700	5.13020700
C	-2.74216700	-3.01251400	-3.63501900
H	-3.17558300	-4.01147800	-3.55827100
H	-3.47781100	-2.29511600	-4.00477300
H	-1.91090000	-3.04883500	-4.34882000
N	0.47753900	0.52948300	0.43120300
C	1.05823100	1.70151600	0.01020000
C	0.92017800	-0.02361900	1.54834200
C	0.67590700	2.31008800	-1.20805200
C	2.08548700	2.29093500	0.80816700
C	1.92781200	0.60082200	2.32583100
H	0.50384400	-0.97664600	1.83741900
C	1.31045800	3.45375000	-1.62829900
H	-0.09998300	1.84360700	-1.80636700
C	2.72047000	3.47169500	0.36029000
N	2.49649400	1.73235800	1.97962300
H	2.26517000	0.12396600	3.24159600
C	2.34425900	4.04087600	-0.84283300
H	1.03839600	3.91686400	-2.56997400
H	3.51214700	3.88926600	0.97108000
C	2.99974400	5.22441100	-1.31375000
N	3.52503600	6.18678000	-1.69971300
N	4.16989800	1.23616600	-2.00306200
C	3.27329100	0.25839300	-2.16438200
C	4.88782700	1.23817600	-0.87423800
C	3.06385500	-0.74607500	-1.21330600
H	2.67606400	0.28196600	-3.07106900

C	4.74939600	0.27345900	0.12655200
H	5.59099600	2.05761600	-0.75121000
C	3.82262300	-0.75286300	-0.05019700
S	1.78612500	-1.98296300	-1.48294000
C	5.57396000	0.36416600	1.37930100
H	3.66067900	-1.51297200	0.70487100
O	2.27819600	-2.93737400	-2.47567000
O	1.46906900	-2.50740700	-0.12376000
O	0.63970700	-1.13113600	-2.04470500
F	6.79542700	-0.18537700	1.21969300
F	4.97937500	-0.27866600	2.41106600
F	5.76035800	1.64936600	1.74926600
N	-6.20707200	2.32482400	0.18811200
H	-6.99771800	1.71726800	0.01541400
C	-6.49829000	3.67992100	0.31593500
C	-7.97755200	3.99113200	0.16575800
H	-8.58519800	3.39191500	0.85369600
H	-8.13177900	5.04939200	0.37666000
H	-8.31464300	3.77842600	-0.85589300
O	-5.65408300	4.53349800	0.51912200
H	-3.79828300	-1.49411700	-0.05065000

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C	-3.97389600	1.24394100	0.26083800
C	-4.84582600	2.31967600	0.29801900
C	-4.37239800	3.61941300	0.54829300
C	-3.00053800	3.80516000	0.78093800
C	-2.12883300	2.72500900	0.76028000
H	-5.90804100	2.16466500	0.12580600
H	-2.62471500	4.80543100	0.98102100
H	-1.07656500	2.89516400	0.96923100
C	-2.58309000	1.40567000	0.50118700
H	-2.26338300	0.61846300	1.51614500
Pd	-1.28566400	0.28214800	-0.69108100
O	-2.77400600	0.00512000	-2.04762700
C	-3.23639900	-1.16043500	-2.32209400
O	-3.15135500	-2.18834800	-1.60585900
Ag	-2.26129200	-2.22073100	0.37181600
O	-2.06856000	-2.00945600	2.51884400
C	-2.16253100	-0.96575300	3.22138300
O	-2.12543300	0.23900600	2.79940500
C	-2.32622500	-1.13894000	4.71937700
H	-1.83467800	-0.32499400	5.25716000

H	-3.39569400	-1.10132500	4.95841000
H	-1.93607700	-2.10777000	5.03681100
C	-3.93366900	-1.27410900	-3.66019400
H	-4.67542600	-2.07456300	-3.63565500
H	-4.39340300	-0.32466500	-3.94247900
H	-3.17634800	-1.52488000	-4.41213300
N	0.36237600	0.62875500	0.50179900
C	1.30407400	1.56124900	0.13917900
C	0.60440600	-0.13017100	1.55766900
C	1.13801400	2.35580300	-1.01920300
C	2.48197400	1.70021200	0.93435200
C	1.77577800	0.05030400	2.33592900
H	-0.10917800	-0.90450800	1.79492500
C	2.12119300	3.24296200	-1.38480100
H	0.24238100	2.22859200	-1.61852100
C	3.47767600	2.62447600	0.54403600
N	2.69221400	0.94486200	2.04724500
H	1.94195100	-0.58385600	3.20197600
C	3.30363500	3.37981800	-0.60151400
H	2.01322500	3.84121100	-2.28243200
H	4.37304400	2.69695500	1.15004400
C	4.31825800	4.30273000	-1.01492000
N	5.13495600	5.05741100	-1.35332700
N	4.03145600	0.22740800	-2.04026100
C	2.85179700	-0.37217400	-2.22695900
C	4.72599300	-0.09972900	-0.94473800
C	2.32768100	-1.31364300	-1.33464900
H	2.28333700	-0.07898400	-3.10459000
C	4.28326800	-1.03243300	-0.00365400
H	5.66909800	0.42011700	-0.79838600
C	3.05830700	-1.66598300	-0.20737500
S	0.69796900	-2.01555200	-1.62849700
C	5.11064500	-1.31943700	1.21739800
H	2.65936900	-2.38077700	0.50258500
O	0.81109000	-2.99526600	-2.70784700
O	0.24518500	-2.50576800	-0.29622200
O	-0.09655900	-0.77967600	-2.07884100
F	6.07609700	-2.22804100	0.97012700
F	4.35216600	-1.80712300	2.22619600
F	5.72098400	-0.20143100	1.66643300
H	-4.36057700	0.24871700	0.06640000
C	-5.32674500	4.78222400	0.60334400
H	-4.81722100	5.73032700	0.40697300
H	-6.13906400	4.66644200	-0.12140800

H	-5.78673100	4.85500700	1.59792700
TS1P_H			
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C	-3.91862700	1.77428600	0.42950200
C	-4.66271100	2.94217400	0.53308700
C	-4.02325300	4.14589900	0.85040200
C	-2.64589500	4.17758700	1.09026700
C	-1.90756300	3.00237500	1.00165800
H	-5.73546400	2.92459500	0.36418100
H	-2.15922300	5.11365000	1.34857600
H	-0.84351200	3.02824500	1.21754200
C	-2.51962500	1.76790900	0.66542400
H	-2.26453900	0.86432400	1.59173200
Pd	-1.35773800	0.57616700	-0.61354600
O	-2.87837700	0.55143800	-1.96088900
C	-3.45475400	-0.53976500	-2.31577700
O	-3.46890600	-1.62107400	-1.67780200
Ag	-2.59157200	-1.88016900	0.28601700
O	-2.35793100	-1.83560700	2.43528200
C	-2.32602400	-0.83285900	3.20111600
O	-2.15319200	0.38276600	2.85183600
C	-2.49797100	-1.07906700	4.68783100
H	-1.91350800	-0.36082800	5.26732000
H	-3.55459600	-0.93556100	4.94328400
H	-2.21851200	-2.10364800	4.94031200
C	-4.16373700	-0.48396200	-3.65104700
H	-4.98039300	-1.20769200	-3.67838200
H	-4.52872800	0.52437500	-3.85716200
H	-3.43669300	-0.75033800	-4.42713400
H	-4.60350700	5.06189800	0.92131600
N	0.33308600	0.66111200	0.56591400
C	1.36493600	1.51097300	0.24833400
C	0.50603700	-0.19361900	1.56041600
C	1.26962200	2.40071200	-0.84712100
C	2.56248800	1.46452400	1.02497900
C	1.70139600	-0.19682300	2.32297500
H	-0.28394900	-0.90188800	1.75878300
C	2.33825100	3.20112300	-1.17093100
H	0.35710300	2.41553000	-1.43405900
C	3.64701500	2.30239600	0.67888900
N	2.70551100	0.61219300	2.07673200
H	1.81034900	-0.90610800	3.13833700
C	3.53976800	3.15299700	-0.40646400

H	2.28286000	3.87125800	-2.02131500
H	4.55332700	2.23484700	1.26900600
C	4.64275700	3.98900300	-0.77606700
N	5.53203500	4.67373500	-1.07829600
N	3.90975000	0.04922900	-2.06507900
C	2.66893600	-0.40253200	-2.27006200
C	4.57859300	-0.43274400	-1.01143700
C	2.05606500	-1.34505300	-1.43734000
H	2.12508900	0.01526400	-3.11211000
C	4.04808700	-1.37914300	-0.13149600
H	5.57524800	-0.03144300	-0.84807200
C	2.75794900	-1.85781800	-0.35428900
S	0.35623100	-1.84395600	-1.74590200
C	4.85438200	-1.84764100	1.04680200
H	2.29181400	-2.57513800	0.31073400
O	0.34607200	-2.74510600	-2.89688700
O	-0.13020700	-2.37869100	-0.44362900
O	-0.30598000	-0.49868200	-2.08959000
F	5.70279200	-2.84149800	0.71368800
F	4.05851600	-2.31656300	2.03558600
F	5.59755800	-0.84348800	1.55934600
H	-4.41405800	0.84032800	0.18490600

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C	-3.97767000	0.73708400	0.22067300
C	-4.95986900	1.71567800	0.20531100
C	-4.58855300	3.04514500	0.43414600
C	-3.26389900	3.40298200	0.70144400
C	-2.29867500	2.40456300	0.72796000
H	-5.99873300	1.46873300	0.01628400
H	-3.00932300	4.44055300	0.88755000
H	-1.27483600	2.67976200	0.96288100
C	-2.61774600	1.04398700	0.48612600
H	-2.20481700	0.28883400	1.48555700
Pd	-1.18988300	0.04735500	-0.68770800
O	-2.63162700	-0.39785000	-2.04756100
C	-2.94983000	-1.61058300	-2.32817900
O	-2.75156800	-2.62084400	-1.61000300
Ag	-1.89866400	-2.54558300	0.38090600
O	-1.74405400	-2.29594100	2.52336300
C	-1.94850700	-1.25979100	3.21385100
O	-2.03233500	-0.06250700	2.77713300
C	-2.10200500	-1.43183800	4.71263200

H	-1.62566000	-2.35712200	5.04186900
H	-1.68998600	-0.57032100	5.24309800
H	-3.17144300	-1.48951200	4.94765800
C	-3.61284400	-1.80271700	-3.67402200
H	-4.25042200	-2.68853000	-3.66066100
H	-4.18269400	-0.91570700	-3.95853900
H	-2.82176300	-1.95424800	-4.41773100
N	0.40881400	0.58052800	0.50306700
C	1.24428300	1.60651700	0.13244900
C	0.73074000	-0.14091400	1.56400900
C	0.99422500	2.37052700	-1.03133500
C	2.40047100	1.87682800	0.92616600
C	1.87616500	0.16973400	2.33975100
H	0.10459600	-0.98577700	1.80755300
C	1.87646300	3.35589700	-1.40324500
H	0.11865500	2.14390300	-1.63083000
C	3.29077200	2.90051400	0.52931400
N	2.69089400	1.15555400	2.04340800
H	2.11017600	-0.43700700	3.20971200
C	3.03694300	3.62479000	-0.62134700
H	1.70499600	3.93277700	-2.30497100
H	4.17248100	3.07390100	1.13489200
C	3.94681500	4.64826800	-1.04169300
N	4.67857600	5.48316600	-1.38581100
N	4.10746800	0.55954300	-2.03043800
C	2.99798000	-0.16181900	-2.21528300
C	4.83235300	0.31191600	-0.93358100
C	2.57589100	-1.14950100	-1.31877300
H	2.40266700	0.06609100	-3.09449000
C	4.49015300	-0.65856200	0.01116700
H	5.71528400	0.92893000	-0.78953700
C	3.33880100	-1.41829900	-0.18988900
S	1.02990400	-2.02073200	-1.60776200
C	5.34240500	-0.85438300	1.23335300
H	3.01705900	-2.16784100	0.52339600
O	1.24080400	-2.98416600	-2.68642400
O	0.63007400	-2.54978700	-0.27402700
O	0.10763700	-0.87498600	-2.06217800
F	6.39059700	-1.66725400	0.99170700
F	4.63431100	-1.40567400	2.24622700
F	5.84106000	0.32077000	1.67317000
H	-4.26026400	-0.29566800	0.04514300
Cl	-5.81395500	4.28731700	0.40278700

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C	-4.01436000	0.92456900	0.26403700
C	-4.94676500	1.94958500	0.23648100
C	-4.52683200	3.27235300	0.46964400
C	-3.17968600	3.55436000	0.75533500
C	-2.26226700	2.51298400	0.79466100
H	-5.99328300	1.74841500	0.03378200
H	-2.87471000	4.57786700	0.94577700
H	-1.22941200	2.73403500	1.04459900
C	-2.64763500	1.17499400	0.53895800
H	-2.22403500	0.35835600	1.46992200
Pd	-1.24513100	0.12506100	-0.64752800
O	-2.70838300	-0.24679400	-2.00386900
C	-3.05176400	-1.44485600	-2.32061700
O	-2.87042900	-2.47893800	-1.63357300
Ag	-2.02876600	-2.47821400	0.36102200
O	-1.85420800	-2.26391700	2.50114100
C	-2.02430100	-1.22626700	3.20007800
O	-2.06218700	-0.02394600	2.77280600
C	-2.19018200	-1.40672900	4.69643000
H	-1.73808500	-2.34601700	5.02026900
H	-1.76110800	-0.55986700	5.23666900
H	-3.26209300	-1.44177200	4.92459800
C	-3.72280100	-1.58136600	-3.66863500
H	-4.37649600	-2.45529600	-3.68060200
H	-4.27707300	-0.67541400	-3.92250400
H	-2.93704500	-1.72339400	-4.41985200
N	0.38305800	0.58342300	0.53392400
C	1.24535300	1.59109600	0.17496200
C	0.69247400	-0.17094200	1.57550600
C	1.00844100	2.38652200	-0.97028700
C	2.41699100	1.80869800	0.96256200
C	1.85419100	0.08832000	2.34581500
H	0.04295000	-1.00160300	1.80686100
C	1.91788200	3.35136200	-1.33058000
H	0.12150700	2.20038200	-1.56684600
C	3.33542800	2.81196600	0.57776800
N	2.69523700	1.05531100	2.06126100
H	2.07819000	-0.54342000	3.20043800
C	3.09375800	3.56745900	-0.55526600
H	1.75626900	3.95180500	-2.21863700
H	4.22804300	2.94450300	1.17764700
C	4.03226400	4.56918800	-0.96480400

