

## Supplementary Information

# DFT Studies on the Mechanism of Palladium catalyzed Arylthiolation of Unactive Arene to Diaryl Sulfide

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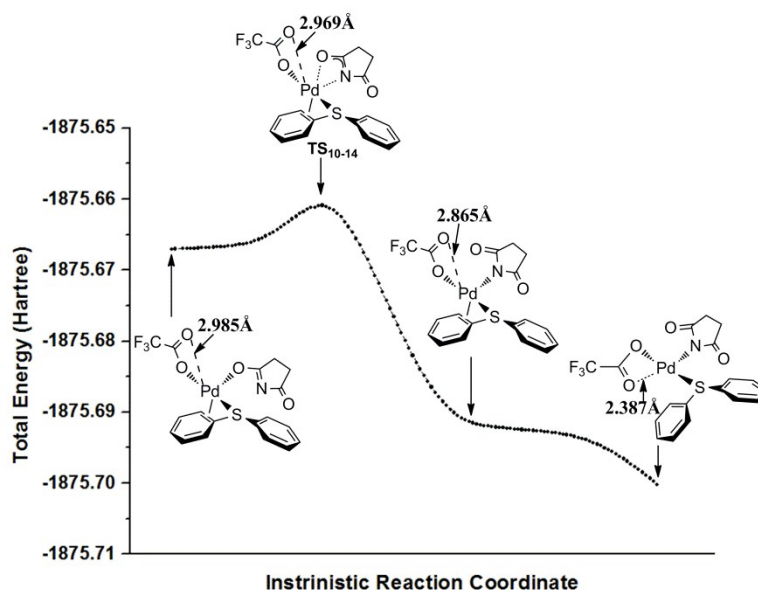
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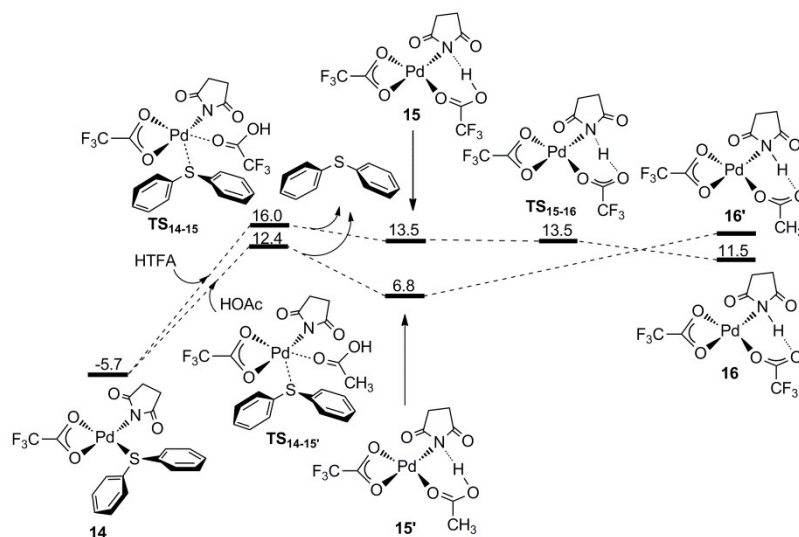
## IRC Calculation of TS<sub>12-14</sub>



**Figure S1.** IRC Calculation for TS<sub>12-14</sub> to verify the formation of **14**. IRC calculation was carried out with a numerical integration step size of 0.3 amu<sup>1/2</sup> Bohr.

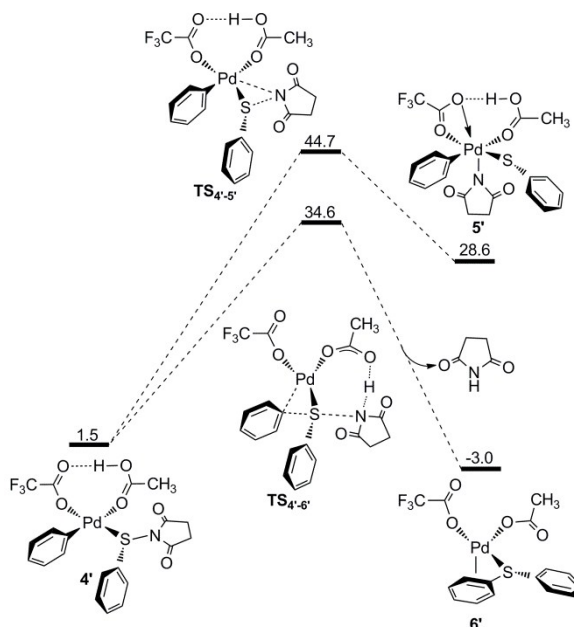
## The comparison of reactions of complex **14** with HTFA and HOAc

The reaction of complex **14** with HTFA has been described in the manuscript. In addition, the reaction of complex **14** with HOAc was also considered and shown in Figure S2. The ligand exchange of diaryl sulfide by HOAc proceeds through transition state TS<sub>14-15</sub> to form intermediate **15'** by releasing the product diaryl sulfide. From **15'**, N-H protonation transition state and corresponding intermediate similar to TS<sub>15-16</sub> and **16** cannot be located. Therefore, fixing N-H bond of 1.01 Å as in the optimized free pyrrolidine-2,5-dione, the fixed optimization gives structure **16'** which is higher than **15'** by 9.1 kcal/mol in electronic energy at the b3lyp level in gas phase. While TS<sub>15-16</sub> is 7.7 kcal/mol higher than **15'** in electronic energy, **16'** is higher than TS<sub>15-16</sub> by 1.4 kcal/mol. Thus, the pathway **14**→TS<sub>14-15</sub>→**15**→TS<sub>15-16</sub>→**16** is more favorable.

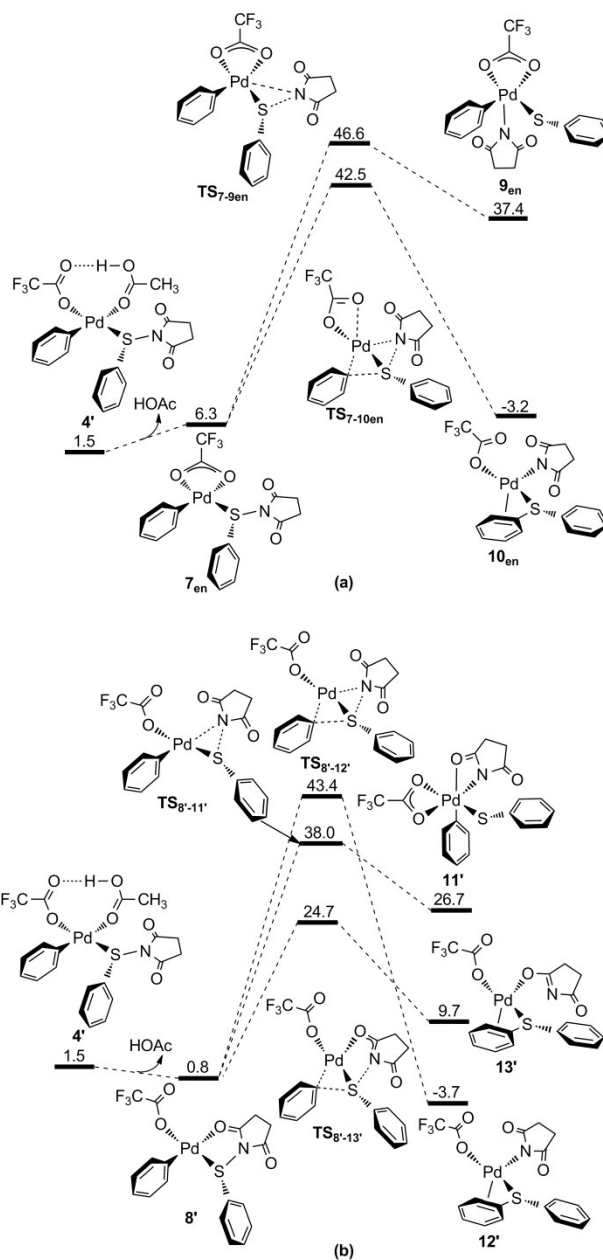


**Figure S2.** Gibbs energy profiles calculated for the reaction of intermediate **14** with HTFA and HOAc, respectively. The calculated relative free energies are given in kcal/mol.

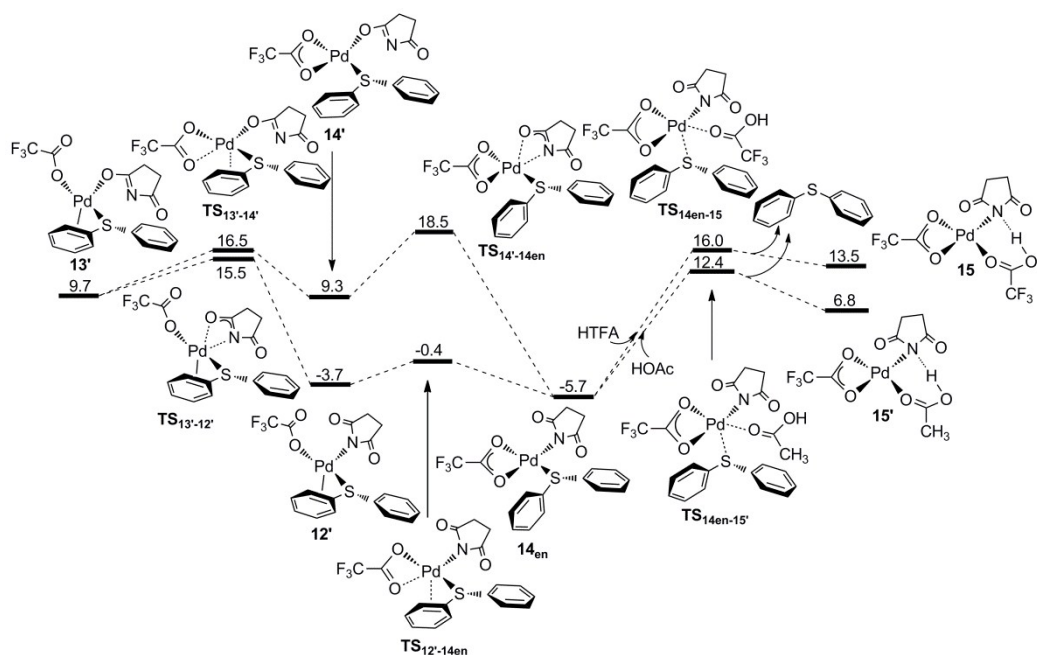
### Reaction pathways from intermediate **4'**



**Figure S3.** Gibbs energy profiles calculated for oxidative addition and concerted  $\sigma$ -bond metathesis giving intermediates **5'** and **6'**. The calculated relative free energies are given in kcal/mol.



**Figure S4.** Gibbs energy profiles calculated for oxidative addition and  $\sigma$ -bond metathesis giving intermediates **9<sub>en</sub>**, **10<sub>en</sub>**, **11'**, **12'**, and **13'**. The calculated relative free energies are given in kcal/mol.



**Figure S5.** Gibbs energy profiles calculated for the isomerization reaction from **13'** to **15**. The calculated relative free energies are given in kcal/mol.