N	4.78810600	5.38590600	-1.30024100
N	4.05225800	0.50628000	-2.05097900
C	2.91870800	-0.17591600	-2.23739700
C	4.78007000	0.21539400	-0.96676200
C	2.47499600	-1.16604400	-1.35415700
H	2.32254400	0.08691100	-3.10626100
C	4.41722400	-0.76158300	-0.03640200
H	5.68351600	0.80152800	-0.82098400
C	3.24041700	-1.48071900	-0.23884800
S	0.89868500	-1.98043500	-1.64045900
C	5.27532200	-1.00532000	1.17338000
H	2.90285700	-2.23360500	0.46348400
O	1.05730300	-2.91603600	-2.75133900
O	0.49941200	-2.53088600	-0.31634000
O	0.00504600	-0.79121400	-2.05060300
F	6.30154200	-1.83649500	0.90368200
F	4.56273100	-1.56213400	2.17994800
F	5.80481500	0.14807100	1.63416800
H	-4.33856900	-0.09491100	0.08529700
C	-5.48159700	4.33931700	0.42878500
N	-6.25596100	5.20623200	0.39633900

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C	-3.95304400	0.39979800	0.22755700
C	-4.98974400	1.32069200	0.16751100
C	-4.68936000	2.66680800	0.37458500
C	-3.40298000	3.11711900	0.66301300
C	-2.38145800	2.17664200	0.73497900
H	-6.01130900	1.02666500	-0.03751100
H	-3.22989100	4.17309300	0.82741800
H	-1.38043400	2.50972500	0.98909700
C	-2.62443200	0.80190300	0.50484200
H	-2.10524400	0.04249600	1.43190900
Pd	-1.10222100	-0.11794100	-0.65260900
O	-2.50844500	-0.66642500	-2.00830300
C	-2.71532600	-1.89951100	-2.31032100
O	-2.42401300	-2.89773900	-1.60846100
Ag	-1.60658500	-2.77753400	0.39077300
O	-1.46440800	-2.50881500	2.52521500
C	-1.74824200	-1.48049500	3.20133000
O	-1.90952600	-0.29830300	2.74836400
C	-1.90487600	-1.64797900	4.70014100
H	-1.58645700	-0.74449300	5.22478800

H	-2.96668800	-1.80882400	4.92151200
H	-1.34578200	-2.51892900	5.04728200
C	-3.35981600	-2.12646900	-3.65886100
H	-3.90978300	-3.06915400	-3.66277200
H	-4.01243400	-1.29242100	-3.92505800
H	-2.55934800	-2.18626400	-4.40558700
N	0.46234200	0.53225000	0.52506300
C	1.20858200	1.62492400	0.15513200
C	0.85030400	-0.17161900	1.57566500
C	0.88756500	2.37720300	-0.99873800
C	2.34767300	1.97891400	0.94120900
C	1.97486700	0.22267000	2.34380400
H	0.29586700	-1.06628300	1.81570400
C	1.68579300	3.43257500	-1.36873300
H	0.02753600	2.08906300	-1.59407900
C	3.15066400	3.07312100	0.54614900
N	2.70509300	1.27282800	2.04828300
H	2.26543200	-0.37081900	3.20576200
C	2.82930700	3.78524100	-0.59512600
H	1.46023800	4.00237500	-2.26301500
H	4.02188400	3.30987300	1.14540500
C	3.65256500	4.87973100	-1.01499800
N	4.31488700	5.77066200	-1.35906600
N	4.11959600	0.82823700	-2.05167100
C	3.06853500	0.02282500	-2.22942600
C	4.87517900	0.63152300	-0.96530300
C	2.73713500	-1.00047700	-1.33477500
H	2.44692200	0.20864200	-3.10031900
C	4.62264500	-0.36939400	-0.02395700
H	5.70822900	1.31557300	-0.82703600
C	3.53257000	-1.21635800	-0.21695100
S	1.26095800	-1.98752800	-1.60964800
C	5.50221600	-0.50352000	1.18757600
H	3.28057000	-1.99389400	0.49438300
O	1.52216800	-2.91507400	-2.70758300
O	0.92000000	-2.55837300	-0.27833500
O	0.24228000	-0.90900400	-2.03843200
F	6.61394900	-1.21906500	0.92577800
F	4.85508200	-1.12467500	2.20063200
F	5.90070800	0.70631900	1.63507400
H	-4.16623000	-0.65182800	0.07060800
N	-5.78270500	3.65610000	0.29744700
O	-5.49013500	4.83719200	0.47123400
O	-6.91252700	3.23357200	0.06354400

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C	-2.26808400	-1.16173600	0.47081800
C	-3.64345500	-1.27697800	0.44309600
C	-4.43383400	-0.14454500	0.17092400
C	-3.82596900	1.10081000	-0.04754300
C	-2.43800200	1.19319000	-0.00186300
H	-4.14368100	-2.22275700	0.62631800
H	-4.42130200	1.98478000	-0.24494400
H	-1.98440300	2.16581000	-0.16101700
C	-1.60524600	0.07974900	0.25535300
H	-0.81171400	0.33342800	1.32637300
Pd	0.19113700	0.03390200	-0.85576300
O	-0.49245700	-1.63675600	-1.80291800
C	-0.16496700	-2.84230500	-1.52454700
O	0.50598500	-3.23854700	-0.54046600
Ag	1.27259300	-1.84605500	1.01060900
O	1.05291000	-0.87294600	2.97340000
C	0.35959300	0.13154100	3.27009000
O	-0.43668900	0.77310200	2.49920700
C	0.48773400	0.70081300	4.67281300
H	0.97915000	1.67902000	4.61516500
H	-0.50493400	0.86037000	5.10352500
H	1.07574400	0.03589900	5.30730800
C	-0.70591600	-3.87660800	-2.49595200
H	-1.78706100	-3.97392800	-2.34473100
H	-0.54502100	-3.54579600	-3.52544600
H	-0.23090500	-4.84428000	-2.32707400
O	1.92924800	-0.09911000	-2.00987400
C	3.00181700	-0.50318600	-1.42558500
O	3.11163800	-0.84118200	-0.22558800
C	4.22557300	-0.58921800	-2.32602800
H	5.12997000	-0.37403500	-1.75180600
H	4.30389000	-1.61505900	-2.70532000
H	4.14061500	0.08723400	-3.17933000
N	0.95262300	1.81720000	-0.13032800
C	1.84478300	1.82584500	0.87742000
C	0.66947400	2.96636900	-0.77095100
C	2.47008100	2.98873800	1.30379200
H	2.06287600	0.86496800	1.31914700
C	1.25093600	4.18271300	-0.39528900
C	2.15973000	4.18412800	0.65773600
H	3.18428500	2.94651000	2.11757300

H	1.00405700	5.09791000	-0.91690100
H	2.62562100	5.11616500	0.96336400
O	-0.20859300	2.81509800	-1.77690100
C	-0.53870100	3.94603000	-2.57822700
H	-1.03296400	4.72217100	-1.98190200
H	0.35446400	4.35845000	-3.06049000
H	-1.22541900	3.57040600	-3.33596400
H	-1.67345200	-2.04397100	0.68879100
O	-5.77212100	-0.35613700	0.15611900
C	-6.62827700	0.74335000	-0.11860900
H	-7.64349600	0.34540600	-0.08770700
H	-6.52141100	1.53118700	0.63755500
H	-6.43043200	1.16440300	-1.11223500

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C	-1.83405300	-1.31017100	0.52568500
C	-3.20227000	-1.50473300	0.51873000
C	-3.54320600	0.85440000	0.03218400
C	-2.16458300	1.02557300	0.05902800
H	-3.61565400	-2.49296600	0.71259200
H	-4.21392500	1.68061100	-0.15267300
H	-1.77519800	2.02518600	-0.09959100
C	-1.25687600	-0.03389400	0.29679600
H	-0.44092900	0.27685500	1.33012500
Pd	0.52389100	0.01571700	-0.85081700
O	-0.05353900	-1.72351100	-1.74810400
C	0.39934500	-2.88910200	-1.47764000
O	1.10942300	-3.21854100	-0.49581300
Ag	1.76421300	-1.75453600	1.03316600
O	1.54727100	-0.74747200	2.97159600
C	0.79891700	0.22243200	3.25179500
O	-0.06740100	0.77306100	2.48762900
C	0.94447000	0.86474100	4.62077100
H	1.40030200	1.85438800	4.49892300
H	-0.04028300	1.01321000	5.07254000
H	1.57473000	0.25409500	5.26917500
C	0.02423600	-3.96038600	-2.48611600
H	-0.99265400	-3.80164100	-2.85339900
H	0.70397700	-3.88544400	-3.34269500
H	0.12424300	-4.95310300	-2.04344200
O	2.23765600	-0.03079200	-2.04035800
C	3.34909400	-0.33717700	-1.46758600
O	3.50607900	-0.62745300	-0.26107200

C	4.55686300	-0.36263300	-2.39282300
H	5.45072400	-0.04523200	-1.85024800
H	4.71552600	-1.39526000	-2.72574000
H	4.39813200	0.26344300	-3.27346000
N	1.16135300	1.86778300	-0.18757100
C	2.07902200	1.97277100	0.79152300
C	0.74423300	2.97747900	-0.82541200
C	2.59254300	3.19624900	1.19645800
H	2.40855500	1.04070900	1.22648700
C	1.20565700	4.24954900	-0.46732000
C	2.13861600	4.35008700	0.55912600
H	3.33121700	3.23279200	1.98839100
H	0.85040600	5.13138600	-0.98376900
H	2.51254400	5.32705200	0.85041000
O	-0.13507700	2.72892600	-1.80895400
C	-0.65841100	3.82147200	-2.56053500
H	-1.21231200	4.51324300	-1.91533800
H	0.14210900	4.35659900	-3.08329100
H	-1.33582200	3.37208200	-3.28556500
H	-1.18528900	-2.15580900	0.73278100
C	-4.07223800	-0.42755900	0.25693200
N	-5.44521200	-0.70484200	0.25318700
H	-5.68339700	-1.67057700	0.43498100
C	-6.50690500	0.14614000	0.00092200
C	-7.86151700	-0.54584400	0.01619700
H	-8.62175000	0.18765000	0.28954400
H	-8.09294600	-0.91684700	-0.98947000
H	-7.90470800	-1.39096500	0.71131800
O	-6.38506400	1.33600800	-0.24135200

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C	-2.67328200	-0.45948400	0.44803300
C	-4.03644400	-0.21234200	0.38541300
C	-4.51967000	1.07298700	0.08825800
C	-3.59382700	2.10265700	-0.12490300
C	-2.22652000	1.85493000	-0.04800100
H	-4.74385600	-1.01913100	0.56430500
H	-3.95465100	3.10404700	-0.34962900
H	-1.53448400	2.67578300	-0.20291000
C	-1.71865600	0.56620800	0.23305300
H	-0.86148400	0.60080300	1.27182400
Pd	0.03592700	0.03807200	-0.84528700
O	-1.03957700	-1.42338700	-1.77514000

C	-0.98053300	-2.67375600	-1.50885600
O	-0.42745500	-3.21345300	-0.51942200
Ag	0.57639400	-2.03687100	1.06179000
O	0.62239800	-1.00316600	2.99436100
C	0.20668100	0.15455400	3.25402500
O	-0.39045800	0.95545400	2.45509100
C	0.46579000	0.71033500	4.64402500
H	1.19811700	1.52268800	4.56979300
H	-0.45408300	1.13797500	5.05290200
H	0.85179800	-0.06677500	5.30550200
C	-1.66180600	-3.56475700	-2.53202000
H	-2.62524000	-3.13752400	-2.82291000
H	-1.03605600	-3.61143700	-3.43032600
H	-1.79418100	-4.57223300	-2.13428300
O	1.67505100	-0.55662100	-1.98486400
C	2.61211700	-1.20278300	-1.38126800
O	2.63301200	-1.51932700	-0.17228400
C	3.76985000	-1.62353200	-2.27440300
H	4.70189400	-1.62317500	-1.70411400
H	3.58606400	-2.64853700	-2.61777200
H	3.85366100	-0.97669200	-3.15040000
N	1.22115700	1.58463300	-0.15017900
C	2.08518600	1.39011400	0.86339700
C	1.22724500	2.75856400	-0.80858400
C	2.97044000	2.37365600	1.28026600
H	2.06332600	0.41034100	1.31685500
C	2.08246000	3.80406700	-0.44194200
C	2.95927000	3.60037900	0.61833400
H	3.65010000	2.17160200	2.09961100
H	2.06611400	4.74455500	-0.97654100
H	3.63412600	4.39690700	0.91708900
O	0.34662600	2.80720000	-1.82148000
C	0.28387900	3.98261700	-2.62487700
H	-0.01691800	4.85216700	-2.02872600
H	1.24675700	4.17733200	-3.11002800
H	-0.47311000	3.77383900	-3.37990200
H	-2.32632000	-1.46111300	0.68498000
C	-6.00211000	1.33948700	0.03778700
H	-6.22514200	2.27251900	-0.48891200
H	-6.53657200	0.52486900	-0.46316600
H	-6.41833300	1.42335700	1.05055600

TS4P_H

0 1

C	-1.42200500	2.50854200	0.46803400
C	-1.68222900	3.87284500	0.41112700
C	-0.64328800	4.76613700	0.12868700
C	0.65572600	4.29324000	-0.07223800
C	0.91098300	2.92547800	0.00008900
H	-2.68831500	4.24542300	0.58375400
H	1.46249700	4.99164900	-0.27915000
H	1.92572700	2.56834200	-0.13897300
C	-0.11936500	1.99384600	0.26097700
H	0.20657900	1.17206700	1.27404900
Pd	0.03025300	0.16807100	-0.83289500
O	-1.71246600	0.65534000	-1.77150400
C	-2.85699200	0.13491900	-1.53180300
O	-3.16898800	-0.59666200	-0.56035800
Ag	-1.73425200	-1.10938100	1.03921500
O	-0.77347200	-0.80480000	2.98170300
C	0.15356300	-0.00017600	3.25533200
O	0.69560400	0.84650400	2.46503100
C	0.74579500	-0.04404200	4.65360600
H	1.77432000	-0.41802400	4.59192700
H	0.79172700	0.96608900	5.07062600
H	0.15956000	-0.69711700	5.30183900
C	-3.92104400	0.45911700	-2.56469000
H	-3.87279000	1.51669000	-2.83757400
H	-3.72220600	-0.12543500	-3.46993400
H	-4.91230700	0.20636900	-2.18494500
O	0.07491600	-1.55166200	-1.99898300
C	-0.18853800	-2.66918400	-1.41228300
O	-0.47836000	-2.82063600	-0.20669900
C	-0.15797200	-3.88556100	-2.32545100
H	0.17648100	-4.76357000	-1.76770100
H	-1.17844500	-4.07870200	-2.67703700
H	0.47964400	-3.71562100	-3.19569900
N	1.89513700	-0.39196000	-0.13571700
C	2.02040100	-1.27738700	0.87025200
C	2.99442400	0.02804900	-0.78921400
C	3.25489200	-1.75597100	1.28458500
H	1.09681700	-1.61120300	1.31907100
C	4.27597900	-0.40016700	-0.42449100
C	4.39745200	-1.30114500	0.62812000
H	3.30820200	-2.47012200	2.09772300
H	5.14923600	-0.04388200	-0.95463200
H	5.38213100	-1.64931600	0.92528200
O	2.72573500	0.87686300	-1.79445600