### Cartesian coordinates for all of the calculated structures

#### Pd(OAc)<sub>2</sub>

Pd	0.02128300	0.00422000	0.00865400
O	1.77118700	-1.03428500	0.34810400
O	1.77766000	1.04576400	-0.28475700
O	-1.73507200	-1.03733500	0.30200500
C	2.44986700	0.00455000	0.03485100
C	-2.40729100	0.00389500	-0.01760700
C	-3.90238400	0.01437900	0.00361200
H	-4.28724500	-0.97606400	-0.24664600
H	-4.24171500	0.27005900	1.01329100
H	-4.28265900	0.76524900	-0.69104300
C	3.94496000	-0.00602700	0.01360200
H	4.28426800	-0.26238700	-0.99590600
H	4.32517700	-0.75647600	0.70874700
H	4.32991100	0.98453800	0.26324800

O	-1.72863300	1.04272500	-0.33084100
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**Pd(TFA)<sub>2</sub>**

Pd	0.01590300	0.01430200	-0.04858800
O	1.77590700	1.05106300	0.29071700
O	1.77452100	-1.02194300	-0.39662800
O	-1.74256300	1.05110600	0.29898000
O	-1.74424800	-1.02190700	-0.38835100
C	3.95530400	-0.01415000	0.02430100
C	2.42187600	0.01149200	-0.04503400
F	4.44822900	-0.82637900	-0.91500200
F	4.32677900	-0.46850700	1.23246600
F	4.44889800	1.21468000	-0.14817800
C	-2.39001700	0.01138100	-0.03336400
C	-3.92303100	-0.01466300	0.04436500
F	-4.41791400	1.21383800	-0.12661700
F	-4.28771400	-0.46793000	1.25499700
F	-4.42089100	-0.82798900	-0.89141100

**HOAc**

C	-1.39677000	-0.11174600	-0.00000900
C	0.09237400	0.12502900	0.00021000
O	0.64263500	1.20296100	-0.00024200
O	0.78054700	-1.04499800	0.00009500
H	1.72160300	-0.80095700	-0.00002500
H	-1.68215900	-0.69278900	0.88154100
H	-1.68174700	-0.69452800	-0.88053300
H	-1.91677900	0.84487200	-0.00102100

**HTFA**

C	-0.60076300	-0.00068300	-0.00008700
F	-0.99713600	-0.67855400	1.09117000
F	-0.99704400	-0.68093700	-1.08969500

F	-1.18825200	1.19600800	-0.00136000
C	0.93497700	0.15959900	-0.00001900
O	1.49767600	1.22230400	-0.00000800
O	1.52154000	-1.04552400	-0.00004200
H	2.48288500	-0.89639300	-0.00000100

**Pd(TFA)<sub>2</sub>(HOAc)<sub>2</sub> 1**

Pd	-0.92891300	-0.87831700	0.00831000
C	2.94961100	-1.49246900	1.81535200
C	1.54023000	-0.99813600	1.66129000
O	1.05459400	-0.88184200	0.51189100
O	0.91483900	-0.74201400	2.76905600
H	0.03062400	-0.24061100	2.63695000
O	-1.20968400	1.09094600	0.35015700
O	-1.07209400	0.88204200	2.60608500
C	-1.89418200	2.92904400	1.65171300
C	-1.32617500	1.49090800	1.55883700
F	-1.80942900	3.40929800	2.89538600
F	-3.19222800	2.92045400	1.28587800
F	-1.23158300	3.75901400	0.82878300
O	-0.76542800	-2.64442900	-2.58793500
O	-0.64789500	-2.84806900	-0.33053600
C	0.04654800	-4.69023200	-1.61680800
C	-0.51745600	-3.24974700	-1.53733100
F	-0.70729900	-5.53156500	-0.88780600
F	1.30031400	-4.71227600	-1.12200400
F	0.08194700	-5.13551100	-2.87551700
C	-4.81036900	-0.29776700	-1.81203400
C	-3.39611800	-0.77549300	-1.64953400
O	-2.91120400	-0.87550000	-0.49854700
O	-2.76775700	-1.03757900	-2.75447900
H	-1.87943100	-1.53035200	-2.61942700

H	-4.78456900	0.74896600	-2.13813900
H	-5.32122700	-0.87786600	-2.58414900
H	-5.33992200	-0.35826300	-0.86096800
H	3.49465000	-1.37101200	0.87868900
H	3.45084700	-0.97083200	2.63356600
H	2.91277200	-2.56010800	2.06394700

**Pd(TFA)<sub>2</sub>(HTFA)<sub>2</sub>**

Pd	-0.92756600	-0.88797800	0.01021900
C	2.89720500	-1.58350400	1.98478100
F	2.92745200	-2.49641100	2.96104900
F	3.66495600	-0.54064600	2.33651100
F	3.37678700	-2.12065100	0.86480300
C	1.44778000	-1.08464600	1.77969100
O	1.02644800	-1.00881000	0.61143900
O	0.85013800	-0.77691500	2.86888100
H	-0.03347200	-0.21080800	2.73892000
O	-1.15654200	1.06778400	0.43513200
O	-1.04633300	0.83415800	2.69055300
C	-1.87426800	2.88672000	1.75310300
C	-1.29247400	1.45469400	1.64357900
F	-1.76809500	3.35778400	2.99699500
F	-3.17536600	2.85831300	1.41134200
F	-1.23298700	3.72067200	0.92053400
O	-0.81170000	-2.61027200	-2.67012100
O	-0.69861900	-2.84370100	-0.41479300
C	0.01621200	-4.66318400	-1.73385100
C	-0.56468100	-3.23085700	-1.62338400
F	1.31908900	-4.63456300	-1.39899500
F	-0.09653100	-5.13579800	-2.97661000
F	-0.62078200	-5.49602700	-0.89693400
C	-4.75317300	-0.19096300	-1.96214900



F	-5.52186000	-1.23401400	-2.31137600
F	-4.78445200	0.72062000	-2.93958400
F	-5.23090400	0.34783900	-0.84217500
C	-3.30374600	-0.69029500	-1.75832200
O	-2.88180000	-0.76702800	-0.59035400
O	-2.70675400	-0.99764000	-2.84797900
H	-1.82358200	-1.56445300	-2.71841400

**Benzene**

C	-1.82464500	-1.72791400	0.00007400
C	-0.42836400	-1.72794500	0.00058400
C	0.26977800	-0.51896700	-0.00009000
C	-0.42833600	0.69028100	-0.00102200
C	-1.82441300	0.69031000	-0.00141700
C	-2.52265900	-0.51883800	-0.00098500
H	-2.36764200	-2.66848700	0.00043600
H	0.11451100	-2.66859900	0.00137400
H	1.35583100	-0.51886700	0.00016400
H	0.11489500	1.63071200	-0.00145100
H	-2.36750400	1.63083200	-0.00224200
H	-3.60871900	-0.51867100	-0.00133500

**1-(phenylthio) pyrrolidine-2,5-dione**

C	3.00714800	0.83060000	-1.02587300
C	3.02358000	-0.70328400	-1.10186700
C	1.90915400	-1.17565000	-0.17237200
C	1.87449000	1.18460300	-0.06667600
H	3.93547000	1.25719900	-0.63525800
H	2.81210500	1.31499100	-1.98643200
H	3.96503000	-1.14761800	-0.76687700
H	2.82510000	-1.09274500	-2.10417400
N	1.32758600	-0.02670500	0.40710300
S	0.05534200	-0.09712200	1.58595300

C	-1.40290600	-0.03208900	0.54190300
C	-2.03370900	-1.22231600	0.15761400
C	-1.93107800	1.20785100	0.15787900
C	-3.19574200	-1.16832700	-0.61289500
H	-1.60619800	-2.17353900	0.45639900
C	-3.09020600	1.25127300	-0.61680400
H	-1.42465600	2.11870000	0.45879800
C	-3.72267700	0.06585400	-0.99904800
H	-3.68751300	-2.08903700	-0.91244600
H	-3.50127800	2.21003400	-0.91870100
H	-4.62786300	0.10430500	-1.59818000
O	1.49506000	2.29037800	0.23794800
O	1.56780400	-2.31444100	0.03839200
<b>2</b>			
Pd	-0.01043900	-0.02237800	-0.20227700
C	1.85354300	-1.86059600	3.19257400
C	1.14412800	-0.76567900	2.45220200
O	1.41317400	-0.56609900	1.24538800
O	0.26395100	-0.08942500	3.12779000
H	-0.05609300	0.73365300	2.61271400
O	0.42927700	1.94846600	-0.11132000
O	-0.29320900	2.15173900	2.03354600
C	0.34611200	4.11435700	0.82361600
C	0.14773400	2.58330500	0.95920700
F	0.54417900	4.68326700	2.01703900
F	-0.76687900	4.65592400	0.27765100
F	1.38497100	4.41413300	0.03067800
O	0.94696100	-2.53434100	-1.83086100
O	-0.48819700	-1.96572900	-0.16108100
C	0.01467300	-4.24402900	-0.40581600
C	0.20781000	-2.78488300	-0.89522500

F	-1.28807800	-4.55207700	-0.26864700
F	0.60458600	-4.39642000	0.80540500
F	0.56813900	-5.12058700	-1.24773100
H	2.92510000	-1.79917400	2.98897500
H	1.65938400	-1.80677500	4.26312000
H	1.49917400	-2.81641600	2.79241800
C	-2.57307400	1.52430400	-1.19050900
C	-1.96711700	0.26225200	-1.42621800
C	-0.91053000	0.15731400	-2.37233000
C	-0.47048200	1.31618700	-3.05599200
C	-1.07107700	2.53516000	-2.80533000
C	-2.12538700	2.64076900	-1.86952200
H	-3.39684200	1.59608800	-0.48742500
H	-2.42932600	-0.63726700	-1.03200000
H	-0.53235300	-0.81423900	-2.67397700
H	0.32897000	1.23087800	-3.78465700
H	-0.73788100	3.42297800	-3.33418400
H	-2.58436300	3.60735900	-1.68894700
<b>TS<sub>2-3</sub></b>			
Pd	-0.06983100	-0.64287600	-0.23040000
C	2.46120300	-2.30072600	2.98736200
C	1.34745300	-1.53738300	2.32586800
O	1.47655600	-1.11181000	1.16243700
O	0.28839000	-1.37187400	3.06807800
H	-0.35855900	-0.67931100	2.68790300
O	-0.31100100	1.25776100	0.43890800
O	-1.19653000	0.60189500	2.42479200
C	-1.22166100	2.92455900	1.83476400
C	-0.87321000	1.43853600	1.56855000
F	-1.40295900	3.15543000	3.14060500
F	-2.36615300	3.23371400	1.18881200

F	-0.25661600	3.74524900	1.39067600
O	-1.18578400	-2.51999100	-2.58872800
O	0.28590800	-2.55514900	-0.87964800
C	0.09571300	-4.51758300	-2.18848900
C	-0.31028300	-3.06087800	-1.86564000
F	-0.24569900	-5.31308900	-1.16024200
F	1.42403400	-4.59221300	-2.36382100
F	-0.50782100	-4.96372600	-3.29266000
H	2.07881400	-3.26401500	3.33699900
H	3.28233600	-2.45247100	2.28870900
H	2.80793000	-1.74926500	3.86627300
C	-3.74568300	0.97446500	-1.53348400
C	-2.86986600	-0.01504000	-1.09890800
C	-1.55194700	-0.10700100	-1.61778800
C	-1.15325800	0.84987900	-2.58649700
C	-2.02985400	1.83660700	-3.02529600
C	-3.32163900	1.90156200	-2.49195600
H	-4.75289000	1.02939600	-1.13136600
H	-3.20449500	-0.74050100	-0.36189900
H	-1.35472700	-1.32979200	-2.09959200
H	-0.15086200	0.79956200	-3.00362600
H	-1.71351900	2.55672700	-3.77403500
H	-4.00438000	2.67672300	-2.82892800
<b>3</b>			
Pd	0.29324000	0.09783500	0.18223200
C	2.03762100	-1.76300800	3.88660600
C	1.31150200	-0.77352300	3.01499800
O	1.55590600	-0.68705300	1.80041300
O	0.44105900	-0.03821500	3.65472300
H	0.09830600	0.74278500	3.09727900
O	0.71337700	2.06361400	0.46460900