C	3.80157400	1.36394400	-2.59249700
H	4.50511100	1.95044400	-1.99004100
H	4.32841100	0.53914800	-3.08494900
H	3.33615500	2.00307600	-3.34185100
H	-2.23066100	1.81969800	0.69445000
H	-0.84550800	5.83289300	0.07712600

TS4P_C1

0 1

C	-2.40998000	-0.84744700	0.49179400
C	-3.79660500	-0.81108800	0.42593500
C	-4.42158800	0.40351600	0.13105000
C	-3.68874900	1.57308300	-0.07282100
C	-2.30055600	1.51313200	0.01213800
H	-4.39274800	-1.70098500	0.59670400
H	-4.20241700	2.50406200	-0.28781400
H	-1.73270000	2.42580300	-0.13109700
C	-1.61685500	0.30686200	0.28406900
H	-0.73658800	0.44667300	1.28749600
Pd	0.18535700	0.04223800	-0.83244100
O	-0.69617000	-1.54267400	-1.76126400
C	-0.45406800	-2.77652500	-1.51838800
O	0.19193300	-3.24478200	-0.54932700
Ag	1.04431300	-1.96506400	1.03680200
O	0.98577100	-0.94975900	2.97414000
C	0.41737300	0.13674100	3.25329000
O	-0.29723100	0.85361100	2.47111900
C	0.61790100	0.70934000	4.64564400
H	1.22445600	1.61933600	4.57063400
H	-0.34682300	0.99590400	5.07387500
H	1.12240800	-0.01120900	5.29109100
C	-1.02705500	-3.73939700	-2.54193600
H	-2.05524500	-3.46015600	-2.78768700
H	-0.43689000	-3.66786300	-3.46229000
H	-0.98801500	-4.76350000	-2.16755900
O	1.85459400	-0.30421700	-2.01424800
C	2.88800500	-0.81892700	-1.43875200
O	2.98000500	-1.13832100	-0.23495600
C	4.06880300	-1.06589200	-2.36499300
H	5.00579400	-0.94774600	-1.81564700
H	4.01599700	-2.10109700	-2.72247900
H	4.04277000	-0.40105000	-3.23100900
N	1.16028800	1.73143800	-0.14376500
C	2.06609100	1.64968800	0.84871000

C	0.98909000	2.89990800	-0.78984300
C	2.81812200	2.74218700	1.25509000
H	2.18855000	0.67308500	1.29275200
C	1.70286700	4.04955600	-0.43282500
C	2.62444800	3.96012900	0.60499800
H	3.53805800	2.62970300	2.05700100
H	1.54515200	4.98270100	-0.95714100
H	3.19152500	4.83918700	0.89606600
O	0.08305800	2.83499600	-1.77911500
C	-0.14978300	3.99239400	-2.57890800
H	-0.54942900	4.81510900	-1.97461000
H	0.76943800	4.31053200	-3.08278500
H	-0.88819900	3.68580300	-3.31872600
H	-1.92238400	-1.78889900	0.72693600
Cl	-6.17083900	0.46324800	0.03405400

TS4P_CN

0 1

C	-2.50675800	-0.77737500	0.53817700
C	-3.88988300	-0.70471200	0.46746000
C	-3.72178600	1.67804700	-0.02115100
C	-2.33740700	1.58640200	0.06804200
H	-4.50535500	-1.58293000	0.63289800
H	-4.20839900	2.62424600	-0.23500400
H	-1.74284400	2.48247200	-0.06818200
C	-1.69143000	0.35939000	0.33106100
H	-0.75538700	0.45218800	1.27640900
Pd	0.10616900	0.05882400	-0.81136200
O	-0.84121600	-1.48621500	-1.74017500
C	-0.61343100	-2.72991200	-1.53214700
O	0.05058600	-3.22935800	-0.59160800
Ag	0.93982500	-2.00789200	1.01350800
O	0.94927400	-1.00410600	2.95110500
C	0.41008600	0.09428600	3.24452700
O	-0.29005900	0.83597700	2.47338000
C	0.63319800	0.64651800	4.64142400
H	1.25149100	1.54890100	4.57187800
H	-0.32332900	0.94115100	5.08247200
H	1.13292800	-0.08935100	5.27305900
C	-1.22877900	-3.65905900	-2.56135500
H	-2.25467700	-3.35195300	-2.78169900
H	-0.65474100	-3.58333400	-3.49154800
H	-1.20572900	-4.69067700	-2.20697000
O	1.72218100	-0.31787200	-2.04030700

C	2.75653400	-0.86916400	-1.49642100
O	2.86963700	-1.20003200	-0.29916700
C	3.90060100	-1.14212400	-2.45975900
H	4.85597300	-1.06238100	-1.93595600
H	3.80243100	-2.17002300	-2.82844000
H	3.87205200	-0.46524100	-3.31622500
N	1.14799400	1.71105500	-0.13282900
C	2.07249500	1.59498300	0.83899500
C	0.99640600	2.88836900	-0.76795300
C	2.86513200	2.66206100	1.23488700
H	2.17513800	0.61223400	1.27450200
C	1.75227400	4.01359700	-0.42014100
C	2.69351300	3.88951400	0.59615700
H	3.59890700	2.52334300	2.01992600
H	1.61053700	4.95463800	-0.93478900
H	3.29293400	4.74927200	0.87982100
O	0.06575900	2.85657300	-1.73535900
C	-0.14723900	4.02370400	-2.52787200
H	-0.50762000	4.85652300	-1.91306100
H	0.77096600	4.31335200	-3.05015800
H	-0.91044400	3.74268100	-3.25245500
H	-2.03848000	-1.72888800	0.77070300
C	-4.50288300	0.52718000	0.17378600
C	-5.92998800	0.61304000	0.08622400
N	-7.08873100	0.68617200	0.01482300

TS4^P_NO₂

0 1

C	-2.27225600	-0.91504400	0.53226600
C	-3.65833200	-0.91172400	0.45290500
C	-3.60479000	1.48556900	-0.01841500
C	-2.21679700	1.45996600	0.08008200
H	-4.24655300	-1.80812600	0.60372700
H	-4.15281500	2.39558800	-0.22780400
H	-1.66578500	2.38458700	-0.04548500
C	-1.51518200	0.26283800	0.33629900
H	-0.57210000	0.38761600	1.26744300
Pd	0.30234600	0.06418600	-0.80699300
O	-0.57240300	-1.51328500	-1.75148300
C	-0.28016400	-2.74684300	-1.56216100
O	0.41637700	-3.22364400	-0.63376100
Ag	1.23615900	-1.98390400	0.99235600
O	1.19770500	-1.00222900	2.93847800
C	0.60525100	0.06619200	3.24068700

O	-0.12650700	0.78115700	2.47396100
C	0.79553200	0.61322100	4.64441100
H	1.35973600	1.55111900	4.58701100
H	-0.17699200	0.84582100	5.08767900
H	1.33646500	-0.10025300	5.26770400
C	-0.86335900	-3.69164000	-2.59563400
H	-1.92597000	-3.47707500	-2.74083800
H	-0.36051600	-3.52368800	-3.55414500
H	-0.72375800	-4.72871500	-2.28741500
O	1.92640200	-0.21951400	-2.04471900
C	2.98808400	-0.72853600	-1.51063600
O	3.12124500	-1.06641100	-0.31794000
C	4.13790000	-0.93745400	-2.48281700
H	5.09140900	-0.82545300	-1.96164300
H	4.08118600	-1.96257300	-2.86756000
H	4.07650500	-0.24904800	-3.32829300
N	1.26545500	1.75720100	-0.11340400
C	2.19802000	1.67525400	0.85423100
C	1.05219300	2.93330300	-0.73305600
C	2.93756500	2.77568400	1.26109900
H	2.35088100	0.69350500	1.27716200
C	1.75211500	4.09049500	-0.37322900
C	2.70221800	4.00089600	0.63837500
H	3.68012000	2.66429900	2.04221200
H	1.56132200	5.02964200	-0.87531900
H	3.25886800	4.88599000	0.93108700
O	0.12044900	2.86678400	-1.69736100
C	-0.16018400	4.03357500	-2.46960000
H	-0.55927900	4.83603500	-1.83866900
H	0.73736300	4.37944700	-2.99351400
H	-0.91321900	3.72390500	-3.19310000
H	-1.75849900	-1.84350800	0.76111700
C	-4.30039100	0.29315300	0.16554600
N	-5.76899000	0.30849700	0.06507600
O	-6.31203700	1.38202900	-0.19521500
O	-6.36442200	-0.75257600	0.24625800

PhNHAc

0 1

C	0.74605200	1.03879900	-0.00003200
C	2.11600600	1.30051400	-0.00003200
C	3.05271800	0.26651400	-0.00001100
C	2.60600700	-1.05603400	0.00002100
C	1.24269600	-1.33485900	0.00002800

C	0.30328200	-0.29229000	-0.00000400
H	0.01984300	1.83827500	-0.00005700
H	2.45055100	2.33423400	-0.00005400
H	4.11597200	0.48667500	-0.00001200
H	3.31849800	-1.87607100	0.00004100
H	0.90014700	-2.36788800	0.00006400
N	-1.06002100	-0.65353500	0.00002400
C	-2.17022200	0.16129600	0.00001700
H	-1.23512500	-1.64831600	-0.00020800
O	-2.12685100	1.38304500	0.00007100
C	-3.49631900	-0.58648600	-0.00004600
H	-3.39867500	-1.67668800	0.00026900
H	-4.06892700	-0.28204900	0.88125100
H	-4.06864200	-0.28250900	-0.88168500

PhMe

0 1

C	-0.19467600	1.20244900	-0.00906500
C	1.20052800	1.20534200	0.00220600
C	1.90384500	-0.00014000	0.00854300
C	1.20016600	-1.20553500	0.00221000
C	-0.19492300	-1.20231500	-0.00906700
C	-0.91304500	0.00021400	-0.01153700
H	-0.73585600	2.14578900	-0.01786200
H	1.73817800	2.14970900	0.00157500
H	2.99019400	-0.00031600	0.01399100
H	1.73764600	-2.15000100	0.00158600
H	-0.73635700	-2.14552400	-0.01788900
C	-2.42302500	0.00008700	0.00943400
H	-2.83075100	-0.88084800	-0.49790300
H	-2.80568800	-0.01122800	1.03884900
H	-2.83059300	0.89181200	-0.47868600

PhH

0 1

C	-1.33846600	-0.39754200	0.00000400
C	-0.32483700	-1.35790600	0.00006600
C	1.01349800	-0.96036500	-0.00005400
C	1.33843100	0.39765300	0.00000700
C	0.32495000	1.35787600	0.00006000
C	-1.01357700	0.96028600	-0.00005600
H	-2.37973500	-0.70694700	-0.00006500
H	-0.57774600	-2.41433100	0.00008000
H	1.80212100	-1.70738400	-0.00015000

H	2.37977200	0.70679300	0.00000900
H	0.57761100	2.41435300	0.00001600
H	-1.80202000	1.70750500	-0.00006000

PhCl

0 1

C	0.17767400	-1.21611400	-0.00000600
C	1.57318400	-1.20747600	0.00001400
C	2.27338000	0.00000300	-0.00000900
C	1.57315800	1.20748900	0.00000500
C	0.17766900	1.21611400	0.00000200
C	-0.50393000	-0.00001500	-0.00002100
H	-0.37623800	-2.14838800	0.00000200
H	2.11119200	-2.15104400	0.00001600
H	3.35914200	0.00002800	-0.00000900
H	2.11118400	2.15104900	0.00000700
H	-0.37628900	2.14835900	0.00001200
Cl	-2.26210600	0.00000000	0.00000400

PhCN

0 1

C	0.09085300	-1.21749200	0.00000000
C	1.48306500	-1.21089500	0.00000800
C	2.17932600	0.00002200	-0.00000500
C	1.48299500	1.21093700	0.00000100
C	0.09081500	1.21747600	0.00000600
C	-0.60965300	-0.00004100	-0.00000700
H	-0.46052700	-2.15165800	-0.00000400
H	2.02524600	-2.15147900	0.00000200
H	3.26530500	0.00007400	-0.00001400
H	2.02518400	2.15151700	-0.00000200
H	-0.46065300	2.15159000	0.00000500
C	-2.04288000	-0.00003100	-0.00000300
N	-3.20595400	0.00001500	0.00000200

PhNO₂

0 1

C	0.42626600	-1.22075000	0.00000300
C	1.81924800	-1.21238700	-0.00000600
C	2.51433000	-0.00000100	-0.00000600
C	1.81924300	1.21238900	0.00000000
C	0.42626600	1.22075100	0.00000700
C	-0.24494800	-0.00000200	0.00000900
H	-0.14286300	-2.14159700	0.00000600

H	2.36161400	-2.15268800	-0.00001100
H	3.60032500	0.00000400	-0.00001100
H	2.36161500	2.15268700	0.00000000
H	-0.14287200	2.14159300	0.00001300
N	-1.71608700	-0.00000100	0.00002500
O	-2.28672600	1.09004800	-0.00002000
O	-2.28672900	-1.09004800	-0.00000700

Pre_TS5

0 1

C	2.26105000	2.97449100	-0.07671400
C	2.60110100	4.23173900	-0.58503800
C	2.88833100	4.37422800	-1.94753300
C	2.83749200	3.27467000	-2.79766200
C	2.49839100	2.01603000	-2.27800700
H	2.64116100	5.09953100	0.06378500
H	3.06215300	3.38267300	-3.85486100
H	2.46934500	1.15421800	-2.94018100
C	2.20971200	1.85683700	-0.92625400
H	3.15166100	5.35452000	-2.33411200
O	1.95325800	2.73404100	1.23760600
C	1.94748200	3.82682800	2.14035000
H	2.94008500	4.28867000	2.21957900
H	1.21754000	4.59002700	1.84017600
H	1.66306400	3.41052400	3.10761600
C	3.13994400	-1.20777000	0.46951900
C	3.75982200	-0.03176500	0.07389500
C	3.51730000	-2.28014400	-0.54199900
C	2.69527400	-1.49124700	1.86554900
H	3.99572700	0.78778300	0.74191800
C	4.53399300	-0.35874900	-1.18660200
C	3.64183600	-1.44337400	-1.83040700
C	5.02466000	-2.56800100	-0.24388100
H	2.86403100	-3.15021800	-0.56052200
O	2.35944600	-0.64784400	2.67778400
O	2.72326500	-2.80671600	2.11273900
C	5.72520500	-1.24194400	-0.67500900
H	4.82323200	0.49572000	-1.79733700
H	2.67610200	-1.07675500	-2.18900100
H	4.14827000	-1.98489100	-2.63552000
H	5.19257500	-2.82446300	0.80506100
H	5.36298100	-3.41356600	-0.85041900
C	2.18035300	-3.21040700	3.38005800
H	6.27201600	-0.76221000	0.14247100