O	-0.23892200	2.15583900	2.52655600
C	0.51748600	4.17627900	1.47062600
C	0.30026700	2.64281300	1.52351600
F	0.22283900	4.75717600	2.63916000
F	-0.26952700	4.71700400	0.51953200
F	1.79698200	4.46457400	1.16792500
O	-0.15747900	-1.95529700	-2.47697200
O	-0.04641000	-1.94931600	-0.20648000
C	-0.14020600	-4.05050700	-1.36833500
C	-0.10384100	-2.50978100	-1.29735000
F	0.11070000	-4.57853700	-0.17175700
F	0.77129300	-4.49013600	-2.24493200
F	-1.35822700	-4.44135400	-1.77447300
H	2.63870900	-2.43498400	3.27571200
H	2.68222200	-1.22095700	4.58569200
H	1.31600200	-2.32859800	4.48198700
C	-3.05596500	0.84973800	-2.34537200
C	-2.23941300	0.42381400	-1.29382300
C	-0.85918800	0.69229100	-1.31467400
C	-0.31571600	1.39658300	-2.40223000
C	-1.13883000	1.80778800	-3.45934500
C	-2.50695200	1.53768600	-3.43075200
H	-4.12255800	0.64405900	-2.31352700
H	-2.68199000	-0.10602800	-0.45418400
H	-0.24352100	-0.97020700	-2.37938400
H	0.74151800	1.64627900	-2.41376300
H	-0.70590000	2.34988400	-4.29563200
H	-3.14428700	1.86403100	-4.24728600
<b>2'</b>			
Pd	0.09034900	0.42547200	-0.22690400
O	-1.79345900	0.02170500	-0.71103100

O	-2.34375500	-0.29314400	1.46877700
O	1.10791600	-1.47751600	-0.33290600
O	2.14700000	0.41302000	0.09338000
C	-3.97694500	-0.72636300	-0.26127400
C	-2.58125400	-0.31198600	0.27402600
F	-3.87430400	-1.68885700	-1.19355500
F	-4.58348200	0.34080400	-0.82566300
F	-4.75562600	-1.17520400	0.72727700
C	2.16823500	-0.85165200	-0.06131600
C	3.49154200	-1.60453800	0.14065200
F	3.68152800	-1.81231700	1.45569600
F	4.51681600	-0.88063800	-0.32946500
F	3.46839700	-2.78475600	-0.48333400
C	0.42854800	2.87756200	1.58657100
C	1.56096900	3.48991100	1.08402200
C	1.71718500	3.68381400	-0.30804200
C	0.73975700	3.26477500	-1.19065500
C	-0.42678600	2.62187900	-0.70020800
C	-0.58568400	2.42999900	0.70139200
H	0.29672000	2.74216300	2.65497900
H	2.33791500	3.83256800	1.76039900
H	2.61146400	4.17308300	-0.68146500
H	0.84741200	3.43155200	-2.25754800
H	-1.26009200	2.42709900	-1.36757600
H	-1.52899900	2.08117800	1.10726200
<b>TS<sub>2-3</sub>'</b>			
Pd	0.16761700	-0.36992700	-0.05832800
O	-1.77087500	-0.98469100	-0.01901400
O	-2.67745300	1.04098200	0.38195300
O	1.29650000	-2.23067500	-0.33864600
O	2.23452400	-0.24083100	-0.16035500

C	-4.12621900	-0.87471500	0.20135200
C	-2.73424300	-0.19958800	0.19094500
F	-4.15124600	-1.84224200	1.12971900
F	-4.36574200	-1.42313100	-1.00005900
F	-5.09304200	0.00550700	0.47195000
C	2.32351000	-1.50507600	-0.30291000
C	3.72468900	-2.13214600	-0.37909300
F	4.21298900	-2.27462500	0.86758000
F	4.55819600	-1.34574100	-1.07439900
F	3.67839500	-3.33487900	-0.95974300
C	0.33443000	2.21155200	1.42079300
C	0.96852200	3.44851400	1.47527800
C	1.15697300	4.18307000	0.29925100
C	0.70098400	3.69339300	-0.92956900
C	0.06512400	2.45718700	-0.98528100
C	-0.13785400	1.68798800	0.18958200
H	0.18054200	1.64593600	2.33592800
H	1.31675100	3.84310800	2.42510700
H	1.65651200	5.14695400	0.34181200
H	0.84314300	4.27665800	-1.83442100
H	-0.29951300	2.08326400	-1.93841100
H	-1.40985300	1.34770000	0.29634900
<b>3'</b>			
Pd	0.43343400	-0.13692900	-0.26112500
O	-1.63565000	-0.31560800	-0.56339000
O	-2.37423000	1.11610800	1.03707600
O	1.38133600	-2.22746500	-0.39506900
O	2.45614700	-0.34384000	0.06889300
C	-3.98863700	-0.22860400	-0.06759900
C	-2.51753400	0.19456700	0.12426500
F	-4.06632000	-1.30107000	-0.85037300

F	-4.65834000	0.78496300	-0.63812300
F	-4.54319900	-0.50259400	1.11903700
C	2.43276000	-1.60965900	-0.12480900
C	3.78023400	-2.34401800	-0.01032800
F	4.31448500	-2.13800600	1.20721300
F	4.63889200	-1.87555700	-0.93325000
F	3.63305200	-3.65961200	-0.19350400
C	0.91747900	2.40920900	1.11348300
C	0.89566400	3.80091300	1.26765600
C	0.31608400	4.60875700	0.28865100
C	-0.24985200	4.02658500	-0.84809200
C	-0.24538000	2.63726600	-1.00560300
C	0.34004400	1.82081900	-0.02307500
H	1.40246500	1.79015100	1.86277100
H	1.34329600	4.24801100	2.15094300
H	0.30726000	5.68802000	0.40855200
H	-0.69576700	4.65144700	-1.61710900
H	-0.68585500	2.19708800	-1.89638800
H	-1.43685900	1.43944900	1.03080300
<b>4</b>			
Pd	-0.08668900	0.20002400	-0.90278700
C	4.34535100	-0.63624400	-1.56141100
C	3.09289800	0.10391700	-1.16435600
O	1.98820400	-0.25324600	-1.60468800
O	3.28136600	1.11348800	-0.35826700
H	2.45867700	1.74041700	-0.30318800
O	1.51218500	2.90193200	-0.37515600
O	-0.15175800	2.11210500	-1.70789400
C	0.21761400	4.44566500	-1.65368100
C	0.58469400	3.00996000	-1.20024000
F	-0.26437400	4.46937500	-2.90596600



F	-0.72960700	4.94091600	-0.82983600
F	1.28197900	5.26167200	-1.60159900
H	4.63150900	-0.31225600	-2.56790000
H	4.14558700	-1.70879000	-1.60313000
H	5.16831400	-0.41377600	-0.88115600
C	-4.32856500	0.44488200	-0.82358200
C	-3.00887600	0.14983900	-1.18615100
C	-1.95636600	0.53287500	-0.34932300
C	-2.21971600	1.22347800	0.83821700
C	-3.54206300	1.51623200	1.19118700
C	-4.59755900	1.12585700	0.36450600
H	-5.14304700	0.14590400	-1.47857900
H	-2.81332800	-0.36590800	-2.12262900
H	-1.40515000	1.52801600	1.48853800
H	-3.74193600	2.05629500	2.11341400
H	-5.62239000	1.35759100	0.64077300
C	2.74724100	-1.34791500	2.73706300
C	3.26785100	-2.65927400	2.12982200
C	2.33163400	-2.97618200	0.96888500
C	1.41495200	-1.07859900	2.05151300
H	3.39904100	-0.49490200	2.52114200
H	2.59859400	-1.37941100	3.81875800
H	4.29305600	-2.60394300	1.75629600
H	3.22666200	-3.49776500	2.83236100
N	1.27342000	-2.03412300	1.01876600
S	0.01800000	-2.02844600	-0.18784800
C	-1.35945300	-2.78053300	0.68425100
C	-1.77212700	-4.02979000	0.20410000
C	-2.01063000	-2.16681700	1.76128200
C	-2.85449500	-4.67074200	0.80868000
H	-1.24846400	-4.49259500	-0.62635200

C	-3.08069500	-2.82675300	2.36342100
H	-1.68790700	-1.19456700	2.11015400
C	-3.50485700	-4.07092400	1.88784500
H	-3.18143400	-5.63795800	0.43960100
H	-3.59331000	-2.35921700	3.19849900
H	-4.34537600	-4.57185900	2.35912900
O	0.61610200	-0.20975800	2.30979000
O	2.43739500	-3.85722100	0.15176400
<b>TS<sub>4-5</sub></b>			
Pd	0.22586600	0.67201900	-0.22708400
C	4.16721700	-0.69454900	-2.22315100
C	3.28325800	0.18937900	-1.38836100
O	2.05387700	0.20544200	-1.54030200
O	3.92104000	0.90127300	-0.49007800
H	3.29729200	1.53887300	-0.00273400
O	2.55999300	2.71819000	0.69913500
O	0.53337300	2.73664200	-0.33062700
C	1.41705300	4.80100800	0.36454900
C	1.54387800	3.26089800	0.23442000
F	1.06792800	5.35734200	-0.80912000
F	0.46419800	5.10193900	1.27077500
F	2.56559600	5.36149300	0.76674800
H	3.68479900	-0.90669000	-3.17754900
H	4.29274000	-1.63470200	-1.67619400
H	5.14824700	-0.24063100	-2.37179600
C	-3.85717500	1.44122600	-0.83249500
C	-2.55272500	0.93320200	-0.90058800
C	-1.66993400	1.19021000	0.15302100
C	-2.06306500	1.92579800	1.26842000
C	-3.37293400	2.41749100	1.32103000
C	-4.26876100	2.17846600	0.27695000

H	-4.54459800	1.24692300	-1.65139300
H	-2.24787300	0.35929800	-1.76956900
H	-1.36947100	2.10873400	2.07775400
H	-3.68283100	3.00002800	2.18455200
H	-5.28199000	2.56640100	0.32770400
C	2.39671200	-0.19320200	3.57980700
C	3.35483400	-0.98682300	2.68423700
C	2.55384200	-1.26225200	1.40908300
C	1.22335100	0.16594100	2.66526600
H	2.81630300	0.72781900	3.99112700
H	2.00832000	-0.78135100	4.41772100
H	4.23745100	-0.40757200	2.39431400
H	3.70230800	-1.93387500	3.10354000
N	1.40298500	-0.47870100	1.44154800
S	-0.03362700	-1.58817300	-0.17786900
C	-0.99440900	-2.35866300	1.07795600
C	-0.65850800	-3.70501400	1.34177100
C	-2.06875900	-1.75756900	1.76127400
C	-1.40069700	-4.43961800	2.26084400
H	0.18293700	-4.15507900	0.82441900
C	-2.78966700	-2.49986500	2.69153700
H	-2.32295000	-0.72438300	1.56620100
C	-2.46462100	-3.83776900	2.93944800
H	-1.14365500	-5.47623100	2.45592000
H	-3.61452400	-2.03347100	3.22146500
H	-3.03971800	-4.40987400	3.66153700
O	0.29611100	0.88943600	2.96669600
O	2.88495800	-2.03153100	0.52762200
<b>5</b>			
Pd	0.01294900	-0.13138500	-0.71776300
C	3.74068800	-1.91976100	-2.33334600

C	2.94112800	-0.76122500	-1.80875200
O	1.73416300	-0.63813500	-2.08672100
O	3.59946100	0.06289400	-1.03986900
H	3.03820200	0.88656700	-0.79664000
O	2.42614500	2.25899100	-0.54885900
O	0.24345400	1.92808100	-1.09526600
C	1.05687200	4.13299500	-1.13809900
C	1.28822800	2.62004800	-0.88352500
F	0.95372200	4.34691100	-2.46857800
F	-0.07712500	4.55867000	-0.56017900
F	2.07043300	4.87344000	-0.67468500
H	3.34802800	-2.23265200	-3.30148400
H	3.61033100	-2.74687300	-1.62654800
H	4.80099100	-1.67329900	-2.39927300
C	-3.79250200	1.48671800	0.01079400
C	-2.52892400	1.17416700	-0.50748300
C	-1.71866300	0.29197200	0.20316200
C	-2.10974700	-0.25279700	1.42096500
C	-3.36644300	0.08441200	1.93176100
C	-4.20888700	0.94766700	1.22767000
H	-4.43397400	2.17133000	-0.53678300
H	-2.18927500	1.63771600	-1.42698700
H	-1.46664100	-0.93749300	1.96058200
H	-3.68328700	-0.33623500	2.88203900
H	-5.18305600	1.20650200	1.63189800
C	2.09455700	0.47775700	3.03479200
C	2.58580000	-0.92758000	2.66956100
C	1.85335300	-1.28724400	1.37401300
C	1.06607600	0.83020800	1.95949600
H	2.88312100	1.23519000	3.00419100
H	1.61839200	0.54435400	4.01678200

H	3.66092700	-0.98510400	2.47908800
H	2.34822100	-1.68744500	3.41998900
N	1.01902900	-0.22962300	1.03864900
S	-0.47847000	-2.30441600	-1.17537200
C	-1.62495000	-3.14723000	-0.12843100
C	-1.13368800	-4.11923400	0.76393000
C	-3.01293300	-2.95406500	-0.25681000
C	-2.02298100	-4.87814500	1.52185000
H	-0.06123100	-4.25773400	0.85479700
C	-3.89327800	-3.73320200	0.48935700
H	-3.38742700	-2.20063300	-0.94117700
C	-3.40139000	-4.69099200	1.38158100
H	-1.64200400	-5.62300300	2.21435000
H	-4.96408800	-3.58930100	0.38051600
H	-4.09228400	-5.29207900	1.96567300
O	0.40821600	1.84548900	1.91848100
O	1.99538200	-2.33328200	0.76538700
<b>TS<sub>4-6</sub></b>			
Pd	0.02308900	-0.00801200	-0.07380200
C	4.50757100	0.00983300	-0.10646800
C	3.11242400	-0.54837300	-0.06840300
O	2.13876500	0.15865300	-0.35371700
O	3.05299300	-1.80694500	0.30421900
H	2.13371800	-2.20259700	0.26757700
O	0.05093700	2.03510900	-0.32671400
O	0.54847800	2.10881000	1.88422100
C	0.44481200	4.15487800	0.61660000
C	0.34772900	2.61701100	0.78280400
F	1.41821100	4.47898500	-0.25947500
F	-0.71633400	4.66118100	0.15008100
F	0.71928000	4.76217800	1.78038900

H	4.84961800	0.16544700	0.92231200
H	4.51012800	0.96332700	-0.63271300
H	5.18904300	-0.70037700	-0.57981300
C	-3.94971000	0.27197400	-1.22159000
C	-2.72012300	-0.35869900	-1.06755200
C	-2.04355700	-0.30470600	0.17570800
C	-2.64928300	0.35172700	1.27068800
C	-3.88284500	0.97325600	1.10857600
C	-4.52754000	0.93686600	-0.13406600
H	-4.46093900	0.24400100	-2.17892400
H	-2.27085000	-0.89679800	-1.89775300
H	-2.14547000	0.38415700	2.23016600
H	-4.34271100	1.49174700	1.94440900
H	-5.49182400	1.42305700	-0.25221000
C	1.56911600	-5.69543900	-0.22871400
C	1.37952000	-5.08123900	-1.62019700
C	0.81454000	-3.68494300	-1.34104400
C	1.20674100	-4.56826200	0.75305100
H	2.58904200	-6.03051100	-0.02147700
H	0.90806200	-6.54623900	-0.03612000
H	2.31508800	-4.97519100	-2.17860000
H	0.68290200	-5.62582000	-2.26350500
N	0.84525900	-3.42069800	0.02777500
S	-0.84092800	-2.03201600	0.40911400
C	-0.83318600	-2.19610700	2.19685700
C	-1.51592600	-3.29368200	2.73458900
C	-0.18294300	-1.27519200	3.02958700
C	-1.54518100	-3.47369400	4.11594100
H	-2.00912200	-4.00323700	2.07804400
C	-0.21642600	-1.47054300	4.41007300
H	0.31649900	-0.40373300	2.61340300

C	-0.89294800	-2.56598000	4.95255600
H	-2.06968700	-4.32615100	4.53620300
H	0.28349900	-0.75888600	5.05986200
H	-0.91382200	-2.71034900	6.02868500
O	1.24486900	-4.65349000	1.96350100
O	0.39655800	-2.90434300	-2.18159300
<b>6</b>			
Pd	0.05538900	0.95448700	-0.30927500
C	4.15259500	-0.12934600	-0.87827500
C	2.68785200	-0.26793800	-0.47796100
O	2.02665200	0.84330700	-0.67112800
O	2.23869000	-1.32882300	-0.03581900
O	0.25228500	2.94577000	-0.64877700
O	-0.57958500	3.37017500	1.42134100
C	0.01679000	5.19996900	-0.02712000
C	-0.12178100	3.69722800	0.33197800
F	1.22312200	5.48105300	-0.54837600
F	-0.92139300	5.53637500	-0.94246500
F	-0.16411400	5.97763700	1.04931300
H	4.69480600	-1.03722200	-0.61357400
H	4.59570700	0.73817900	-0.38281300
H	4.21906300	0.04145900	-1.95676900
C	-3.73246900	0.61181800	-1.81063900
C	-2.78897300	-0.35375900	-1.49692700
C	-2.03357500	-0.21919900	-0.31228900
C	-2.22409500	0.89729300	0.54311900
C	-3.17552700	1.87440000	0.18088600
C	-3.91937100	1.73238100	-0.97933800
H	-4.32495100	0.50611500	-2.71439200
H	-2.62370400	-1.20588100	-2.14820400
H	-1.75310900	0.95687400	1.51875200

H	-3.30676000	2.73206300	0.83126100
H	-4.65265800	2.48537600	-1.25001200
S	-0.59318800	-1.26622900	-0.06056900
C	-0.66866200	-1.64333700	1.71051400
C	-1.86654600	-2.13380000	2.24349300
C	0.47889700	-1.51842600	2.49761600
C	-1.91774200	-2.47824600	3.59388500
H	-2.74748800	-2.24290900	1.61883100
C	0.41007900	-1.87364900	3.84627600
H	1.40246500	-1.17245300	2.04951900
C	-0.78200600	-2.34685900	4.39625800
H	-2.84573700	-2.85269500	4.01527100
H	1.29586000	-1.77479800	4.46616500
H	-0.82672400	-2.61664000	5.44700500
7			
Pd	-0.27784600	0.73737100	-0.30635900
O	0.12330300	2.76655200	-0.84251300
O	1.87402000	1.44249800	-0.50083400
C	2.30977400	3.76899800	-0.97583800
C	1.37414200	2.56383600	-0.77350400
F	3.48388800	3.38372700	-1.50014700
F	1.76472700	4.68748300	-1.78432900
F	2.55319800	4.34765600	0.21843900
C	-4.37881800	-0.10371700	-1.21395200
C	-2.98749900	-0.22395900	-1.11312200
C	-2.25403400	0.73581400	-0.40551900
C	-2.91432000	1.81381200	0.19690900
C	-4.30514100	1.92122600	0.09726200
C	-5.03941200	0.96390100	-0.60617800
H	-4.94032200	-0.84835400	-1.77225100
H	-2.49011500	-1.05581700	-1.60541200



H	-2.35121800	2.57809000	0.72509200
H	-4.81093200	2.76178700	0.56528000
H	-6.11907300	1.05346300	-0.68450100
C	3.56785900	-1.22425800	1.59842600
C	3.69450600	-2.40283200	0.61928600
C	2.30191500	-2.61603700	0.03744200
C	2.08755400	-0.87796800	1.64218900
H	4.09523000	-0.32950300	1.25408300
H	3.91827400	-1.44466200	2.60971100
H	4.38852400	-2.21635300	-0.20420700
H	4.00866600	-3.33308600	1.10213200
N	1.43988300	-1.69588700	0.68351300
S	-0.21264200	-1.51218300	0.19066000
C	-1.11584000	-2.00974300	1.66443200
C	-1.49295400	-3.35601500	1.74272600
C	-1.46346900	-1.09810100	2.66640400
C	-2.21852500	-3.79563100	2.85013600
H	-1.22339500	-4.04479000	0.94810000
C	-2.19363900	-1.55119100	3.76448900
H	-1.15616500	-0.06288300	2.58562000
C	-2.56852500	-2.89410900	3.85736400
H	-2.51550400	-4.83752900	2.91987400
H	-2.46887900	-0.85246900	4.54839700
H	-3.13881600	-3.23763500	4.71536700
O	1.53016900	-0.06941100	2.34414100
O	1.95778900	-3.41118000	-0.80182500
<b>8</b>			
Pd	0.22924800	0.18057800	-0.73315400
O	2.33585300	-0.38673500	1.27370600
O	2.27006000	0.23920100	-0.90850900
C	2.84593100	-0.11586700	0.18788800

C	4.38626100	-0.17869700	0.02843100
F	4.98543400	-0.57903300	1.16002700
F	4.88285800	1.03227500	-0.29671200
F	4.73052200	-1.04329200	-0.94891600
C	0.83426100	2.65067200	0.75632800
C	0.80718300	4.02920400	0.99135300
C	0.14930800	4.88704800	0.10733400
C	-0.48647000	4.36317100	-1.01837000
C	-0.47142400	2.98405000	-1.25999100
C	0.18931200	2.12836100	-0.37034900
H	1.36407200	1.99173300	1.43659100
H	1.31231000	4.43040400	1.86627000
H	0.13604300	5.95728700	0.29301400
H	-0.99670700	5.02262700	-1.71581300
H	-0.96582300	2.59208800	-2.14477800
C	-1.54054500	-3.85264900	-1.65745200
C	-3.07734000	-3.80562600	-1.56109100
C	-3.41836700	-2.40422400	-1.06503500
C	-1.07619100	-2.46819000	-1.25153300
H	-1.08407000	-4.58253800	-0.98235700
H	-1.16781200	-4.06799300	-2.66258600
H	-3.49288400	-4.53482000	-0.86056000
H	-3.57482600	-3.96301800	-2.52222600
N	-2.18907600	-1.71135400	-0.91534200
S	-2.06808200	-0.03399500	-0.39406700
C	-2.30211200	-0.20049900	1.38564600
C	-3.61390500	-0.10347200	1.86845400
C	-1.21369500	-0.37982700	2.25094800
C	-3.83790300	-0.19963600	3.24149100
H	-4.43954600	0.02870500	1.17768000
C	-1.45894100	-0.47372600	3.62143700

H	-0.19662500	-0.42795000	1.86872900
C	-2.76299900	-0.38399500	4.11453600
H	-4.85021100	-0.12709200	3.62684700
H	-0.62350500	-0.60820100	4.30138000
H	-2.94173100	-0.45246500	5.18361500
O	0.07615200	-2.05353800	-1.22749600
O	-4.50046200	-1.93060000	-0.82715200
<b>TS<sub>7-9</sub></b>			
Pd	-0.08142200	0.19429700	-0.41095000
O	0.53157000	2.13734900	-0.92188900
O	2.03829200	0.67529600	-1.68310300
C	2.49860700	3.03296700	-1.93962800
C	1.63052600	1.83423100	-1.50648000
F	3.39813100	2.67752300	-2.86594200
F	1.75129000	4.03183800	-2.43571500
F	3.16805100	3.50466800	-0.86398300
C	-4.20935800	1.11849100	-0.52953000
C	-2.97459500	0.48908200	-0.74017700
C	-1.89120400	0.86532600	0.05720100
C	-2.01078700	1.81789000	1.06793000
C	-3.25586900	2.42459900	1.26655200
C	-4.35157600	2.07882200	0.47128600
H	-5.05630200	0.84252400	-1.15186600
H	-2.87465500	-0.25906100	-1.51848500
H	-1.15813700	2.08017300	1.68296400
H	-3.35958900	3.17635300	2.04423400
H	-5.31328200	2.55662100	0.63321600
C	2.82406700	-0.42306500	2.81125500
C	3.57080100	-1.20145700	1.71710100
C	2.48640500	-1.58736500	0.70448900
C	1.45758100	-0.11098200	2.19523900