H	6.43379800	-1.40798100	-1.49230400
H	2.29006400	-4.29370600	3.40994900
H	2.72636000	-2.73867600	4.20068900
H	1.12587800	-2.92910000	3.43096000
Pd	1.46842400	0.13075700	-0.21491500
N	-0.40380800	1.02253200	-0.50251000
O	0.40252700	-1.62676600	0.46530800
C	-1.22513300	1.21715400	0.57614100
C	-0.87157400	1.27058800	-1.71181600
S	-0.34393400	-2.40148100	-0.63162200
C	-0.77428800	0.96005900	1.89421000
C	-2.56044400	1.67150600	0.34886100
C	-2.19780000	1.73136000	-1.90211900
H	-0.20350300	1.10196800	-2.54641800
C	-2.04675500	-1.95462500	-0.25951000
O	-0.20409800	-3.84934300	-0.44543900
O	-0.06840500	-1.84401900	-1.97526600
C	-1.64084400	1.12700600	2.94604600
H	0.24542700	0.62660100	2.05368400
C	-3.43170800	1.83962000	1.44988700
N	-3.02920000	1.92802600	-0.90314900
H	-2.56551800	1.91313400	-2.90780700
C	-2.50911900	-1.97488500	1.06123800
C	-2.89765800	-1.53168200	-1.27091900
C	-2.98111000	1.56335400	2.72731500
H	-1.31444200	0.92133400	3.95938400
H	-4.44579500	2.16886200	1.25699700
N	-3.74156100	-1.59367400	1.40628000
H	-1.84762500	-2.28671500	1.86408400
C	-4.18227200	-1.12218200	-0.91324600
H	-2.54659500	-1.48981300	-2.29533100
C	-3.86136300	1.71517700	3.84731800
C	-4.55636500	-1.17306700	0.43071000
C	-5.14613900	-0.62315000	-1.95131400
N	-4.56577900	1.84287900	4.76322700
H	-5.54513600	-0.84252700	0.73705200
F	-5.92486300	-1.61502900	-2.43306300
F	-4.49632900	-0.08298100	-3.01050800
F	-5.96760500	0.32188500	-1.45028800
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C	1.79526700	2.81206300	-0.27894800
C	1.49306100	4.00675000	-0.93964900

C	1.54588400	4.06073200	-2.33531500
C	1.91128500	2.93643600	-3.07411400
C	2.20984900	1.74502400	-2.40838400
H	1.21562800	4.89162100	-0.37874000
H	1.96551800	2.98202100	-4.15759900
H	2.49320100	0.87153400	-2.98619700
C	2.12817700	1.65034300	-1.01354000
H	1.30843000	4.99311200	-2.83910000
O	1.78973400	2.67074200	1.07363400
C	1.42226700	3.77722800	1.88310300
H	2.09786000	4.62781500	1.73006200
H	0.38949100	4.08732400	1.68187800
H	1.50512000	3.42450100	2.91139000
C	3.31600200	-0.66038700	0.45802800
C	3.68570900	0.62694000	-0.07207500
C	4.09262600	-1.70232600	-0.34418000
C	3.00288400	-0.84625300	1.90402100
H	3.81506300	1.46471900	0.60372900
C	4.68341300	0.32437100	-1.17523400
C	4.16539400	-1.02347700	-1.72486700
C	5.57028900	-1.56115400	0.12340700
H	3.67927400	-2.70799000	-0.29968900
O	2.55870700	0.01488000	2.64589800
O	3.24245500	-2.11084000	2.28890600
C	5.96375800	-0.14887700	-0.40940600
H	4.85374400	1.13544700	-1.88320600
H	3.19166600	-0.96555200	-2.21809600
H	4.88210900	-1.50512200	-2.39732000
H	5.66933400	-1.65552400	1.20728600
H	6.18361900	-2.34367000	-0.33484200
C	2.79494500	-2.45334400	3.60931300
H	6.24417300	0.54629800	0.38834000
H	6.80406500	-0.19918700	-1.10863100
H	3.08761400	-3.49272500	3.75385700
H	3.26386500	-1.80762400	4.35584500
H	1.70853100	-2.35100100	3.66748500
Pd	1.42133000	-0.17100800	-0.27956600
N	-0.52954300	0.51525900	-0.85130900
O	0.75945800	-2.04612600	0.45672100
C	-1.34781600	1.10031700	0.07675400
C	-0.95749100	0.42082200	-2.09541700
S	-0.21598500	-2.85898800	-0.41030900
C	-0.94730300	1.20206400	1.43130100
C	-2.62580100	1.58869300	-0.33075900

C	-2.22741900	0.92617100	-2.47493100
H	-0.31050800	-0.07925200	-2.80426000
C	-1.80802600	-2.24463000	0.16771300
O	-0.14327700	-4.28285200	-0.07365200
O	-0.13926500	-2.47430800	-1.83705000
C	-1.80011600	1.76358600	2.34920700
H	0.02985300	0.83031300	1.72284200
C	-3.48927800	2.16159500	0.63147000
N	-3.04551500	1.50333900	-1.62363300
H	-2.55782700	0.83202900	-3.50602300
C	-2.00704800	-1.96889500	1.52246200
C	-2.83678600	-1.99632900	-0.73364900
C	-3.08212300	2.24537500	1.95125800
H	-1.51355800	1.83252100	3.39250100
H	-4.46443900	2.50518000	0.30786800
N	-3.14401900	-1.45311400	2.00443200
H	-1.20572300	-2.14362900	2.23422100
C	-4.01818400	-1.44933000	-0.23869400
H	-2.69489400	-2.18809200	-1.79053300
C	-3.95241700	2.81631900	2.93592000
C	-4.12351700	-1.19625900	1.13299200
C	-5.16722300	-1.11711100	-1.14702300
N	-4.64850200	3.28437800	3.74091500
H	-5.02803100	-0.75083000	1.53918900
F	-6.14100900	-2.04971000	-1.08764800
F	-4.77647200	-1.02781900	-2.43751900
F	-5.73247800	0.06377400	-0.80598500

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C	2.01831200	2.63387800	-0.55055800
C	1.04866800	3.31901200	-1.29130600
C	0.76368300	2.92785300	-2.60061000
C	1.43262600	1.85653300	-3.18729700
C	2.37720400	1.14749200	-2.44287100
H	0.53621700	4.17124900	-0.86269900
H	1.22620300	1.56946000	-4.21308200
H	2.93037100	0.34972700	-2.91898800
C	2.67960900	1.48483900	-1.09772000
H	0.01733700	3.47978400	-3.16499600
O	2.42973900	3.01254300	0.67077600
C	1.71694000	4.02792300	1.36720900
H	1.83246900	5.00137600	0.87525700
H	0.65461100	3.77451700	1.44358200

H	2.15817600	4.06110800	2.36284700
C	3.24814400	-0.41010000	0.42548100
C	3.83166000	0.82201400	-0.31084300
C	4.12198400	-1.58992400	0.00832200
C	2.82497000	-0.29439800	1.85234900
H	4.23549900	1.56818900	0.37701200
C	4.94964400	0.16953600	-1.16210500
C	4.41566100	-1.25349900	-1.46296800
C	5.52697800	-1.36902000	0.64016000
H	3.67403300	-2.56047500	0.21561800
O	2.23573600	0.66222200	2.34310700
O	3.08550900	-1.41613400	2.54894500
C	6.09996200	-0.17054300	-0.18305000
H	5.25656500	0.77614800	-2.01891600
H	3.52408200	-1.31015800	-2.09018200
H	5.18734500	-1.89762300	-1.89793600
H	5.47039500	-1.16495100	1.71130700
H	6.13655700	-2.26956400	0.51137300
C	2.50025800	-1.48982900	3.85624600
H	6.36945900	0.68523400	0.44471600
H	6.99598100	-0.46327600	-0.73981800
H	2.80786100	-2.45490200	4.25765200
H	2.85810900	-0.67302600	4.48813400
H	1.41102900	-1.43853700	3.78005000
Pd	1.38319600	-0.25301800	-0.41290600
N	-0.61755300	0.30480900	-1.08852300
O	0.88102200	-2.06543000	0.53305600
C	-1.39743800	1.08290000	-0.27641400
C	-1.09572200	-0.03708100	-2.26899300
S	-0.20240700	-2.96331400	-0.09407800
C	-0.95740100	1.44010300	1.02265600
C	-2.67722600	1.51442000	-0.73743700
C	-2.36855700	0.41085700	-2.70711700
H	-0.48659600	-0.69613500	-2.87418200
C	-1.71419200	-2.20589900	0.52830500
O	-0.12298000	-4.31441800	0.46571000
O	-0.26735500	-2.81732600	-1.56341300
C	-1.77194900	2.19110100	1.83359500
H	0.01394000	1.10108000	1.37274900
C	-3.49756200	2.29495300	0.11062400
N	-3.14300000	1.17829600	-1.97283000
H	-2.73725500	0.11346300	-3.68561000
C	-1.76903700	-1.69523600	1.82649600
C	-2.82937500	-2.08982400	-0.29408100

C	-3.05184400	2.62591200	1.37778200
H	-1.45638000	2.44701100	2.83885300
H	-4.47304000	2.59607800	-0.25148800
N	-2.84432700	-1.07019200	2.32176700
H	-0.90092500	-1.76916000	2.47488300
C	-3.94659700	-1.43118800	0.21242000
H	-2.80072200	-2.46753900	-1.30913300
C	-3.87857300	3.40574000	2.25024600
C	-3.90585200	-0.93932400	1.52190700
C	-5.18364900	-1.23857200	-0.61771700
N	-4.53822500	4.04368200	2.96408100
H	-4.75826100	-0.40368500	1.93192500
F	-6.15737900	-2.10776900	-0.27628100
F	-4.93580600	-1.40910600	-1.93423300
F	-5.69250100	0.00519600	-0.45317400

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C	2.10965000	2.54370100	-2.43824100
C	2.71226300	2.00890500	-1.29537500
C	3.05594400	0.61717300	-1.23354600
C	2.84038000	-0.15219700	-2.40800300
C	2.25545600	0.39439400	-3.55222000
C	1.88211900	1.73523200	-3.55365400
H	1.41839200	2.17048200	-4.43403900
Pd	1.19067600	-0.33303000	-0.37331000
C	2.75843600	-0.60726100	0.93016800
C	4.78363400	-1.10297900	-0.26674100
C	3.28416800	-2.02446900	1.16438900
C	3.80576900	0.06833400	0.00041600
C	3.88970500	-2.36701000	-0.20604600
H	4.48119700	-3.28813600	-0.18777000
H	3.13519500	-2.45800700	-0.98960700
C	5.60888700	-1.28849300	1.02941500
H	6.44375800	-1.97353000	0.85184400
H	6.03051700	-0.34288400	1.38512500
C	4.57465300	-1.90270000	2.02642700
H	4.88693000	-2.89587500	2.36510000
H	4.42138000	-1.28968700	2.91685800
H	3.18237300	-1.17765500	-2.43430600
H	1.83491800	3.59046600	-2.47128300
H	4.30879100	0.90809300	0.48417700
H	2.09942700	-0.22600900	-4.42827000
H	2.54209800	-2.71577700	1.56317400

H	5.38843900	-0.96815900	-1.16756200
O	3.03765700	2.73514700	-0.21164300
C	2.61316600	4.09177700	-0.12542600
H	1.52655200	4.16850900	-0.24061100
H	2.90126400	4.42279300	0.87170800
H	3.11003400	4.70995200	-0.88240500
C	2.21632100	0.14955300	2.09775300
O	1.93802100	1.34191300	2.11232200
O	1.97342300	-0.65764600	3.15446100
C	1.38814600	-0.03628700	4.31218800
H	1.42740600	-0.79364900	5.09457900
H	1.95584300	0.85117700	4.59926300
H	0.35015000	0.24586000	4.11710500
N	-0.53701000	0.30013300	-1.60048700
C	-1.23158600	1.40140200	-1.15438800
C	-1.11803300	-0.47154400	-2.49753600
C	-2.52773500	1.67028200	-1.67949600
C	-0.68781900	2.24671100	-0.15637100
C	-2.41581000	-0.17927100	-3.01238700
H	-0.60109800	-1.36851800	-2.81407400
C	-3.25514900	2.78218300	-1.19703600
N	-3.10278900	0.86856900	-2.62513600
C	-1.41504000	3.31647800	0.30911700
H	0.29156300	2.02838100	0.25757500
H	-2.86713100	-0.86419900	-3.72028900
C	-2.70907900	3.59268000	-0.21566800
H	-4.24198200	2.96656000	-1.60541500
H	-1.01358900	3.95505800	1.08843700
N	-0.29091300	-1.28417400	0.76137000
C	-0.86265700	-2.31810300	0.11866500
C	-1.04206000	-0.51550800	1.57084200
C	-2.23227000	-2.54823300	0.16144000
H	-0.22250400	-2.93557300	-0.50081900
C	-2.40307900	-0.74230300	1.72848700
H	-0.54281800	0.31528400	2.05145900
C	-3.02239100	-1.75012800	0.98231700
S	-2.91711600	-3.68878800	-1.08255900
C	-3.19580600	0.21614800	2.57225100
H	-4.09453100	-1.91670300	1.01023800
O	-2.08853600	-4.90124600	-0.93452100
O	-4.34457900	-3.78919200	-0.73027100
O	-2.62151600	-2.90123500	-2.32103900
F	-4.29157300	-0.35724800	3.09302200
F	-2.45046300	0.70487300	3.59287200

F	-3.60176500	1.28070500	1.83985200
C	-3.44086700	4.71748700	0.28588800
N	-4.01603600	5.63963000	0.69869200

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C	-3.15493200	-0.50693800	-3.10187800
C	-3.55626800	-0.47437100	-1.76291500
C	-3.33065700	0.69302300	-0.95932900
C	-2.76553300	1.82198300	-1.60520400
C	-2.38679100	1.78850200	-2.94849800
C	-2.57444700	0.62233700	-3.68435700
H	-2.27810700	0.58299300	-4.72879300
Pd	-1.30819600	0.26289100	-0.04055500
C	-2.72421800	0.36978400	1.45189000
C	-4.27429500	2.15199400	0.99671400
C	-2.64148400	1.53634900	2.44086600
C	-3.88147400	0.74497600	0.48258500
C	-2.94793900	2.74104200	1.53661800
H	-3.11603900	3.65798600	2.11231300
H	-2.15381400	2.92642600	0.81295300
C	-5.04696400	1.93529900	2.31990200
H	-5.51755500	2.87012100	2.64046500
H	-5.84062800	1.18792100	2.21563000
C	-3.92824500	1.49360500	3.31646600
H	-3.82993500	2.20168300	4.14584100
H	-4.10712400	0.50808100	3.75108100
H	-2.63901100	2.73730700	-1.04728000
H	-3.31721300	-1.39523000	-3.69976300
H	-4.71637800	0.04371100	0.54552600
H	-1.94764800	2.66853900	-3.40639700
H	-1.71233100	1.57549200	3.00939500
H	-4.81560800	2.74664300	0.25534900
O	-4.20287600	-1.48331800	-1.15138800
C	-4.30551400	-2.74345500	-1.80255100
H	-3.31582600	-3.11359800	-2.09408400
H	-4.74625200	-3.41580100	-1.06722900
H	-4.95075900	-2.68274300	-2.68711900
C	-2.65071600	-1.01781200	1.99521400
O	-2.88987200	-2.05111900	1.38257000
O	-2.19504700	-1.03424200	3.26991800
C	-2.07850700	-2.32479400	3.89257800
H	-1.88250200	-2.11819500	4.94455700
H	-3.00431000	-2.89179700	3.77371600

H	-1.25037000	-2.89214800	3.46249800
O	1.42752300	4.20129000	-1.39700600
C	0.26297700	4.01093100	-0.88518200
O	-0.05734400	3.03079700	-0.17559700
C	-0.78097500	5.05831600	-1.25063000
H	-1.60537000	5.05019200	-0.53380100
H	-0.33038200	6.05256500	-1.29364200
H	-1.18080200	4.83673600	-2.24824200
N	0.06738300	-0.14871400	-1.70934500
C	0.38638500	-1.45527900	-1.97226300
C	0.81434100	0.79268100	-2.25473600
C	1.53871000	-1.75319300	-2.75870700
C	-0.40332900	-2.51013000	-1.45041500
C	1.93202200	0.47069800	-3.07218700
H	0.56011200	1.81698800	-2.02036000
C	1.90706700	-3.10352000	-2.96541600
N	2.30331100	-0.76707900	-3.31097400
C	-0.02920100	-3.81478300	-1.66159300
H	-1.29142100	-2.26867600	-0.87444600
H	2.52707700	1.27213300	-3.50248700
C	1.14143400	-4.11793100	-2.41628300
H	2.79426500	-3.31207600	-3.55196700
H	-0.61500000	-4.62897400	-1.24938900
N	0.29003000	-0.33682400	1.18794900
C	1.32466900	0.51223900	1.32541600
C	0.45861400	-1.64117100	1.46114000
C	2.59032200	0.05374900	1.68468400
H	1.12124800	1.55492700	1.09950400
C	1.69001400	-2.15446100	1.84857400
H	-0.41052800	-2.27644100	1.35197400
C	2.78647100	-1.29714400	1.94884400
S	3.98947600	1.20606700	1.68967700
C	1.82917700	-3.64092100	2.02769300
H	3.77383800	-1.65134800	2.22491900
O	3.47242000	2.42804200	2.33124200
O	5.09253700	0.47460600	2.31869000
O	4.21459700	1.40634700	0.18457500
F	2.86691900	-3.95794400	2.81646500
F	0.70924100	-4.17929600	2.56898100
F	2.01638200	-4.25412200	0.83580400
C	1.51147500	-5.48862200	-2.60805900
N	1.79443400	-6.60599300	-2.75873100
Ag	2.88204500	2.87663700	-0.61450000

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C	-4.56757300	-2.08361900	-2.43385100
C	-4.61879900	-1.82921100	-1.06016900
C	-3.50901500	-1.26557500	-0.40244200
C	-2.35337800	-0.93259300	-1.14482600
C	-2.30615800	-1.22858200	-2.52761700
C	-3.40558200	-1.78993300	-3.16126300
H	-3.38045000	-2.00114500	-4.22680100
Pd	-0.68370700	-0.70603000	0.09278400
C	-2.03473000	-1.00421000	1.63463800
C	-4.17802300	0.14264400	1.69169600
C	-2.10721800	0.18010900	2.61383100
C	-3.48686300	-1.11628300	1.08580500
C	-3.01524400	1.14994200	1.82963100
H	-3.29466300	2.03808100	2.40742800
H	-2.57862100	1.46708800	0.88179800
C	-4.46315100	-0.17400700	3.17501500
H	-5.07153500	0.61673800	3.62695200
H	-5.00398100	-1.11788000	3.29640700
C	-3.03231900	-0.20890100	3.80168800
H	-2.93215600	0.52426700	4.60886000
H	-2.77252600	-1.18561700	4.21927400
H	-1.96332500	0.39358900	-1.09073300
H	-5.41947000	-2.51420700	-2.94707400
H	-3.96579100	-2.01139100	1.49755700
H	-1.41864800	-0.96736500	-3.09673300
H	-1.13686600	0.55976700	2.93212000
H	-5.05413600	0.46972300	1.12623100
O	-5.69749400	-2.09968200	-0.26969500
C	-6.81773200	-2.74299000	-0.85616200
H	-6.54066000	-3.71361300	-1.28697800
H	-7.53249800	-2.89564200	-0.04636300
H	-7.27760100	-2.11906700	-1.63367100
C	-1.47541500	-2.30225400	2.11649500
O	-1.78704200	-3.40892700	1.70665900
O	-0.51612000	-2.13405900	3.07123600
C	0.10276800	-3.34015800	3.53627000
H	0.80866300	-3.02891700	4.30682800
H	-0.64217200	-4.02451100	3.94965700
H	0.62641900	-3.84677500	2.71925200
O	-2.19025400	3.77366400	-1.62508700
C	-2.49621300	2.55426500	-1.60738100
O	-1.62060100	1.65459500	-1.32096600

C	-3.91327200	2.12574100	-1.89989000
H	-4.37167600	1.76429100	-0.97255100
H	-4.49391000	2.96282400	-2.28813100
H	-3.91722400	1.29129000	-2.60752800
N	0.87782500	-0.55531600	-1.47984800
C	1.68414200	-1.64723400	-1.66942000
C	1.33071400	0.62093900	-1.87273500
C	2.98466900	-1.47339400	-2.22957700
C	1.24541000	-2.93503700	-1.27393600
C	2.62848700	0.77137300	-2.43145600
H	0.68002300	1.47353900	-1.72220000
C	3.83082800	-2.59709200	-2.37243500
N	3.44633800	-0.24427000	-2.59993700
C	2.08330400	-4.01424800	-1.42110700
H	0.24720900	-3.04304000	-0.85809200
H	2.97866200	1.76478100	-2.69818900
C	3.38881300	-3.84610300	-1.97062300
H	4.82138200	-2.44828100	-2.78582500
H	1.76093600	-5.00579600	-1.12290000
N	0.96428200	-0.05299400	1.32089600
C	1.04831900	1.28766700	1.26241200
C	2.09060400	-0.76886300	1.45579500
C	2.26971400	1.95147900	1.22540100
H	0.11491200	1.83412200	1.19547800
C	3.34657700	-0.16766700	1.47823400
H	1.97560200	-1.84409100	1.51200600
C	3.44639800	1.21808900	1.33186500
S	2.27905700	3.72090300	0.85503800
C	4.57816100	-1.03091100	1.52442600
H	4.40538800	1.72449600	1.30308800
O	1.10297400	4.26805700	1.56654700
O	3.61929800	4.19879100	1.19869800
O	2.01913800	3.70572500	-0.65901500
F	5.60454700	-0.40269300	2.12146400
F	4.34647500	-2.18525700	2.18369300
F	4.97732200	-1.36075100	0.27330200
C	4.24367500	-4.98863700	-2.10266800
N	4.92679800	-5.92368300	-2.20472900
Ag	-0.10846900	4.00093700	-1.01935200

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C	-4.12715800	-2.43937900	-2.57631100
C	-4.21719800	-2.35367600	-1.18080000

C	-3.11661000	-1.91952700	-0.41910200
C	-1.90414300	-1.59279000	-1.06094500
C	-1.82163100	-1.68396400	-2.46539200
C	-2.92807600	-2.10174000	-3.20915200
H	-2.85865600	-2.17943600	-4.29139400
Pd	-0.44190400	-0.92804800	0.12792700
C	-1.75080300	-1.46419900	1.64079600
C	-4.06219700	-0.71508300	1.67263600
C	-2.03736100	-0.28802000	2.59600800
C	-3.15831400	-1.83607900	1.07476200
C	-3.10000500	0.48625100	1.79044600
H	-3.53650200	1.32806100	2.34109900
H	-2.71407500	0.84481900	0.83276900
C	-4.28719500	-1.05420000	3.16170200
H	-5.04061000	-0.39024700	3.59983100
H	-4.63508500	-2.08333300	3.29547500
C	-2.88133100	-0.80256000	3.79355200
H	-2.92841600	-0.04076100	4.57951400
H	-2.44760500	-1.70143500	4.24098700
H	-1.94422400	0.40359900	-1.54168400
H	-4.97135400	-2.77004900	-3.16972400
H	-3.48662400	-2.80542700	1.46757700
H	-0.89098100	-1.44718200	-2.97385600
H	-1.14882100	0.26515600	2.89968700
H	-4.98593500	-0.55962300	1.11055100
O	-5.34296400	-2.66274700	-0.46875400
C	-6.46455100	-3.17036800	-1.17153100
H	-6.21703800	-4.09586700	-1.70679900
H	-7.22237400	-3.38015600	-0.41510300
H	-6.85915800	-2.43575500	-1.88645900
C	-0.99759900	-2.62843400	2.18296900
O	-1.17464600	-3.80105600	1.89821200
O	-0.00774600	-2.24693600	3.05174300
C	0.79556400	-3.31588100	3.56238800
H	1.48467200	-2.85399100	4.27088800
H	0.17688600	-4.06565700	4.06184300
H	1.34989400	-3.80520500	2.75451000
O	-3.10304700	3.22480000	-1.40837000
C	-3.05393200	2.00816900	-1.62097900
O	-1.88124100	1.39851400	-1.52886500
C	-4.26026500	1.18248200	-1.94586700
H	-4.50740200	0.57247500	-1.06903400
H	-5.10104800	1.83166800	-2.18917400
H	-4.04911500	0.48642600	-2.76282600

N	1.08567800	-0.51095200	-1.43528100
C	2.06757400	-1.45303500	-1.61287100
C	1.31643900	0.70669300	-1.89200700
C	3.29920300	-1.08159900	-2.22997500
C	1.87364100	-2.78027600	-1.15691400
C	2.54929200	1.05426700	-2.50823500
H	0.55077900	1.45812600	-1.74915000
C	4.32323900	-2.04663200	-2.36578800
N	3.52663900	0.19002900	-2.66951400
C	2.88189900	-3.70339300	-1.29760800
H	0.92129500	-3.04033400	-0.70263000
H	2.70586000	2.08061100	-2.82693600
C	4.11990600	-3.33515900	-1.90189300
H	5.25767800	-1.74643400	-2.82520800
H	2.74580100	-4.72293000	-0.95398900
N	1.03477900	0.18750900	1.34563700
C	0.85594900	1.49991400	1.12531700
C	2.27975800	-0.27274200	1.52037600
C	1.91961100	2.38182000	0.96790200
H	-0.17052900	1.83087100	1.02103000
C	3.39598600	0.55860200	1.42737600
H	2.37633600	-1.33661300	1.70397400
C	3.22052000	1.90740500	1.11743500
S	1.60980600	4.02508900	0.28922400
C	4.76588200	-0.05393700	1.53689200
H	4.06332900	2.57774000	0.98990600
O	0.31425000	4.46245900	0.96793900
O	2.77920000	4.84087600	0.61367800
O	1.33516300	3.74874200	-1.15384200
F	5.71682500	0.87259300	1.73992100
F	4.82218700	-0.94742600	2.54575400
F	5.08029400	-0.72226600	0.40105200
C	5.15685400	-4.31632100	-2.02748900
N	5.99038300	-5.12092700	-2.12416500
Ag	-1.29046400	4.04355500	-0.45862400

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C	4.35593100	-3.95470700	-0.17195100
C	4.80835500	-2.65059900	-0.40098400
C	3.90258400	-1.57506400	-0.41590300
C	2.53826800	-1.81157400	-0.19957500
C	2.08245200	-3.12373700	0.01534500
C	2.99115700	-4.18178300	0.02878300

H	2.64095300	-5.19884500	0.18955100
Pd	1.28865400	-0.28238900	-0.31840000
C	3.05102100	0.75716800	-0.74564300
C	5.13986700	0.48713000	0.46692400
C	3.29338600	1.79236800	0.37384000
C	4.31579700	-0.16358500	-0.68250000
C	4.03223100	0.94917000	1.43066300
H	4.39978500	1.55164200	2.26799500
H	3.43325700	0.12085600	1.81714200
C	5.69680400	1.83405400	-0.04196400
H	6.44661400	2.23250100	0.65012600
H	6.17467700	1.73071900	-1.02185700
C	4.43147600	2.74640000	-0.08619200
H	4.51621600	3.57873400	0.62161300
H	4.24214200	3.17690600	-1.07243400
H	5.04525100	-4.79063400	-0.15956200
H	4.87240200	-0.10957700	-1.62448600
H	1.02118800	-3.33247000	0.13996900
H	2.40606800	2.31865000	0.72523200
H	5.89596100	-0.18679500	0.87224500
O	6.11843200	-2.32269600	-0.63065400
C	7.07049200	-3.36935700	-0.67294400
H	6.83889100	-4.09243600	-1.46613400
H	8.03045100	-2.89497100	-0.88495900
H	7.13160900	-3.89893200	0.28746900
C	2.73945300	1.26715600	-2.11261900
O	3.07890600	0.76291300	-3.16623000
O	1.99500800	2.41746000	-2.07302100
C	1.53773400	2.89042600	-3.34399600
H	0.98437200	3.80764400	-3.13529100
H	2.37983200	3.09374600	-4.00994000
H	0.88487100	2.14961300	-3.81595700
C	-0.07175100	-1.38787000	2.11853600
C	-1.42875700	-1.50572700	1.83502000
C	0.40526100	-0.12945000	2.50384500
H	0.61168700	-2.22398500	2.04031200
C	-2.32756200	-0.44528500	1.92510300
C	-0.46848100	0.95936200	2.60751200
H	1.45378600	0.00870500	2.73619600
C	-1.82780600	0.79744300	2.31640500
H	-3.37255700	-0.54810800	1.66061100
H	-2.49866800	1.64621500	2.37609800
I	-2.16583800	-3.45563900	1.20706800
Ag	-3.51674900	-2.30037900	-0.91460100

N	-0.33605200	1.17271100	-0.64986500
C	-1.47249300	0.61047100	-1.08224500
C	-0.34406700	2.48035300	-0.34485600
C	-2.66828300	1.31636400	-1.19513200
H	-1.41797500	-0.43699600	-1.35854400
C	-1.48989700	3.25873300	-0.46621500
H	0.59454600	2.90281700	-0.01819000
C	-2.68335300	2.67141400	-0.89196200
S	-4.20006400	0.44762200	-1.58387100
C	-1.46494200	4.72357100	-0.13010500
H	-3.59872400	3.24496000	-0.99563000
O	-5.08379500	1.41788000	-2.22620200
O	-3.74564900	-0.71157000	-2.46527100
O	-4.64014600	-0.10892200	-0.26030500
F	-2.31115600	5.00427500	0.88645800
F	-0.23339900	5.13663400	0.23821400
F	-1.85042100	5.47111000	-1.18244000
C	0.11655400	2.27818900	2.97982800
O	1.28962300	2.44992000	3.24720200
O	-0.79958400	3.26578400	2.96589500
C	-0.31103600	4.56495100	3.34971200
H	-1.15560100	5.23817200	3.21797200
H	0.02139100	4.54646500	4.39025200
H	0.51960000	4.86085700	2.70744600