H	3.30331200	0.50972800	3.11719900
H	2.66023900	-1.01986400	3.71500100
H	4.30329700	-0.58003600	1.19167900
H	4.08429900	-2.10250700	2.05928400
N	1.35340800	-0.82174500	1.00426100
S	-0.43253000	-2.01941800	-0.06764700
C	-1.16901400	-2.56099100	1.43581700
C	-0.92320700	-3.91005200	1.77182100
C	-1.99570200	-1.77074900	2.25715300
C	-1.51315600	-4.46145800	2.90469100
H	-0.27247300	-4.50804000	1.14147600
C	-2.56243700	-2.33168700	3.39708200
H	-2.18142800	-0.73538800	2.00359400
C	-2.32991500	-3.67302100	3.72042700
H	-1.32821900	-5.50110500	3.15661500
H	-3.19528000	-1.72080300	4.03340700
H	-2.78524900	-4.10254500	4.60782700
O	0.61151000	0.62885600	2.66002600
O	2.58894600	-2.40514200	-0.18042100
<b>9</b>			
Pd	0.20283200	-0.05434400	-0.47015900
O	0.35777900	1.72228300	-1.74044800
O	1.81852300	0.08950600	-2.09676300
C	1.97189000	2.04595600	-3.50044900
C	1.35533300	1.22897000	-2.35128100
F	1.38097700	1.68132800	-4.65995000
F	1.78285700	3.35942600	-3.33045000
F	3.28603900	1.81109800	-3.60881000
C	-3.34586000	1.86081500	0.63609200
C	-2.19028000	1.40888800	-0.01443100
C	-1.38686800	0.46646500	0.63021200

C	-1.67781100	-0.00160200	1.90863200
C	-2.82891300	0.47315200	2.54598800
C	-3.66406600	1.39642900	1.91204000
H	-3.98069200	2.58996600	0.14057800
H	-1.92276800	1.80522200	-0.98854300
H	-1.03881400	-0.72833400	2.39599700
H	-3.06964300	0.11163500	3.54202900
H	-4.55586200	1.75833100	2.41531500
C	3.22457600	1.41732900	2.27786700
C	2.78143500	0.13971200	2.99902300
C	1.71373400	-0.47970500	2.09478000
C	2.34897100	1.48897100	1.02431000
H	4.27240600	1.40239800	1.96480500
H	3.07380500	2.33072100	2.85969800
H	3.58033100	-0.59353800	3.13926900
H	2.33378300	0.32217000	3.98051400
N	1.51171600	0.35986400	1.01363400
S	-0.02927100	-2.29559300	-0.36268800
C	-1.32251200	-3.01289200	0.59169100
C	-0.99389300	-3.89823100	1.63636500
C	-2.67209000	-2.81324200	0.23957200
C	-2.00532700	-4.57177300	2.31540700
H	0.04619100	-4.02923600	1.91154900
C	-3.67398000	-3.49936400	0.91836100
H	-2.91797700	-2.12913000	-0.56537700
C	-3.34291600	-4.37652500	1.95659500
H	-1.75213600	-5.25069900	3.12403800
H	-4.71294200	-3.35057000	0.64042900
H	-4.12828400	-4.90825200	2.48591500
O	2.38896400	2.36294700	0.18858400
O	1.15206100	-1.54003700	2.31624800

TS<sub>7-10</sub>

Pd	0.77636800	-0.89767300	1.09318300
O	3.15300600	-3.03978300	0.87122100
O	2.81780100	-0.81091300	1.19506300
C	3.52061800	-1.88886500	1.06859700
C	5.03436200	-1.57658000	1.20188900
F	5.42450300	-0.69356200	0.25914400
F	5.30531300	-1.03799600	2.40940900
F	5.78130800	-2.68141200	1.06629300
C	0.88582100	1.45819600	-0.59798400
C	1.03569200	2.82614800	-0.82448400
C	0.72801800	3.74741900	0.18472800
C	0.26270300	3.30754500	1.42504100
C	0.09894000	1.93919500	1.66622700
C	0.49164600	1.03158800	0.67755600
H	1.12324200	0.73948100	-1.37555900
H	1.39104100	3.17273600	-1.79059000
H	0.83009400	4.81142600	-0.00744400
H	0.00421400	4.02338400	2.20003500
H	-0.29708400	1.59907600	2.61778800
C	0.30886100	-5.18948900	1.31781300
C	0.66897100	-4.94273400	-0.15666300
C	0.36122100	-3.46696400	-0.39488500
C	0.01694700	-3.80274700	1.89777800
H	1.11378000	-5.64674900	1.89777000
H	-0.58528500	-5.80834600	1.44719400
H	1.73905900	-5.06902100	-0.34299400
H	0.11802600	-5.55781800	-0.87223100
N	0.11830100	-2.87623000	0.85311800
S	-1.50081700	-1.04246500	0.85849400
C	-2.30229600	-0.96334600	2.41238800

C	-3.70113900	-1.16472900	2.41297000
C	-1.63289900	-0.69622700	3.62601800
C	-4.41419300	-1.07044300	3.60229800
H	-4.21127100	-1.38596300	1.48062300
C	-2.35627100	-0.62121700	4.80907300
H	-0.55426900	-0.58683500	3.62811800
C	-3.74501000	-0.80023000	4.80064200
H	-5.48985300	-1.21624100	3.59875500
H	-1.83823500	-0.42846100	5.74322300
H	-4.30373200	-0.73570900	5.72939500
O	-0.23967500	-3.53392100	3.05259800
O	0.34758300	-2.87362900	-1.45213700

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Pd	-0.20435900	0.10493100	-0.67074800
O	2.56918300	-1.95071100	-0.51892500
O	1.79502500	0.20089600	-0.65242600
C	2.68583600	-0.74233700	-0.59381100
C	4.10358100	-0.10244400	-0.64328800
F	4.28390300	0.56242400	-1.80550200
F	4.27139300	0.78002500	0.36412000
F	5.06281700	-1.03001000	-0.54494100
C	-0.50513300	2.42823700	-1.68164100
C	0.46929800	3.43574400	-1.57374600
C	0.53764100	4.22137600	-0.43225700
C	-0.37090100	4.01886100	0.61996000
C	-1.33163900	3.01979900	0.55035100
C	-1.39358800	2.21468800	-0.60184600
H	-0.61933500	1.88465000	-2.61575300
H	1.15931400	3.59190000	-2.39604200
H	1.29162700	4.99762100	-0.35149500
H	-0.31600500	4.64150900	1.50769700

H	-2.01667100	2.84771900	1.37234200
C	0.09934800	-3.98731800	0.49501600
C	-0.03639800	-4.12986500	-1.02910000
C	-0.26735100	-2.70297300	-1.53226200
C	-0.13825600	-2.50206100	0.76839100
H	1.10238600	-4.23023700	0.85577400
H	-0.61476800	-4.58587300	1.06789900
H	0.86333600	-4.51955700	-1.51139200
H	-0.87634300	-4.75993200	-1.33767100
N	-0.35139300	-1.86396200	-0.43282100
S	-2.46885500	0.77051900	-0.78003400
C	-3.31415500	0.62380300	0.80176300
C	-4.61509800	1.14080400	0.87452500
C	-2.72434100	-0.02655100	1.89225900
C	-5.32749000	1.02415500	2.06750500
H	-5.06265400	1.62391200	0.01130800
C	-3.45646500	-0.13738900	3.07670300
H	-1.72734100	-0.45879500	1.82710600
C	-4.74753000	0.38657400	3.16725100
H	-6.33420700	1.42505600	2.13374700
H	-3.00904000	-0.64471700	3.92569200
H	-5.30719600	0.29149100	4.09305000
O	-0.15493500	-1.96377600	1.86814300
O	-0.37721100	-2.34902400	-2.69324100

**TS<sub>8-11</sub>**

Pd	0.16205100	0.36799000	0.61597600
C	0.96466600	2.62680800	-0.97277400
C	1.19938800	3.97471000	-1.25916200
C	1.22605400	4.91872500	-0.22827900
C	1.02636100	4.51764000	1.09433000
C	0.79397900	3.17182400	1.40023300



C	0.71425700	2.25242800	0.35110100
H	0.96357300	1.88938100	-1.77049100
H	1.37178700	4.28044200	-2.28738600
H	1.42493700	5.96224800	-0.45461200
H	1.06897500	5.24627300	1.89935800
H	0.69023600	2.84813100	2.42949500
C	-0.42112800	-4.13399100	0.78379900
C	0.04056500	-3.84878700	-0.65436900
C	-0.04306600	-2.32582600	-0.79168500
C	-0.71498800	-2.75293800	1.38700500
H	0.33932300	-4.62587700	1.39689500
H	-1.32690800	-4.74455600	0.84339700
H	1.07143300	-4.15736000	-0.85082900
H	-0.58724400	-4.30937700	-1.42251100
N	-0.40708800	-1.78239400	0.43323900
S	-2.00717800	0.03968600	0.25438500
C	-2.83873600	0.16935000	1.77665600
C	-4.13851900	-0.38777200	1.84566900
C	-2.27952100	0.80677500	2.90931300
C	-4.87420700	-0.27705300	3.01701300
H	-4.54933600	-0.89489500	0.97851900
C	-3.01603500	0.87879500	4.08292900
H	-1.27020600	1.20065400	2.86396200
C	-4.31178300	0.34915500	4.13622200
H	-5.87581600	-0.69151700	3.06957800
H	-2.58361800	1.34979800	4.95962400
H	-4.88421700	0.42046200	5.05630500
O	-1.14437300	-2.53210000	2.50139800
O	0.17885100	-1.67240600	-1.79579700
O	1.44860800	0.61270900	3.20201900
O	2.14203700	0.02059500	1.13131700

C	2.29079000	0.22695900	2.39422900
C	3.73862900	-0.06185200	2.86304500
F	4.08058200	-1.33801000	2.59105200
F	4.61043000	0.74642300	2.22791600
F	3.87830100	0.13186700	4.18118900

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Pd	0.04605600	-0.59514000	-0.34618600
C	0.91542000	1.40491900	-2.33571400
C	1.31865100	2.67975000	-2.75714600
C	1.23401900	3.77565400	-1.89968100
C	0.73558500	3.60842100	-0.60737000
C	0.33207900	2.34507000	-0.15849500
C	0.45190700	1.26917200	-1.03320300
H	0.93371100	0.57509700	-3.03068900
H	1.68730300	2.80090400	-3.77177300
H	1.54550700	4.75888200	-2.23979300
H	0.65658100	4.45672000	0.06700700
H	-0.05079800	2.21955400	0.84642000
C	-0.28606900	-4.11084000	-2.40094900
C	-0.26312600	-3.36454500	-3.74691700
C	-0.12461800	-1.87029400	-3.39393200
C	-0.18657300	-2.98495900	-1.39273200
H	0.55386500	-4.79877000	-2.26530300
H	-1.20351900	-4.67970900	-2.22396900
H	0.57493600	-3.64671200	-4.38973100
H	-1.17865900	-3.49508300	-4.33053400
N	-0.07621200	-1.77342600	-2.00678200
S	-2.23347800	-0.24878200	-0.61025700
C	-2.71212700	0.32072500	0.99055900
C	-2.86546200	-0.58556900	2.05850600
C	-3.01411300	1.68282000	1.18623000

C	-3.31372600	-0.13354700	3.29609600
H	-2.62740600	-1.63277100	1.90299000
C	-3.47568100	2.12371000	2.42422300
H	-2.89062100	2.37616200	0.36087000
C	-3.62123300	1.21846200	3.47959500
H	-3.42709600	-0.83393100	4.11805600
H	-3.71772600	3.17245900	2.56880400
H	-3.97494700	1.56639500	4.44581100
O	-0.20086700	-3.04342600	-0.15380800
O	-0.06050900	-0.96213800	-4.19680100
O	0.41853200	0.03750100	1.60104300
O	2.17686500	-0.83772700	0.58030500
C	1.64438300	-0.34109400	1.59065900
C	2.44047700	-0.12111100	2.88846800
F	3.63375500	-0.71747300	2.83198500
F	2.62787100	1.19877300	3.07868900
F	1.76305400	-0.60767500	3.94094200