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C	-4.79266600	-3.47865700	-0.15155900
C	-4.70164400	-2.43096100	0.76685900
C	-3.53401000	-1.64604100	0.84618600
C	-2.44051400	-1.92799900	0.01433000
C	-2.53589600	-2.98741500	-0.90499500
C	-3.70292100	-3.74570300	-0.98289700
H	-3.76356700	-4.56773900	-1.69173200
Pd	-0.76097500	-0.85734600	0.32498700
C	-2.00043000	0.13487100	1.73040500
C	-4.34469600	0.69907700	1.41140500
C	-2.26997500	1.58684500	1.27879600
C	-3.42887800	-0.50045400	1.79602700
C	-3.48714400	1.40625300	0.35032400
H	-3.90345700	2.36189100	0.01211900
H	-3.27974600	0.77971900	-0.51672400
C	-4.33322100	1.71775100	2.57030200
H	-5.12564200	2.46290000	2.44326000

H	-4.49265600	1.23136100	3.53853400
C	-2.92113900	2.36963700	2.45433100
H	-2.99547100	3.42804800	2.17964700
H	-2.33758400	2.31210000	3.37372200
H	-5.68604900	-4.08734900	-0.22209500
H	-3.65036000	-0.83764400	2.81414500
H	-1.70638100	-3.25685400	-1.54746700
H	-1.41700800	2.10329900	0.83699300
H	-5.34088300	0.37920700	1.10479700
O	-5.69850200	-2.08730600	1.63911800
C	-6.88665900	-2.85927500	1.63293400
H	-6.68301700	-3.91101100	1.87210800
H	-7.52765000	-2.42969300	2.40465800
H	-7.39792000	-2.80351300	0.66269100
C	-1.20701800	-0.10148800	2.98088200
O	-1.25799500	-1.10419500	3.66838700
O	-0.38178400	0.93953700	3.28816800
C	0.51186200	0.72219600	4.38951300
H	1.11497700	1.62810100	4.45251100
H	-0.04737200	0.56146600	5.31398200
H	1.14388400	-0.15058400	4.20094600
C	-1.76194800	0.07952000	-2.55964400
C	-0.51643800	0.10437600	-1.93065900
C	-2.29630400	1.29446500	-2.97649900
H	-2.32602200	-0.84006000	-2.65150500
C	0.26064300	1.25865200	-1.83401000
C	-1.58639500	2.49170500	-2.80727900
H	-3.28473100	1.33178300	-3.42186300
C	-0.30394900	2.46505600	-2.24506900
H	1.26211900	1.23208100	-1.42613400
H	0.26021400	3.38451100	-2.13796500
I	0.70379500	-1.92309200	-2.09066100
Ag	3.33876500	-1.37041400	-1.61079900
N	1.16597800	0.09275000	1.00532400
C	2.24300300	-0.70234100	1.11925000
C	1.32685300	1.40884400	1.20934300
C	3.52529500	-0.19621500	1.33113000
H	2.08783500	-1.77061700	1.01276200
C	2.55689800	1.97009200	1.54192700
H	0.44952500	2.02701200	1.10062900
C	3.69228800	1.16143500	1.57790600
S	4.95037600	-1.25514300	0.96437600
C	2.62308900	3.43579100	1.87091900
H	4.68130100	1.56555900	1.76546400

O	6.07239500	-0.75765700	1.75941900
O	4.46492200	-2.63252400	1.15202100
O	5.12956600	-0.91291700	-0.53442100
F	3.85367600	3.93817300	1.66770200
F	1.75216500	4.14592700	1.11991600
F	2.30207700	3.65533300	3.16597900
C	-2.23732300	3.75412000	-3.24659600
O	-3.34310000	3.81403600	-3.74712300
O	-1.46076700	4.83477200	-3.01966800
C	-2.03362500	6.09144000	-3.41449600
H	-2.96491200	6.27238300	-2.87188300
H	-1.28695500	6.84407200	-3.16202100
H	-2.24054800	6.09554000	-4.48763100

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C	-4.80241000	-2.61405400	-1.75750300
C	-4.33117700	-2.77952000	-0.45328700
C	-3.14074000	-2.14826600	-0.03932300
C	-2.42082500	-1.39173300	-0.96958400
C	-2.88015600	-1.21633900	-2.27565600
C	-4.07118000	-1.83234400	-2.65592200
H	-4.44137800	-1.70100400	-3.66882400
Pd	-0.72308100	-0.59073200	-0.26269500
C	-1.22814800	-1.64492500	1.53669400
C	-3.43260300	-1.73253100	2.53452500
C	-1.35230200	-0.89039000	2.85491500
C	-2.61331500	-2.33780800	1.35017700
C	-2.79079100	-0.34833900	2.74603000
H	-3.12311000	0.12754700	3.67479300
H	-2.93052900	0.34857000	1.92475100
C	-2.97495200	-2.46348800	3.81388200
H	-3.62049800	-2.20467500	4.65919200
H	-3.00290700	-3.55189900	3.69970100
C	-1.52745200	-1.91714700	4.02211100
H	-1.43868700	-1.37264500	4.96786100
H	-0.76727600	-2.69689200	4.01974300
H	-5.72269200	-3.08469000	-2.08129700
H	-2.50834600	-3.41798100	1.52761600
H	-2.33546800	-0.60436700	-2.98322300
H	-0.55582800	-0.16843100	3.03472900
H	-4.50719100	-1.75729300	2.35389100
O	-4.94945100	-3.53662400	0.50277400
C	-6.14312200	-4.21776500	0.14719600

H	-5.96942200	-4.92600000	-0.67260800
H	-6.45351500	-4.76302300	1.03977900
H	-6.93330800	-3.51405600	-0.14374700
C	-0.06487400	-2.53699900	1.23220600
O	0.25081800	-2.66975700	0.03599800
O	0.60673400	-3.09441100	2.21695500
C	1.76023200	-3.91771700	1.85764800
H	2.06329300	-4.38192100	2.79408100
H	1.45967900	-4.66741900	1.12454200
H	2.56279300	-3.29714800	1.45388000
C	-3.07144200	1.37828300	-0.15540000
C	-1.68898000	1.18626000	-0.27315200
C	-3.60691300	2.66343600	-0.21119800
H	-3.74064300	0.53768400	-0.03210100
C	-0.86343800	2.29614900	-0.50221900
C	-2.77935400	3.77437200	-0.40291300
H	-4.67601300	2.82020100	-0.11260600
C	-1.40279700	3.58153200	-0.55817800
H	0.19860500	2.17149100	-0.67152900
H	-0.75373700	4.43174600	-0.73413200
I	0.59819600	-0.12089300	-2.87096400
Ag	3.21031500	-0.36856700	-2.24493000
N	1.14120500	0.15279000	0.81839300
C	2.26636100	-0.52406000	0.55644600
C	1.21942300	1.24923500	1.59009600
C	3.51964200	-0.09676600	0.98233800
H	2.16321900	-1.43999300	-0.01220100
C	2.43193000	1.70784900	2.09957400
H	0.29298200	1.77725800	1.77845500
C	3.61631100	1.03777800	1.77573900
S	4.95355100	-0.99698700	0.33737400
C	2.44172000	2.90124100	3.01774200
H	4.58568400	1.38251300	2.11964600
O	6.09574700	-0.59398200	1.16077800
O	4.51399600	-2.40698600	0.36608700
O	5.04337700	-0.44350500	-1.08751400
F	3.60669800	3.56945000	2.94503500
F	1.44530600	3.76040100	2.71536400
F	2.26785800	2.52365600	4.30249800
C	-3.41093800	5.12005200	-0.44875300
O	-4.60256400	5.32512100	-0.32176700
O	-2.50716400	6.10510600	-0.64713300
C	-3.05384700	7.43015000	-0.70482700
H	-3.56043400	7.67635300	0.23208800

H	-2.20209800	8.09069600	-0.86760900
H	-3.76977000	7.51315800	-1.52673500

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C	-3.04955000	-4.54699600	1.04292600
C	-2.76233100	-3.57877900	2.00893500
C	-2.00992700	-2.43527700	1.67102200
C	-1.52823400	-2.30973100	0.36687900
C	-1.79209600	-3.27593600	-0.60503700
C	-2.55765300	-4.38755900	-0.25443900
H	-2.77612300	-5.14534600	-1.00176500
Pd	-0.40726000	-0.68386100	0.02137500
C	-0.69873800	-0.31265000	2.12142500
C	-2.79160600	-0.56859100	3.33825600
C	-1.29960300	0.98986100	2.64237300
C	-1.64424500	-1.41627000	2.70343300
C	-2.80656500	0.71038700	2.48148200
H	-3.42137500	1.50139500	2.92365000
H	-3.11631500	0.56005500	1.45070100
C	-2.25022600	-0.01998500	4.67326600
H	-3.04857400	0.46385100	5.24505000
H	-1.82599200	-0.80875000	5.30286400
C	-1.18323900	1.01658000	4.20355800
H	-1.43125000	2.02818100	4.53993600
H	-0.17774800	0.79305900	4.55639100
H	-3.63790700	-5.42219900	1.28970900
H	-1.12424900	-1.94279700	3.51670200
H	-1.41997000	-3.17449400	-1.61566600
H	-0.90571400	1.89473600	2.18774900
H	-3.72677100	-1.12304000	3.41633500
O	-3.15643200	-3.64925300	3.31337900
C	-3.89174000	-4.79014800	3.73261600
H	-3.31619200	-5.71193900	3.58281600
H	-4.08143100	-4.64775200	4.79730600
H	-4.84711400	-4.86724700	3.19856100
C	0.74993500	-0.65506200	2.28431300
O	1.20275900	-1.50040200	1.48447900
O	1.46990800	-0.03825800	3.18290100
C	2.90443700	-0.34801200	3.27956900
H	3.38793500	0.58380500	3.56286500
H	3.01765400	-1.11297900	4.04986200
H	3.29532000	-0.68365700	2.32084900
C	-3.33490900	-0.23333400	-0.74381800

C	-2.00385700	0.18876500	-0.86305800
C	-4.34026900	0.40397200	-1.46942700
H	-3.60020100	-1.05327600	-0.09067400
C	-1.70089500	1.23776700	-1.74392400
C	-4.03962900	1.46599600	-2.32838400
H	-5.37319100	0.08473600	-1.37746400
C	-2.70995900	1.87671600	-2.46558900
H	-0.67490500	1.54473500	-1.90262200
H	-2.46164200	2.68821900	-3.14031400
C	-5.15935700	2.10796700	-3.07044600
O	-6.32286900	1.76843400	-2.98200200
O	-4.73711900	3.11813700	-3.86034500
C	-5.77004800	3.78680300	-4.60059800
H	-5.26261200	4.56305500	-5.17316100
H	-6.27858000	3.08450000	-5.26610000
H	-6.50394100	4.22547000	-3.91976300
N	0.37982600	-1.42061900	-2.08383900
C	1.67669200	-1.81441900	-2.31311200
C	-0.40113800	-1.26828900	-3.14014900
C	2.56235800	-2.10209300	-1.24872800
C	2.15215300	-1.91710100	-3.66328300
C	0.07454700	-1.44422500	-4.46253800
H	-1.42893100	-0.97735400	-2.96426200
C	3.88789500	-2.36990500	-1.49915500
H	2.19829400	-2.09222000	-0.23119300
C	3.51155000	-2.22257100	-3.90259200
N	1.32878400	-1.73128100	-4.73076700
H	-0.60697000	-1.31361100	-5.29978400
C	4.37082200	-2.42796300	-2.83751300
H	4.57687600	-2.50459700	-0.67481100
H	3.84970400	-2.28685900	-4.93011900
C	5.74854800	-2.73648700	-3.08406900
N	6.85872200	-3.00892400	-3.29375300
N	0.93612900	1.15809100	-0.06900300
C	2.25675500	0.91037700	0.02516900
C	0.50484800	2.38642800	0.25394500
C	3.17536100	1.82824100	0.50929900
H	2.60640600	-0.07319600	-0.23960000
C	1.36631500	3.37520800	0.72601100
H	-0.55697900	2.57419100	0.15123100
C	2.72199200	3.09172500	0.88436000
S	4.89689300	1.27961900	0.75687600
C	0.75999700	4.68240800	1.15386700
H	3.40824900	3.81735200	1.30717100

O	4.77279600	-0.20070500	0.60058200
O	5.65449600	1.96547000	-0.30307600
O	5.14943600	1.73026900	2.14625200
F	-0.05391600	5.18171500	0.19732000
F	-0.00534900	4.51305500	2.26235600
F	1.68921300	5.60749200	1.43781000
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C	3.18032600	4.28632100	-1.10573500
C	2.84194800	3.91213200	0.19956700
C	2.12099600	2.72734100	0.43452500
C	1.74358700	1.94432200	-0.66645700
C	2.06826800	2.31242600	-1.97723600
C	2.77711600	3.49208800	-2.18476200
H	3.03995100	3.79529700	-3.19404300
Pd	0.49544600	0.42376000	-0.15154800
C	0.38292900	1.44281400	1.70193700
C	2.40419300	1.81986200	2.96719800
C	0.49478700	0.59157800	2.96333800
C	1.56017300	2.42453900	1.79265600
C	2.00413700	0.32233400	3.01377200
H	2.31686400	-0.15065900	3.95064200
H	2.34796800	-0.29418400	2.18782400
C	1.69803700	2.30638400	4.25297200
H	2.26394200	2.00660000	5.14077800
H	1.58926400	3.39463400	4.27984200
C	0.32655400	1.55936800	4.18274600
H	0.14026200	0.96597500	5.08268500
H	-0.52444200	2.23449600	4.06438500
H	3.74615600	5.19090000	-1.29264500
H	1.16803300	3.38742800	2.14409900
H	1.79026500	1.67819000	-2.81218400
H	-0.17474300	-0.26469100	2.99690500
H	3.46906200	2.05569900	2.91663700
O	3.14823600	4.63385100	1.31379400
C	3.79244300	5.88985900	1.14781500
H	3.19037100	6.56611600	0.52862000
H	3.89476800	6.30687200	2.15040500
H	4.78670200	5.77189500	0.69921900
C	-0.95662300	2.11232600	1.42109200
O	-1.08179500	3.13225700	0.76586600
O	-1.96873500	1.44794400	1.98688300
C	-3.31199300	1.96292100	1.77142500

H	-3.98031700	1.19186400	2.15375500
H	-3.42053600	2.91197500	2.30117800
H	-3.48497000	2.11016900	0.70434000
C	3.62434700	-0.07667600	0.24066200
C	2.46181700	-0.16620700	-0.52688000
C	4.70422600	-0.90464100	-0.05516300
H	3.71628200	0.64567000	1.03612700
C	2.43641400	-0.97608800	-1.66676100
C	4.65486500	-1.78990100	-1.13743200
H	5.60925300	-0.85987900	0.54140000
C	3.52001700	-1.80688700	-1.95395900
H	1.59720200	-0.94424100	-2.34674300
H	3.48852700	-2.45320500	-2.82372200
C	5.84317900	-2.64788600	-1.39588300
O	6.85561900	-2.63312000	-0.72419600
O	5.67031300	-3.45209100	-2.46617800
C	6.78169900	-4.30990200	-2.77000500
H	6.47654200	-4.88348500	-3.64505300
H	7.67316700	-3.71622000	-2.98765300
H	6.99296600	-4.97261600	-1.92704800
N	-0.69521100	-0.25526000	-2.26420300
C	-1.77202600	0.57292700	-2.45019200
C	-0.85796000	-1.52809300	-2.58052100
C	-1.68745000	1.94448200	-2.10570800
C	-3.01456100	0.03650900	-2.91886100
C	-2.07540000	-2.02987300	-3.10546500
H	-0.02569600	-2.20207000	-2.39693100
C	-2.80611500	2.73759400	-2.18389200
H	-0.74495000	2.35282600	-1.76105800
C	-4.15447300	0.86975700	-2.98973300
N	-3.13716400	-1.27203800	-3.26544900
H	-2.15883700	-3.08067000	-3.37268800
C	-4.05096300	2.19897800	-2.62434300
H	-2.75379400	3.78037600	-1.89250100
H	-5.09517400	0.42784700	-3.29145200
C	-5.19606100	3.05846400	-2.67823800
N	-6.10442000	3.78189800	-2.73020900
N	-0.84388500	-1.11192500	0.54754400
C	-2.16385600	-0.91476200	0.40942700
C	-0.40736600	-2.28176800	1.04256000
C	-3.11179000	-1.85773000	0.77199000
H	-2.49533800	0.01783600	-0.02092600
C	-1.29740100	-3.29153900	1.40161200
H	0.66507800	-2.39987100	1.14600300

C	-2.67300700	-3.08126200	1.27002900
S	-4.86392800	-1.37573500	0.64677100
C	-0.74776300	-4.61439700	1.86094400
H	-3.39566100	-3.84493700	1.53814700
O	-4.82811300	-0.37029100	-0.45038900
O	-5.55463200	-2.64313100	0.35151300
O	-5.10710300	-0.79431500	1.99048000
F	-0.47194100	-5.41671200	0.80754700
F	0.40758200	-4.45458400	2.54636800
F	-1.61396400	-5.26881100	2.65212200

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C	-0.39824200	-3.93518000	-1.79828400
C	-0.70313200	-3.66579000	-0.46051700
C	-1.64504200	-2.64176600	-0.08366100
C	-2.36749600	-2.01796800	-1.15475000
C	-2.06236700	-2.33620100	-2.49053600
C	-1.07664700	-3.26134400	-2.80758300
H	-0.84915200	-3.47920800	-3.84685000
Pd	-0.23713900	-0.68298600	-0.03887200
C	-0.77947900	-1.26582500	1.87787800
C	-3.10090100	-1.88943800	2.07132200
C	-1.61237200	-0.32238900	2.74889900
C	-1.77525400	-2.39932800	1.45137100
C	-2.97564800	-0.35101400	2.04503700
H	-3.76394900	0.13691400	2.62798800
H	-2.95276200	0.08928300	1.05242200
C	-2.98829800	-2.15048200	3.59472500
H	-3.96016900	-1.99422400	4.07346700
H	-2.67507900	-3.17587000	3.81635900
C	-1.94874200	-1.08594400	4.06435900
H	-2.38781100	-0.38909900	4.78585300
H	-1.06521400	-1.52234700	4.53278700
H	0.33773500	-4.68947900	-2.04638300
H	-1.49461300	-3.34360300	1.91759700
H	-2.62778700	-1.84762200	-3.27679600
H	-1.15462500	0.65377900	2.90860900
H	-3.99608100	-2.31782900	1.62341700
O	-0.17701700	-4.37282800	0.55254000
C	1.02357400	-5.11235600	0.34663900
H	1.78247900	-4.48570100	-0.13137900
H	1.36489500	-5.39609600	1.34094000
H	0.83607500	-6.00880700	-0.25586900

C	0.59490400	-1.62985500	2.38640400
O	1.31250000	-2.50911300	1.92864200
O	1.00151100	-0.80271200	3.36318900
C	2.33993100	-1.01656600	3.88215800
H	2.40326700	-0.36961700	4.75635900
H	2.46353400	-2.06415700	4.16378600
H	3.09787200	-0.73431100	3.14655300
C	-4.78739200	-1.54334900	-0.66997900
C	-3.51320300	-1.06870600	-1.00487600
C	-5.86906200	-0.67147000	-0.59694300
H	-4.92728300	-2.60071700	-0.46886300
C	-3.36071100	0.28919200	-1.32249300
C	-5.70002100	0.68886600	-0.87880300
H	-6.85758700	-1.02613600	-0.32636200
C	-4.43826400	1.16618300	-1.25362800
H	-2.37510500	0.66346800	-1.58169800
H	-4.30822600	2.21769300	-1.48154500
C	-6.89162000	1.57681900	-0.77283200
O	-8.00055400	1.19686500	-0.45332000
O	-6.60113200	2.86041000	-1.07139700
C	-7.70729100	3.77273200	-0.98486400
H	-7.30173900	4.74860500	-1.25125400
H	-8.49856100	3.47919500	-1.67929700
H	-8.11195900	3.78555200	0.03027400
N	0.76860600	-0.38836700	-2.11266400
C	2.12357100	-0.58963300	-2.13690500
C	0.23465100	0.32058900	-3.09198200
C	2.76042100	-1.38120600	-1.14988000
C	2.91402300	0.05283000	-3.14386100
C	1.02612500	0.88234600	-4.12281700
H	-0.83988000	0.46923400	-3.07176700
C	4.13151500	-1.44406000	-1.09905400
H	2.15616500	-1.89513500	-0.40826500
C	4.32356300	-0.04869200	-3.09008500
N	2.33812400	0.77769400	-4.14174100
H	0.55300100	1.44844500	-4.92199200
C	4.92199300	-0.76100100	-2.06870400
H	4.62778300	-1.97265200	-0.29498800
H	4.90775300	0.46441400	-3.84433800
C	6.34951700	-0.85499000	-2.00102600
N	7.50446300	-0.97916700	-1.98056300
N	0.82295800	0.99690000	0.61351900
C	2.11987700	0.80528600	0.91005900
C	0.35163700	2.25173300	0.51583200

C	3.02047600	1.84834800	1.04971600
H	2.46822700	-0.20865600	1.02445100
C	1.18897700	3.35095800	0.69532400
H	-0.70377600	2.36609000	0.30076700
C	2.54880300	3.15415800	0.94806700
S	4.78360100	1.41131900	1.20290900
C	0.61276600	4.73028600	0.52384200
H	3.22931500	3.98906400	1.07839300
O	5.23093600	1.52100200	-0.20672100
O	5.31832600	2.41496000	2.13867400
O	4.71585100	0.00932300	1.70639600
F	0.57880500	5.08392700	-0.78098100
F	-0.66086900	4.78909400	0.97812900
F	1.33103800	5.65791600	1.17728600

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C	-0.87843800	-5.07118700	-1.47103900
C	-0.46178500	-4.03627400	-0.62986800
C	-1.23690700	-2.86105600	-0.45552500
C	-2.45522000	-2.75782300	-1.18038800
C	-2.87709500	-3.81500300	-1.99811500
C	-2.09488400	-4.95781400	-2.14221200
H	-2.42454600	-5.76297400	-2.79194100
Pd	-0.20895800	-1.01839100	-0.09001200
C	-0.53254100	-1.30518100	1.94297300
C	-2.68354500	-2.25482000	2.02100700
C	-1.52927400	-0.42598900	2.69796900
C	-1.26503500	-2.49332700	1.52994300
C	-2.83448800	-0.71997800	1.94791600
H	-3.72211600	-0.36614400	2.48080800
H	-2.84306300	-0.31997700	0.93889600
C	-2.56054100	-2.45140800	3.56918100
H	-3.56282100	-2.49610800	4.00576600
H	-2.04728500	-3.38218900	3.82951200
C	-1.78730400	-1.17959400	4.03671700
H	-2.40150900	-0.55976400	4.69724100
H	-0.86213500	-1.41163800	4.57098200
H	-0.26947800	-5.95810100	-1.59825700
H	-0.78764500	-3.44831000	1.71507000
H	-3.80459400	-3.71136500	-2.55268600
H	-1.23210100	0.61540500	2.80972500
H	-3.45177700	-2.86683900	1.54997000
O	0.67515100	-4.08786900	0.10552300

C	1.48036900	-5.25995900	0.09199100
H	1.91021500	-5.43200800	-0.90174300
H	2.27540900	-5.06740700	0.81212800
H	0.90407100	-6.13946400	0.40238900
C	0.87635000	-1.42528300	2.45910700
O	1.56819800	-2.42513300	2.37867900
O	1.26572000	-0.26997600	3.02069400
C	2.62302500	-0.17808700	3.52744400
H	2.55785200	0.42393600	4.43424700
H	3.00505100	-1.17545600	3.74514100
H	3.24810500	0.33051400	2.78740000
C	-4.61682500	-1.53157900	-0.72891600
C	-3.28238600	-1.52289000	-1.16149500
C	-5.32168600	-0.33823100	-0.58594300
H	-5.07727300	-2.47196300	-0.44099700
C	-2.72343000	-0.30136300	-1.56830500
C	-4.71311400	0.88348500	-0.89953300
H	-6.33339600	-0.32867000	-0.19450500
C	-3.42267600	0.89266600	-1.43981800
H	-1.72429800	-0.29279700	-1.97970700
H	-2.96733000	1.83424800	-1.72392200
C	-5.43308700	2.15255600	-0.59594500
O	-6.58327000	2.22165200	-0.21227300
O	-4.62405900	3.21846000	-0.75863900
C	-5.18134900	4.49732700	-0.42349000
H	-4.36166500	5.20400500	-0.54391400
H	-6.01011900	4.74018200	-1.09364500
H	-5.54332000	4.49451800	0.60755300
N	0.98925700	-0.88597700	-2.03561900
C	2.32874700	-0.93495900	-1.73281500
C	0.63915100	-0.19687900	-3.10923600
C	2.79135400	-1.70843100	-0.63938400
C	3.24947400	-0.11710500	-2.46226800
C	1.58693500	0.50654500	-3.89202200
H	-0.41449100	-0.16016900	-3.36576800
C	4.09897400	-1.59324300	-0.23361100
H	2.09867900	-2.35443700	-0.11200800
C	4.58621500	0.00303300	-2.01109700
N	2.85684700	0.58453800	-3.55968900
H	1.26246600	1.04180800	-4.78145300
C	4.99871400	-0.71404100	-0.90408500
H	4.45111500	-2.14983800	0.62749300
H	5.24419500	0.69062900	-2.52423100
C	6.34332300	-0.60128900	-0.42522300

N	7.44177700	-0.56788300	-0.04784900
N	0.44517400	0.95270000	0.24155800
C	1.74510800	1.23569900	0.41396900
C	-0.43414700	1.96347300	0.15390900
C	2.23352000	2.53245900	0.44496900
H	2.42714900	0.40862400	0.53204400
C	-0.02227900	3.29287000	0.19657500
H	-1.47795100	1.69670400	0.05027300
C	1.33562400	3.59191100	0.33271300
S	4.04295800	2.72683000	0.52293800
C	-1.08243600	4.35072500	0.05379400
H	1.69755300	4.61375700	0.36886700
O	4.41246600	2.69651700	-0.91377200
O	4.22999000	4.01274100	1.21685700
O	4.45125700	1.50551000	1.27395100
F	-1.68670600	4.27216400	-1.16065900
F	-2.06442200	4.19467600	0.97307300
F	-0.58794900	5.59087100	0.18278400

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C	-5.54692100	1.73202900	-0.90641000
C	-4.58772400	0.70557200	-0.90962800
C	-3.23683100	1.03414200	-0.70455700
C	-2.89072500	2.38844600	-0.60301000
C	-3.83770100	3.41584600	-0.57691100
C	-5.17673500	3.06632700	-0.71852100
H	-5.94562100	3.83301100	-0.71744200
Pd	-1.43516300	0.14618000	-0.29847500
C	-1.51772600	-1.95605200	0.68546200
C	-3.25418700	-1.16467900	2.02271000
C	-1.13205500	-1.95623700	2.15458300
C	-2.81287600	-1.46761500	0.60699800
C	-1.92754500	-0.74412400	2.68725200
H	-1.98200800	-0.72353000	3.77991500
H	-1.56195000	0.22180900	2.32454600
C	-3.44577500	-2.58848000	2.65183400
H	-3.90790000	-2.49519300	3.63928500
H	-4.09352300	-3.22393400	2.04116300
C	-1.98501800	-3.12734200	2.75117900
H	-1.69001900	-3.29741500	3.79071900
H	-1.82873400	-4.06155600	2.20636800
H	-6.59310800	1.49713900	-1.06213300
H	-3.49333000	-1.68868000	-0.20111000

H	-3.52659800	4.45246000	-0.48564200
H	-0.06719200	-2.01299900	2.36931700
H	-4.10903500	-0.49570600	2.12159000
O	-4.91502600	-0.60070800	-1.13701900
C	-6.26661200	-0.93292800	-1.41901100
H	-6.62381200	-0.41480300	-2.31695300
H	-6.27484500	-2.00938500	-1.59463100
H	-6.92468000	-0.69430500	-0.57373100
C	-0.92063000	-2.83378200	-0.37191600
O	-1.36201800	-2.91694600	-1.50230500
O	0.14906900	-3.48045800	0.09230800
C	0.86977500	-4.31505600	-0.85976300
H	1.82945500	-4.52114700	-0.39264900
H	0.29274300	-5.22495300	-1.04076500
H	1.03239500	-3.77067300	-1.79021600
C	-0.72103800	3.32613800	0.39126100
C	-1.41641200	2.59411200	-0.59837700
C	0.65677600	3.43099600	0.33652100
H	-1.28157700	3.77970100	1.20288500
C	-0.67678600	2.00847300	-1.66602500
C	1.39009500	2.81232200	-0.69976700
H	1.21347400	3.95478800	1.10598000
C	0.72696500	2.12957100	-1.70904700
H	-1.21031100	1.60070300	-2.52007800
H	1.28985500	1.66899500	-2.51233100
C	2.88416200	2.85585300	-0.61186700
O	3.47824200	3.47354900	0.25081400
O	3.45292500	2.09090400	-1.54709300
C	4.89167800	1.93691000	-1.49313700
H	5.09305200	0.96929100	-1.95194900
H	5.35728700	2.75952600	-2.04242500
H	5.22096100	1.95988800	-0.45298600
N	0.61956000	-0.23590300	0.14840800
C	1.39249700	-0.89284100	-0.73589100
C	1.18817900	0.33752300	1.21863600
C	2.76019700	-1.03860900	-0.55792400
H	0.91621400	-1.30811500	-1.61612500
C	2.56326800	0.28204300	1.43140200
H	0.53618000	0.87618100	1.89304900
C	3.36219300	-0.43284900	0.54244100
S	3.70897300	-2.06015500	-1.72707900
C	3.14857000	0.98148800	2.62775700
H	4.43659100	-0.50045100	0.67494600
O	2.75674600	-2.23666100	-2.85058700