**TS<sub>8-12</sub>**

Pd	0.22250900	-0.89352600	-0.56448300
O	2.26683400	-1.10499500	1.50237500
O	2.29000000	-0.79966500	-0.74256700
C	2.82545200	-0.93349800	0.41688900
C	4.36878400	-0.81281800	0.37141200
F	4.93163500	-1.18103600	1.53274500
F	4.72222100	0.47095300	0.13159400
F	4.89935300	-1.57365500	-0.60486400
C	0.05770500	1.56618300	1.20833000
C	0.45195200	2.89974200	1.28456500
C	0.29837900	3.74094000	0.17693900
C	-0.25121700	3.25766700	-1.01462400
C	-0.64705100	1.92546200	-1.09857800

C	-0.47884100	1.06302600	0.00634700
H	0.18939100	0.91336300	2.06315200
H	0.88512000	3.28362300	2.20329500
H	0.60390800	4.78114800	0.24553700
H	-0.37341300	3.91776000	-1.86803500
H	-1.08993300	1.54851600	-2.01649200
C	-1.69936900	-4.72029500	-1.42926100
C	-3.21838600	-4.65925400	-1.18659600
C	-3.47245000	-3.23015600	-0.68649700
C	-1.20953900	-3.32673100	-1.06195300
H	-1.18100700	-5.45200300	-0.80264100
H	-1.42335100	-4.93263500	-2.46610300
H	-3.56882700	-5.36837300	-0.43145000
H	-3.81173500	-4.83074200	-2.08913500
N	-2.24272500	-2.55993500	-0.64789900
S	-1.89169100	-0.56471200	-0.10820500
C	-2.16097800	-0.89540300	1.64243300
C	-3.46371600	-0.71132700	2.11843300
C	-1.13208000	-1.34281100	2.48253300
C	-3.73735300	-0.96835300	3.46227200
H	-4.25261000	-0.39849700	1.44310000
C	-1.42577900	-1.59725100	3.82274200
H	-0.11957200	-1.47561100	2.10661600
C	-2.72122800	-1.40885300	4.31247500
H	-4.74587500	-0.83028300	3.83960600
H	-0.63465700	-1.93890600	4.48321800
H	-2.93842700	-1.60764800	5.35783900
O	-0.01561100	-2.96797200	-1.14318500
O	-4.53534400	-2.74049400	-0.37319900
<b>12</b>			
Pd	0.13475900	0.25974300	-0.89251000

O	2.43857600	0.47479600	0.85195900
O	2.11258100	0.07340200	-1.35314900
C	2.82529300	0.23833100	-0.28875700
C	4.34068300	0.13198500	-0.59185800
F	5.07343200	0.24031900	0.52475900
F	4.71642600	1.12247500	-1.43175600
F	4.63951800	-1.04236000	-1.17664200
C	-0.51147100	2.83636300	1.28230500
C	0.51354800	3.76617800	1.34395300
C	1.23729100	4.12873300	0.19257600
C	0.90529600	3.58573700	-1.03635600
C	-0.15026100	2.65493800	-1.13655300
C	-0.84868600	2.26554500	0.03934000
H	-1.04283200	2.54066900	2.17863200
H	0.77048400	4.21018400	2.30084200
H	2.04932000	4.84439700	0.27064000
H	1.43728000	3.87860400	-1.93552600
H	-0.51765000	2.37570800	-2.12201100
C	-1.26724500	-3.80782700	-1.49177600
C	-2.76692500	-4.08466600	-1.33075000
C	-3.34960700	-2.70938000	-0.94098000
C	-1.18360700	-2.31200900	-1.19379500
H	-0.63167700	-4.35627000	-0.78987900
H	-0.87831700	-4.00232700	-2.49586300
H	-2.99846700	-4.81331100	-0.54874000
H	-3.24833900	-4.43408200	-2.24880200
N	-2.33624800	-1.74439000	-0.91523100
S	-1.98559700	0.88571500	-0.23961600
C	-2.30725300	0.25215600	1.41451600
C	-3.64992800	0.11283600	1.77523400
C	-1.27453600	-0.15047900	2.27084400

C	-3.96335400	-0.41560700	3.02817200
H	-4.43627900	0.38121700	1.07816100
C	-1.60603600	-0.67260600	3.52086500
H	-0.23431000	-0.06606500	1.96896900
C	-2.94510000	-0.80295000	3.90026600
H	-5.00393500	-0.53355300	3.31318500
H	-0.81348700	-0.98643800	4.19325700
H	-3.19359800	-1.21716000	4.87280500
O	-0.03508900	-1.74008200	-1.22803300
O	-4.51733500	-2.48863500	-0.68498400

**TS<sub>12-13</sub>**

Pd	0.26448000	0.21861600	0.28526800
O	1.08434600	2.25459400	1.98662400
O	2.18786600	0.74143600	0.73528600
C	2.11318600	1.73582400	1.55206500
C	3.49927100	2.29451800	1.94914700
F	4.30741200	1.31971000	2.40175900
F	4.08973700	2.86195100	0.87477700
F	3.39407500	3.22830400	2.90426100
C	-0.67661600	2.20951300	-1.16159500
C	-0.28107200	3.55573200	-1.18485000
C	-0.91387100	4.47920100	-0.36378400
C	-1.95480500	4.06951800	0.48311700
C	-2.34775800	2.73876700	0.53988400
C	-1.70323200	1.79646700	-0.27830600
H	-0.26082500	1.51819300	-1.89173100
H	0.51010100	3.86569500	-1.85986200
H	-0.61128400	5.52131700	-0.38204400
H	-2.45738800	4.79900800	1.11093700
H	-3.13963700	2.42910000	1.21099500
C	0.50767600	-4.11663500	0.56842900

C	-0.76103000	-4.93664700	0.30119300
C	-1.83124700	-3.86405000	0.00688000
C	0.00786700	-2.68560300	0.37689200
H	1.32738800	-4.31451200	-0.12872700
H	0.91098500	-4.23052800	1.57917400
H	-0.67496700	-5.60709100	-0.55885000
H	-1.07859200	-5.54470100	1.15295500
N	-1.26354500	-2.58746200	0.06214000
S	-1.96193400	0.00482800	-0.26471700
C	-2.90970800	-0.28854100	1.23883000
C	-4.05492400	-1.07878900	1.10803000
C	-2.48702000	0.18239700	2.48806400
C	-4.80681600	-1.37311900	2.24604100
H	-4.32335400	-1.50120700	0.14615800
C	-3.25278000	-0.11793300	3.61471600
H	-1.57651100	0.76641700	2.58311200
C	-4.41210000	-0.88901300	3.49429500
H	-5.69239200	-1.99377200	2.15369100
H	-2.93467600	0.24448100	4.58748800
H	-4.99954400	-1.12351400	4.37699800
O	0.83291700	-1.71699300	0.53708000
O	-3.00272600	-4.08595600	-0.23440700

**13**

Pd	0.87488200	-0.44440700	-0.16643000
O	1.28038600	1.19750800	1.06810600
O	2.86373600	-0.29087800	0.69426600
C	2.47021400	0.77501000	1.23727700
C	3.43809500	1.62636900	2.07325100
F	4.46592900	0.89491100	2.51279100
F	3.91681300	2.62584300	1.30748900
F	2.80535900	2.16459200	3.12554200

C	-0.37362000	2.24925600	-1.83655500
C	-0.50853600	3.54418300	-2.34148800
C	-1.73394600	4.20569100	-2.26375100
C	-2.83317900	3.56671100	-1.68462800
C	-2.71266900	2.27195200	-1.18246700
C	-1.47544300	1.61843500	-1.25088200
H	0.58319100	1.73928900	-1.89084400
H	0.35119800	4.03438800	-2.78800800
H	-1.83383600	5.21455600	-2.65231300
H	-3.79113700	4.07460800	-1.62519900
H	-3.56998500	1.77836400	-0.73720900
C	0.42167300	-4.32401100	-2.01226600
C	-0.82327000	-5.14194700	-1.64530500
C	-1.63767400	-4.17710600	-0.75629600
C	0.18527700	-3.03672700	-1.22997100
H	0.50655400	-4.09889700	-3.08015100
H	1.36839600	-4.77674300	-1.70257100
H	-1.42574900	-5.44293600	-2.50647800
H	-0.59422500	-6.04890100	-1.07776500
N	-0.92294500	-2.99680400	-0.53198500
S	-1.35825300	-0.11875700	-0.75234600
C	-2.22055400	-0.12815300	0.83813500
C	-3.05799400	-1.21556100	1.11061400
C	-2.03543700	0.90238300	1.76902400
C	-3.73076900	-1.25232100	2.33366500
H	-3.15502600	-2.03830300	0.41043900
C	-2.71895300	0.84794800	2.98262000
H	-1.36698300	1.72811800	1.55305500
C	-3.56762900	-0.22598700	3.26508300
H	-4.37923900	-2.09478700	2.55317900
H	-2.58037400	1.64283700	3.70932000



H	-4.09537000	-0.26409800	4.21356500
O	1.04866300	-2.08444600	-1.30423100
O	-2.75392900	-4.39697000	-0.32235200

**TS<sub>12-14</sub>**

Pd	0.05997700	0.36139400	-0.93470100
O	2.48838100	0.62768500	0.75586100
O	1.99426000	0.21971000	-1.42156100
C	2.78262300	0.37293900	-0.40214000
C	4.26558400	0.20823500	-0.82417500
F	5.08331700	0.31500900	0.23106800
F	4.60886800	1.16329400	-1.71499000
F	4.47578500	-0.99071900	-1.39872600
C	-0.43387200	2.69075700	1.34448900
C	0.62245900	3.57964700	1.44629300
C	1.28192800	4.05630600	0.29687800
C	0.86900000	3.66309300	-0.96470600
C	-0.21715500	2.77435300	-1.11138200
C	-0.84671400	2.27727300	0.06311800
H	-0.92134000	2.29694500	2.22857300
H	0.95826500	3.89552700	2.42881600
H	2.11540900	4.74297600	0.40440700
H	1.35851300	4.04573900	-1.85406200
H	-0.64914100	2.60926800	-2.09465400
C	-0.27702700	-3.60174600	-2.32789700
C	-0.64490500	-3.33661300	-3.79818300
C	-0.78186200	-1.79770700	-3.88538900
C	-0.21235700	-2.19502600	-1.75332300
H	-1.01987900	-4.19387200	-1.78366900
H	0.69018600	-4.09526000	-2.19181800
H	-1.58492100	-3.80209400	-4.10787300

H	0.12426700	-3.66605100	-4.50282100
N	-0.49087400	-1.24503300	-2.63895100
S	-2.09625000	1.02326500	-0.27488100
C	-2.50933200	0.33478300	1.33537900
C	-3.67285300	0.80687900	1.95605000
C	-1.72892300	-0.67213800	1.91576200
C	-4.04615100	0.27722300	3.19120100
H	-4.27636800	1.57420200	1.48077100
C	-2.12063900	-1.19310900	3.15024600
H	-0.85017100	-1.05175200	1.40480100
C	-3.26975500	-0.71953900	3.78718100
H	-4.94376700	0.63992000	3.68228500
H	-1.52394900	-1.97517400	3.60916600
H	-3.56566500	-1.13298100	4.74667000
O	0.07973900	-1.90963500	-0.55599800
O	-1.10010600	-1.18185200	-4.88302000

**TS<sub>13-14</sub>**

Pd	0.84838000	-0.36264800	-0.27378800
O	1.60735600	1.18284800	1.08010700
O	2.86422200	-0.45195500	0.30129500
C	2.72237200	0.59259600	1.00480800
C	3.94066600	1.18323700	1.73073700
F	4.84732900	0.23785500	1.99911000
F	4.51260900	2.11563700	0.94403000
F	3.57029400	1.76849600	2.87801800
C	-0.83598100	2.75596600	-0.55604300
C	-0.94171200	4.05169400	-1.06013300
C	-1.69261500	4.30425700	-2.21200600
C	-2.34449500	3.25943500	-2.86824500
C	-2.25044800	1.95726500	-2.37407400
C	-1.50011400	1.71412700	-1.21825200