O	4.90010000	-1.22674900	-2.00953500
O	3.96849500	-3.27458500	-0.91945000
F	2.42838800	2.08223000	2.94754700
F	3.14520800	0.18107100	3.71719300
F	4.41734200	1.35991300	2.40536600

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C	0.07843000	5.24206400	-0.77676700
C	-0.26944900	3.99119100	-0.25101500
C	0.63734100	2.91217200	-0.28857800
C	1.90733400	3.11786700	-0.87220300
C	2.25680100	4.37716900	-1.38597100
C	1.34080200	5.42285600	-1.34444400
H	1.60641100	6.39412600	-1.75104700
Pd	0.13382000	1.06913400	0.38488400
H	-0.61805500	6.07151700	-0.74352100
H	3.23842200	4.51862100	-1.82798800
O	-1.47102600	3.73583100	0.34535800
C	-2.47359100	4.74275600	0.32941400
H	-2.71236800	5.04902300	-0.69637500
H	-3.35299200	4.28699700	0.78611500
H	-2.16983200	5.62114600	0.91199000
C	4.12541000	2.16750200	-0.18673100
C	2.90502200	2.01369100	-0.86355600
C	4.97698200	1.08048500	-0.00514400
H	4.37349000	3.13325900	0.24432300
C	2.61083300	0.76624800	-1.43396600
C	4.63125900	-0.17817800	-0.51173200
H	5.90448700	1.17881300	0.54979700
C	3.45936300	-0.32185100	-1.26362200
H	1.70220200	0.64276500	-2.01049600
H	3.20200800	-1.28957700	-1.67715400
C	5.50241000	-1.34246300	-0.18730900
O	6.52911700	-1.27313900	0.45988700
O	4.99002300	-2.49114700	-0.66687400
C	5.70966700	-3.68864500	-0.33921400
H	5.11272500	-4.50210600	-0.74831500
H	6.70619100	-3.66857900	-0.78760700
H	5.80514400	-3.78847600	0.74462800
N	-1.43611000	1.05484900	-0.95388400
C	-2.73428000	0.94378500	-0.52618500
C	-1.18756900	0.88080400	-2.24689400
C	-3.09601100	1.20476900	0.81782800

C	-3.72798600	0.49399900	-1.45285800
C	-2.21490500	0.54553900	-3.15369400
H	-0.16532000	0.99910400	-2.57993600
C	-4.37095700	0.93007800	1.24261600
H	-2.34300600	1.59639000	1.49259200
C	-5.03160000	0.19812800	-0.98359600
N	-3.45440900	0.32663600	-2.76947000
H	-1.98178700	0.43235300	-4.20931300
C	-5.34304100	0.39684500	0.34430800
H	-4.65099600	1.09144100	2.27730600
H	-5.74567200	-0.20843400	-1.68753700
C	-6.65281900	0.09570500	0.83697500
N	-7.72302700	-0.10201600	1.24439100
N	-0.21304100	-1.03482400	0.79888900
C	-1.46017500	-1.51903900	0.90331600
C	0.77133700	-1.87533500	0.43147900
C	-1.81161700	-2.80132000	0.50853300
H	-2.22769900	-0.85894800	1.27468400
C	0.51311700	-3.20585400	0.10889400
H	1.77159500	-1.46192400	0.38720200
C	-0.80496500	-3.67320500	0.10394700
S	-3.59536700	-3.11976100	0.30810700
C	1.67233500	-4.06817000	-0.30842100
H	-1.05625400	-4.68347000	-0.20092000
O	-3.81629100	-2.49184100	-1.02559900
O	-3.71696200	-4.58698700	0.35277800
O	-4.20068900	-2.35893600	1.42983600
F	2.19920100	-3.64838300	-1.48849300
F	2.67767200	-4.01489300	0.59736400
F	1.32251800	-5.35499700	-0.46070900
O	1.67869500	0.90161600	1.79155600
C	2.24888100	1.78260700	2.45250300
O	2.00566200	3.06826700	2.32087300
H	1.39164700	3.20001500	1.54946100
C	3.30602600	1.43219500	3.45210300
H	4.25617900	1.33528800	2.91423700
H	3.40565300	2.21350300	4.20706900
H	3.07500800	0.46943100	3.91086500

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C	-0.80472300	-1.44591900	4.06358500
C	-0.76154300	-1.58735400	2.67375700
C	0.34926700	-1.14105700	1.92473800

C	1.40419800	-0.50757300	2.61009200
C	1.35205600	-0.34576200	4.00664500
C	0.26031400	-0.82333200	4.72111900
H	0.22749100	-0.71361700	5.80106000
Pd	0.32009200	-1.31119700	-0.08492600
H	-1.65525100	-1.80207500	4.63311700
H	2.17706400	0.14072900	4.51816200
O	-1.77924400	-2.12020300	1.93304800
C	-3.00067400	-2.46155000	2.57930700
H	-3.39579400	-1.60888500	3.14605900
H	-3.68981800	-2.71103700	1.77288900
H	-2.86763600	-3.31485700	3.25607200
C	2.81928000	1.43792800	1.94267700
C	2.53526200	0.06769500	1.83877000
C	3.76034500	2.03129800	1.10844000
H	2.25168400	2.04477200	2.64177700
C	3.27337400	-0.70803300	0.92966800
C	4.46007100	1.25740500	0.17341100
H	3.94559300	3.09934700	1.14245400
C	4.23200500	-0.12386400	0.10813900
H	3.08973900	-1.77529900	0.86055200
H	4.78583200	-0.72685800	-0.60188200
C	5.38449500	1.95653300	-0.75875700
O	5.47987400	3.16612300	-0.84684200
O	6.09397400	1.09830100	-1.52078900
C	6.98109800	1.71165900	-2.46912100
H	7.46189500	0.88646400	-2.99403800
H	6.41995800	2.33894900	-3.16657600
H	7.72220800	2.32817800	-1.95427100
N	0.38943700	0.72488100	-0.32385000
C	-0.42922100	1.62336100	0.31425100
C	1.33229300	1.19104100	-1.12770000
C	-1.53815300	1.19323600	1.07811100
C	-0.17249900	3.01928200	0.15645100
C	1.55502000	2.58410500	-1.26338100
H	1.93045600	0.46469300	-1.66040100
C	-2.34140400	2.11874000	1.69642500
H	-1.76130300	0.13676200	1.13268100
C	-1.00406100	3.95497500	0.81527400
N	0.84032200	3.48364500	-0.62605500
H	2.36623800	2.93525400	-1.89517700
C	-2.06996300	3.51182000	1.57672900
H	-3.20520100	1.79874600	2.26762300
H	-0.79125400	5.00968900	0.68749800

C	-2.92884900	4.45032400	2.23520700
N	-3.63220300	5.19889200	2.77957000
O	0.21957200	-3.38691600	-0.06216100
C	0.72014600	-4.22690700	0.69137000
O	1.33257600	-3.92907300	1.82455800
H	1.21874200	-2.95846300	1.99740700
C	0.66188200	-5.68771700	0.36830800
H	1.65654000	-6.13120000	0.47185400
H	0.00003700	-6.18948300	1.08286100
H	0.28487400	-5.81787900	-0.64598400
O	0.51031200	-1.40993800	-2.19569800
S	-0.66265400	-1.91629300	-3.06570300
C	-2.08624800	-1.25751300	-2.17016100
O	-0.80232800	-3.37787400	-3.02592500
O	-0.64106600	-1.23689200	-4.36632300
C	-2.81707600	-2.06242300	-1.29307800
C	-2.41778200	0.08653900	-2.29541500
N	-3.82930100	-1.59695200	-0.54845300
H	-2.56231500	-3.11233000	-1.19297200
C	-3.45514300	0.57941200	-1.50645800
H	-1.86491600	0.72364200	-2.97770500
C	-4.13132700	-0.29876500	-0.65505300
C	-3.82685200	2.03189200	-1.57749400
H	-4.94047800	0.06456800	-0.02776600
F	-2.71966500	2.81216500	-1.65955500
F	-4.58367900	2.31278400	-2.65562700
F	-4.51741200	2.42922500	-0.48482000

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C	-0.11598500	2.10244700	3.12010500
C	0.06534600	0.82414800	2.58781800
C	1.18419700	0.50047300	1.77127600
C	2.17749100	1.50395300	1.55266000
C	1.96057000	2.79468800	2.05724100
C	0.82694000	3.08279500	2.81504500
H	0.67995500	4.09206000	3.18942900
Pd	0.52792200	-0.67426000	0.11992100
H	-0.97371600	2.34662100	3.73435100
H	2.66930100	3.58894200	1.85519800
O	-0.80650100	-0.19676100	2.78892900
C	-1.92228000	-0.00247400	3.65597000
H	-2.56978200	0.80191000	3.28489700
H	-2.46698700	-0.94531000	3.63227300

H	-1.59015100	0.23397100	4.67329900
C	4.60293900	1.98612200	1.13253900
C	3.46272800	1.20007400	0.86652000
C	5.81921500	1.73139100	0.51375400
H	4.55012300	2.78623500	1.86160700
C	3.62037600	0.12323200	-0.02650000
C	5.94653200	0.67105700	-0.39075000
H	6.69131200	2.33964300	0.72769000
C	4.83535000	-0.13908600	-0.64906700
H	2.77790100	-0.52653000	-0.24642400
H	4.92253700	-0.97230100	-1.33675200
C	7.27224800	0.44687600	-1.02912400
O	8.25652000	1.12937800	-0.82137700
O	7.26191000	-0.60589000	-1.87373000
C	8.51273000	-0.88132700	-2.52194600
H	8.32774200	-1.74825200	-3.15605700
H	8.82927100	-0.02367200	-3.12118200
H	9.28588600	-1.10132600	-1.78129400
N	0.11047300	1.08332000	-0.86685200
C	-1.10533100	1.70694900	-0.75078600
C	0.98312600	1.56147500	-1.73611300
C	-2.08963100	1.22990300	0.14495200
C	-1.37685800	2.84931000	-1.56580500
C	0.68623900	2.70294500	-2.52149200
H	1.93674300	1.05521000	-1.82018800
C	-3.30153200	1.86894200	0.22744500
H	-1.87827400	0.35109200	0.74075600
C	-2.63726200	3.48518100	-1.47113600
N	-0.46040400	3.33990600	-2.44541300
H	1.42901800	3.07593900	-3.22187200
C	-3.58683900	2.99876100	-0.59102200
H	-4.07263600	1.50129100	0.89188900
H	-2.83087700	4.34074200	-2.10726200
C	-4.87760900	3.61356800	-0.50013400
N	-5.92659400	4.10608000	-0.41256900
O	0.87037700	-2.48624400	0.96965600
C	1.60002500	-2.67223800	1.99203800
O	2.17081700	-1.74956600	2.65222900
H	1.72619500	-0.64309000	2.18480100
C	1.76640300	-4.09892200	2.45465300
H	2.79456800	-4.26680600	2.78363000
H	1.10685900	-4.26513000	3.31419300
H	1.49333800	-4.78755900	1.65433000
O	-0.13140900	-1.52670200	-1.66180800

S	-1.09002300	-2.74356100	-1.77714700
C	-2.43198600	-2.28359900	-0.66140000
O	-0.51343800	-3.97780400	-1.23885800
O	-1.66713900	-2.74663300	-3.12621800
C	-2.36079300	-2.57917000	0.70338600
C	-3.52625500	-1.58336700	-1.15318600
N	-3.30261100	-2.19914800	1.57750500
H	-1.50966200	-3.12669300	1.09322700
C	-4.50800600	-1.18669400	-0.24516500
H	-3.59083500	-1.35036600	-2.21047900
C	-4.35247100	-1.51779300	1.10258200
C	-5.70228400	-0.39995200	-0.70651200
H	-5.09843300	-1.21027300	1.83055500
F	-5.37417700	0.44251000	-1.71226600
F	-6.69688700	-1.18888300	-1.15151200
F	-6.20922000	0.35739800	0.29944600

(AgI)₂

0 1

Ag	-0.00022100	-1.43509900	0.00000000
I	-2.42888000	0.00012500	0.00000000
Ag	0.00000000	1.43501800	0.00000000
I	2.42907600	-0.00005300	0.00000000

ArI

0 1

C	0.08013900	-1.13505700	-0.00010200
C	-1.31102700	-1.05111900	-0.00006100
C	-1.94310400	0.19802300	0.00007200
C	-1.17233700	1.36635400	0.00016500
C	0.21822600	1.29611600	0.00012600
C	0.82840300	0.04170400	-0.00000700
H	0.56905900	-2.10237600	-0.00020500
H	-1.90844200	-1.95533900	-0.00013200
H	-1.67947000	2.32518100	0.00026500
H	0.81282200	2.20228200	0.00019900
I	2.97269800	-0.08087900	-0.00006800
C	-3.42407700	0.34294200	0.00011300
O	-4.00945600	1.40812600	0.00028800
O	-4.05727000	-0.85084900	-0.00001900
C	-5.49035200	-0.77921800	-0.00005500
H	-5.84694000	-0.25223300	-0.88890800
H	-5.83436800	-1.81360600	-0.00107400
H	-5.84704600	-0.25400900	0.88982000

NBE-CO₂Me

0 1

C	1.77926300	1.09918600	-0.86669100
C	1.06069100	0.92599100	0.51139000
C	2.00329200	-1.10142200	0.18351300
C	2.42685300	-0.30002600	-1.09906800
H	1.07575300	1.38287700	-1.65370500
H	2.54142300	1.88268400	-0.80123900
H	2.07935000	-0.78520900	-2.01535400
H	3.51869200	-0.23233700	-1.15115800
C	2.07379200	0.02106500	1.24853100
H	1.72111100	-0.30280800	2.23235000
H	3.07087400	0.46671100	1.34083800
C	-0.06103300	-0.07284000	0.27285000
C	0.50251000	-1.28057900	0.07648100
H	-0.00660800	-2.18827300	-0.22699800
H	0.75915400	1.85833500	0.98824200
H	2.58627500	-2.00724200	0.36100900
C	-1.46561200	0.32063600	0.11070000
O	-1.86221800	1.47185000	0.13048800
O	-2.28620300	-0.74509100	-0.06437700
C	-3.67099200	-0.41869000	-0.23339200
H	-4.18471300	-1.37305700	-0.35403800
H	-4.05156200	0.11465300	0.64217100
H	-3.81495700	0.20967000	-1.11689000