H	-0.23988600	2.55643700	0.32741900
H	-0.42840800	4.86391200	-0.55461700
H	-1.76491000	5.31601400	-2.59958500
H	-2.92495300	3.45292400	-3.76495700
H	-2.75042300	1.13759500	-2.88031000
C	0.57403000	-3.97273200	-2.50423000
C	0.10265500	-4.91920100	-1.38436300
C	-0.14340700	-3.98433200	-0.17904200
C	0.61887600	-2.62581700	-1.79687100
H	-0.11362900	-3.92016200	-3.35436000
H	1.56347200	-4.21099900	-2.90576200
H	-0.81766400	-5.46092400	-1.61959000
H	0.85314300	-5.66611500	-1.10793500
N	0.23270100	-2.69325900	-0.52064800
S	-1.37827000	0.00090200	-0.68194700
C	-2.16149100	-0.02898400	0.95310300
C	-2.00215300	-1.19798700	1.71111800
C	-2.96879200	1.02029200	1.40322500
C	-2.65266700	-1.29474800	2.94116600
H	-1.38710100	-2.02282100	1.36303400
C	-3.61026800	0.90224600	2.63719500
H	-3.10191000	1.91510200	0.80696900
C	-3.45198900	-0.24967100	3.40874600
H	-2.52615700	-2.19755900	3.53046700
H	-4.23556800	1.71666500	2.99074700
H	-3.95185200	-0.33333400	4.36903800
O	0.97042600	-1.53207200	-2.30508300
O	-0.61112600	-4.32518800	0.89403500
<b>14</b>			
Pd	0.48202800	-0.53935700	-0.06665000
O	1.15411500	1.04149400	1.19389300

O	2.52377000	-0.58682300	0.60602000
C	2.30287500	0.49730300	1.21084000
C	3.44925900	1.21569800	1.93993900
F	4.42187400	0.36133000	2.27233000
F	3.96366800	2.15928500	1.12792100
F	2.99959800	1.81516200	3.05200300
C	-0.96507000	2.52436500	-0.94938600
C	-1.08287200	3.74095800	-1.62240500
C	-2.07612000	3.92216400	-2.58811400
C	-2.96076400	2.88487100	-2.88719600
C	-2.85473700	1.66237100	-2.22247900
C	-1.85940000	1.49004000	-1.25359700
H	-0.19111900	2.38127900	-0.20321700
H	-0.39061400	4.54546600	-1.39377100
H	-2.15675600	4.87058200	-3.11070800
H	-3.73031900	3.02144600	-3.64069700
H	-3.53384100	0.84811800	-2.45498600
C	0.80189600	-3.70782100	-2.93476000
C	-0.18533300	-4.35010800	-1.94872100
C	-0.43311200	-3.27133800	-0.88947900
C	1.02870700	-2.29293800	-2.38944500
H	0.42281800	-3.63936900	-3.95828000
H	1.76667100	-4.22151100	-2.98264900
H	-1.14254100	-4.62522100	-2.40179300
H	0.20446600	-5.24511300	-1.45509200
N	0.31726600	-2.16106700	-1.20368700
S	-1.76501700	-0.13421700	-0.47888300
C	-2.47019400	0.09822300	1.17666100
C	-2.57138500	-1.06121800	1.95713800
C	-2.92984500	1.33113000	1.64233700
C	-3.13886400	-0.96766900	3.22701800

H	-2.20222800	-2.00800900	1.57217500
C	-3.49950700	1.40208200	2.91577900
H	-2.84967900	2.22237700	1.03138600
C	-3.60341600	0.25905200	3.70862000
H	-3.21739100	-1.86050200	3.83998900
H	-3.85898600	2.35815000	3.28448500
H	-4.04465300	0.32315200	4.69869700
O	1.70817600	-1.42143400	-2.89985600
O	-1.18361900	-3.37552100	0.07273400

**TS<sub>14-15</sub>**

Pd	0.76130500	-0.56079000	-0.01705700
O	1.87876300	0.88579000	0.94940400
O	2.61989400	-1.18990700	1.04360200
C	2.72409900	0.02128700	1.35931400
C	3.84822700	0.47872500	2.30170200
F	4.11607400	1.77946100	2.13091100
F	3.46281600	0.28522900	3.57666700
F	4.96472800	-0.22671100	2.08280100
C	-0.99217400	2.68641400	1.12255900
C	-1.34497900	3.97627800	0.72927700
C	-2.64231400	4.25229200	0.28655600
C	-3.59564500	3.23479900	0.24497300
C	-3.25879500	1.94223500	0.65459300
C	-1.95679600	1.66802600	1.09218100
H	0.02220700	2.46590200	1.43632400
H	-0.59804000	4.76419800	0.75257900
H	-2.90596700	5.25737400	-0.02892100
H	-4.60435200	3.44308000	-0.09876000
H	-4.00012000	1.14944800	0.63705200
C	0.25959600	-4.16802700	-2.23134000
C	-0.44692900	-4.57027100	-0.93009100

C	-0.43989100	-3.30189300	-0.07416700
C	0.50525400	-2.66545600	-2.09157800
H	-0.32309400	-4.35730400	-3.13703400
H	1.22839200	-4.65903600	-2.36480600
H	-1.48467100	-4.88451800	-1.08177100
H	0.05288800	-5.36986100	-0.37757700
N	-0.00114400	-2.22559200	-0.85535700
S	-1.55677600	-0.03891900	1.47981100
C	-0.94594000	0.00666200	3.17581500
C	-0.21782200	-1.10633000	3.61818400
C	-1.22975900	1.06106000	4.04986500
C	0.23685300	-1.14673400	4.93604000
H	-0.02601000	-1.93186100	2.94058100
C	-0.76278300	1.00682600	5.36447700
H	-1.80559300	1.91582600	3.71404200
C	-0.02740500	-0.09139600	5.81162700
H	0.80500400	-2.00829300	5.27429500
H	-0.98080500	1.82966500	6.03928300
H	0.33551100	-0.12554400	6.83438800
O	1.03310300	-1.93952100	-2.91114000
O	-0.76758000	-3.23091800	1.09555400
C	-1.82404600	1.58862000	-3.16438800
F	-1.72569100	1.13918000	-4.42522400
F	-3.12329900	1.74868500	-2.86655300
F	-1.20926200	2.76625500	-3.07239600
C	-1.18093400	0.56594900	-2.20422000
O	-0.14289900	0.82322800	-1.61582000
O	-1.87656100	-0.54333800	-2.12358700
H	-1.37083800	-1.19645400	-1.56488400
<b>15</b>			
Pd	0.27195400	0.18998200	-0.05428700

O	1.11299500	2.12045600	-0.32179200
O	2.32289700	0.31523500	-0.00278700
C	2.24424900	1.57379900	-0.19285100
C	3.53262800	2.40933700	-0.21700300
F	3.92971700	2.64019400	1.04583100
F	3.32294200	3.57923600	-0.82522400
F	4.50267400	1.74643700	-0.85852100
C	0.91750600	-4.00508000	-0.20038100
C	0.90448500	-3.77789800	1.31858100
C	0.39815600	-2.34663300	1.50341700
C	0.42463000	-2.68917300	-0.80431600
H	1.91156900	-4.21692500	-0.60405100
H	0.26018800	-4.81555700	-0.52929500
H	1.89256700	-3.85378900	1.78130700
H	0.24507700	-4.46213600	1.86075900
N	0.05177100	-1.81330600	0.24064400
O	0.33521700	-2.41817400	-1.98261400
O	0.28203300	-1.74604700	2.54996500
C	-4.12798600	0.29286100	-0.15802400
F	-4.61376500	0.38613100	1.08929500
F	-4.88416300	-0.55985700	-0.85694600
F	-4.16658900	1.49218000	-0.73434000
C	-2.67530500	-0.22413700	-0.08030200
O	-1.74787900	0.58808300	-0.19513500
O	-2.57228200	-1.49063200	0.13579900
H	-1.57155600	-1.72691600	0.20119600

**TS<sub>14-15'</sub>**

Pd	0.72976700	-0.56624000	0.02022300
O	1.83468600	0.91559000	0.93893400
O	2.71430900	-1.11123600	0.99334800
C	2.75439200	0.10268400	1.29720000

C	3.89614600	0.64465000	2.17214000
F	4.10236600	1.94885900	1.94136800
F	3.57227900	0.48912900	3.47011800
F	5.03401400	-0.01997200	1.93647800
C	-1.00685300	2.66509200	1.09774300
C	-1.40286900	3.96197800	0.77182300
C	-2.73894800	4.24006200	0.46882000
C	-3.68769600	3.21718900	0.49707700
C	-3.30479000	1.91702900	0.83510100
C	-1.96480900	1.64136500	1.13586100
H	0.03323700	2.44560300	1.31155900
H	-0.66128700	4.75496300	0.74437900
H	-3.03823300	5.25184600	0.21101700
H	-4.72761800	3.42828500	0.26558600
H	-4.03961300	1.11884500	0.87149300
C	0.14715500	-4.17805200	-2.19227900
C	-0.55091600	-4.56577000	-0.88288200
C	-0.50196400	-3.29831700	-0.02611400
C	0.45873300	-2.68793300	-2.03892800
H	-0.46335700	-4.32829200	-3.08711500
H	1.08994200	-4.70920900	-2.35397900
H	-1.59714100	-4.85812300	-1.01812100
H	-0.05952000	-5.37603900	-0.33795400
N	-0.01376400	-2.24382000	-0.79652900
S	-1.52509000	-0.06684400	1.48003500
C	-0.94772700	-0.03748100	3.19116700
C	-0.25780700	-1.16928400	3.64671400
C	-1.21829100	1.02487500	4.05917500
C	0.16956700	-1.22159900	4.97292000
H	-0.07500300	-1.99841500	2.97126700
C	-0.77917600	0.95786000	5.38313300



H	-1.76229700	1.89605500	3.71319700
C	-0.08356000	-0.15979600	5.84433300
H	0.70774100	-2.09817900	5.32160200
H	-0.98689500	1.78720100	6.05327800
H	0.25804100	-0.20396600	6.87407600
O	1.01202200	-1.98193700	-2.86090000
O	-0.84023200	-3.22164000	1.14237800
C	-1.50065900	1.54789900	-3.43347600
C	-1.05366400	0.61055900	-2.34815300
O	-0.06579700	0.82217000	-1.64853700
O	-1.82414800	-0.46562000	-2.22445400
H	-1.40053200	-1.08077800	-1.58126900
H	-2.58246900	1.69284200	-3.38692900
H	-1.26386400	1.09805100	-4.40326500
H	-0.97899900	2.49894500	-3.33774200
<b>15'</b>			
Pd	0.69565100	-0.33161100	-1.11988800
O	1.86275100	1.11194500	-0.06949400
O	2.25113900	-1.05031700	0.02795600
C	2.53716700	0.14133700	0.37551900
C	3.67590800	0.37512000	1.37910700
F	4.18582200	1.60250600	1.23619800
F	3.19380700	0.25029500	2.62826300
F	4.64916300	-0.52662500	1.20341200
C	0.42055800	-4.25441300	-2.76315800
C	-0.46415600	-4.41274200	-1.51798600
C	-0.64431900	-2.99227400	-0.97638300
C	0.70230700	-2.75283900	-2.86049000
H	-0.05805100	-4.58821700	-3.68871000
H	1.37723200	-4.77953200	-2.69137200
H	-1.44805500	-4.84266000	-1.72779100

H	-0.00968700	-5.02379900	-0.73292300
N	-0.01212200	-2.08706600	-1.84821900
O	1.40567500	-2.20054200	-3.68161400
O	-1.24731300	-2.67203800	0.02719600
C	-2.49408700	1.63581900	-3.40050700
C	-1.61773300	0.57542800	-2.80641000
O	-0.65438000	0.88386000	-2.07536500
O	-1.93495100	-0.65276500	-3.10830100
H	-1.27487400	-1.27611100	-2.66789600
H	-3.53072700	1.45678600	-3.10127900
H	-2.44958800	1.56813600	-4.49154300
H	-2.16888700	2.62110600	-3.07111100

**TS<sub>15-16</sub>**

Pd	0.18709900	0.15395400	-0.03413700
O	1.06934200	2.05642900	-0.27538000
O	2.25103400	0.22893800	0.01574700
C	2.19313200	1.49063200	-0.15810300
C	3.49272300	2.30847100	-0.17822500
F	3.89769900	2.51858100	1.08571600
F	3.29870600	3.48712200	-0.77299000
F	4.44989500	1.63675100	-0.83037200
C	1.14829700	-3.88587500	-0.23028800
C	1.10670600	-3.67581800	1.28942600
C	0.29043900	-2.40620300	1.50761300
C	0.36996000	-2.71888300	-0.82857700
H	2.15929300	-3.87447400	-0.64754000
H	0.67985800	-4.81955800	-0.55571700
H	2.09401200	-3.52769700	1.73679500
H	0.63004800	-4.49608700	1.83402400
N	-0.14237000	-1.89259900	0.23360700
O	0.17784300	-2.48890200	-1.99654600

O	0.01743900	-1.88294000	2.55901800
C	-4.13933200	0.33301400	-0.15116500
F	-4.42722400	0.92449600	1.02067900
F	-5.04160000	-0.62352000	-0.38330600
F	-4.21571300	1.24751500	-1.12532100
C	-2.71110700	-0.25753100	-0.07392700
O	-1.78419100	0.59672200	-0.16274300
O	-2.59982600	-1.49688400	0.09614500
H	-1.35999300	-1.77328200	0.17594200

**16**

Pd	0.15499200	0.07419800	-0.00533900
O	1.04630700	1.98184600	-0.22428400
O	2.22635200	0.15275600	0.07108800
C	2.16734900	1.41774600	-0.09391200
C	3.46707900	2.23563100	-0.08552800
F	3.85881200	2.41944300	1.18664200
F	3.28182300	3.42448100	-0.65987500
F	4.42982100	1.57276900	-0.74000400
C	1.71720900	-3.34506700	-0.33430800
C	1.72399100	-3.12244900	1.18630900
C	0.41910300	-2.40931000	1.51006500
C	0.43242800	-2.70899300	-0.84654600
H	2.56097900	-2.86760600	-0.84139500
H	1.72014400	-4.39920400	-0.62482100
H	2.54748800	-2.48055600	1.51500200
H	1.77576500	-4.04392300	1.77152200
N	-0.19858700	-1.99962700	0.25702700
O	-0.03183700	-2.75357100	-1.95365900
O	-0.06653600	-2.19147300	2.58698900
C	-4.12370100	0.49198700	-0.22404500
F	-4.25334400	1.42053500	0.73901200

F	-5.15323200	-0.35416200	-0.14201500
F	-4.16775500	1.10725100	-1.41767600
C	-2.77406600	-0.25585000	-0.06014200
O	-1.77606100	0.54917500	-0.15974200
O	-2.77462700	-1.47287200	0.13940600
H	-1.27208800	-1.95809200	0.24245400
<b>17</b>			
Pd	0.31742700	-0.00335700	0.50884000
O	0.87657400	1.87087900	-0.19602700
O	2.35397500	0.29193100	0.17012000
C	2.08474800	1.48187100	-0.18026900
C	3.21565500	2.46186200	-0.52296300
F	3.60164300	3.09025400	0.60063100
F	2.79548900	3.37329900	-1.40505600
F	4.26379300	1.80586400	-1.03154000
C	-3.90210800	0.32697300	0.03594800
F	-4.28476500	0.47489500	1.31408100
F	-4.80072800	-0.43721700	-0.59172700
F	-3.88682200	1.53842800	-0.54771400
C	-2.48571300	-0.29705200	-0.04393200
O	-1.65450700	0.27227800	0.74163700
O	-2.29033300	-1.22776000	-0.83866500
C	0.59084900	-4.26764000	1.24754500
C	0.05983800	-2.97795300	0.69075100
O	0.36357000	-1.89888100	1.25855500
O	-0.68524700	-3.08886300	-0.35880000
H	-1.22231100	-2.23522100	-0.60160900
H	1.18717000	-4.76584100	0.47708000
H	-0.24493100	-4.92884400	1.49238900
H	1.20100500	-4.08053000	2.12952400

**diaryl sulfide**

S	-0.00001400	-1.61770700	-0.00001500
C	-1.40990700	-0.50896100	0.05921600
C	-2.52677800	-0.82296400	-0.72489500
C	-1.45344200	0.59918700	0.91665400
C	-3.67953600	-0.03962300	-0.64514500
H	-2.48854700	-1.67412900	-1.39761000
C	-2.59971300	1.38984400	0.97209400
H	-0.59245400	0.84069700	1.53106900
C	-3.71810200	1.07113200	0.19745700
H	-4.54177500	-0.29226700	-1.25544900
H	-2.62353500	2.25091500	1.63393300
H	-4.61165200	1.68572100	0.25088000
C	1.40990200	-0.50899100	-0.05922100
C	2.52667800	-0.82287500	0.72507300
C	1.45353900	0.59902600	-0.91682400
C	3.67945000	-0.03955600	0.64533000
H	2.48834900	-1.67392800	1.39792500
C	2.59982000	1.38967100	-0.97225800
H	0.59261700	0.84045300	-1.53136400
C	3.71812100	1.07105800	-0.19745100
H	4.54161700	-0.29210800	1.25577400
H	2.62372600	2.25064200	-1.63422100
H	4.61168500	1.68562800	-0.25088000

**pyrrolidine-2,5-dione**

C	-0.76934600	1.25936100	-0.00005100
C	0.76934900	1.25935800	0.00004000
C	1.17760600	-0.21442000	-0.00000600
C	-1.17760400	-0.21447500	0.00000300
H	-1.20612300	1.74185600	0.87870800
H	-1.20607200	1.74183400	-0.87884500
H	1.20603000	1.74178700	0.87889600

H	1.20615900	1.74198400	-0.87862300
O	-2.29641700	-0.67619800	0.00001200
O	2.29639500	-0.67621500	-0.00002600
N	0.00000400	-0.95937600	0.00000700
H	0.00012600	-1.97147000	0.00001600
<b>18</b>			
Pd	0.54712600	-0.12485100	0.63227700
C	1.95163800	-2.66444100	3.81664800
C	1.11058900	-1.58290300	3.20380000
O	1.58644900	-0.87337900	2.28976700
O	-0.09605400	-1.46560900	3.67094300
H	-0.51949700	-0.58096900	3.37762800
O	0.09636000	1.67324900	1.46509600
O	-0.96320300	0.89163900	3.32537700
C	-0.88610600	3.24471100	2.90276600
C	-0.55388900	1.76975000	2.55947900
F	-1.39626000	3.36907400	4.12860800
F	-1.81239100	3.70758000	2.01765700
F	0.19601500	4.02814600	2.80481100
O	2.00283000	-0.97074300	-1.96982300
O	1.02915800	-1.90689500	-0.14956300
C	2.23536400	-3.33955200	-1.56809700
C	1.73136800	-1.91232300	-1.23737800
F	1.20611000	-4.20788000	-1.62725500
F	3.08477800	-3.76666100	-0.61140600
F	2.87600200	-3.37043400	-2.74096700
H	1.85755200	-3.55913200	3.19085200
H	2.99971400	-2.36229100	3.80979600
H	1.61447600	-2.89979700	4.82620300
C	-3.65140100	2.48275500	-0.14733000
C	-2.99326400	3.60700300	-0.96193300

C	-1.75206300	2.98861300	-1.59010900
C	-2.65246500	1.33432700	-0.15319600
H	-3.86672600	2.75534900	0.88704900
H	-4.58207000	2.12082800	-0.59594900
H	-2.66136000	4.43383600	-0.32733900
H	-3.62510200	4.02486200	-1.74882000
N	-1.61050800	1.68925000	-1.03223300
S	-0.21643000	0.72105700	-1.40624400
C	-0.96719500	-0.55388400	-2.43273500
C	-0.75495800	-0.43294000	-3.81072700
C	-1.70821200	-1.61262500	-1.89724500
C	-1.30790000	-1.38489600	-4.66696000
H	-0.15909700	0.38538600	-4.20089000
C	-2.25385200	-2.55583100	-2.76833800
H	-1.85639800	-1.68936100	-0.82760600
C	-2.05521000	-2.44348100	-4.14649600
H	-1.14625800	-1.30210800	-5.73715800
H	-2.82929200	-3.38346600	-2.36532100
H	-2.47866000	-3.18656700	-4.81568300
O	-2.72047800	0.29041800	0.45611900
O	-1.00432600	3.47073800	-2.40297700

**TS<sub>18-19</sub>**

Pd	0.65317900	-0.12707900	-0.73747000
C	0.80675000	-2.08642000	3.21844400
C	0.55814000	-0.94821400	2.26943500
O	1.13021900	-0.94251500	1.16009900
O	-0.26488300	-0.04273800	2.70209700
H	-0.37925000	0.73899100	2.06304600
O	1.08375000	1.81491100	-0.26125500
O	-0.45592400	2.13339400	1.37690200
C	0.79210700	4.00881400	0.58677600

C	0.41069700	2.50514700	0.57548400
F	1.65924400	4.22959100	1.59487700
F	-0.29734100	4.76217400	0.79521100
F	1.36595700	4.39967400	-0.55665100
O	2.73604600	-2.00690700	-1.29767900
O	0.47276100	-2.04704200	-1.28235100
C	1.57269200	-4.10448500	-1.60631300
C	1.66062300	-2.57700300	-1.36866900
F	0.86435800	-4.36148700	-2.73275900
F	0.95156000	-4.71396700	-0.58105500
F	2.78542100	-4.64386900	-1.74826300
H	0.06487400	-2.86456800	3.00648600
H	1.79930700	-2.50352700	3.04724700
H	0.68685000	-1.76366900	4.25321200
C	-3.75396200	0.41232800	-0.30107400
C	-3.63706800	1.77662400	-0.99347200
C	-2.24643300	1.76355000	-1.63874800
C	-2.32298900	-0.12794700	-0.30239700
H	-4.13091600	0.44616100	0.72333000
H	-4.37885700	-0.29144700	-0.86137500
H	-3.65472300	2.60831900	-0.28168000
H	-4.39208500	1.97758700	-1.75671200
N	-1.56148600	0.65096700	-1.17438100
S	0.39328600	0.80125900	-2.80585700
C	-0.43798400	-0.08436200	-4.06226800
C	-1.04090500	0.73473800	-5.04774900
C	-0.45150200	-1.48806900	-4.20512100
C	-1.60689200	0.15385900	-6.17610200
H	-1.06396400	1.80929800	-4.90146700
C	-1.03506600	-2.05075900	-5.33411200
H	-0.03009500	-2.11757800	-3.43505100



C	-1.60480000	-1.23752800	-6.32129000
H	-2.06146400	0.78253900	-6.93531300
H	-1.04372300	-3.13042800	-5.44585800
H	-2.05538100	-1.68987000	-7.19983900
O	-1.92114100	-1.06915700	0.35152700
O	-1.83752400	2.60613300	-2.41546900
<b>19</b>			
Pd	0.47776800	-0.09006400	0.22423400
C	-0.66907800	-2.03547100	4.04249900
C	-0.35650100	-0.82815500	3.20822800
O	0.51787900	-0.87464500	2.32240400
O	-1.06517500	0.23426600	3.47888300
H	-0.75591000	1.03075600	2.93375800
O	1.15468100	1.74821000	0.63175200
O	-0.23000000	2.37809000	2.33139000
C	1.39172900	3.92427500	1.49765400
C	0.66022100	2.55256100	1.50093000
F	2.39612500	3.87233500	2.39618100
F	0.54986700	4.89778600	1.86120400
F	1.90837100	4.22636400	0.30298900
O	2.34221500	-1.18608200	0.12555400
O	0.39334100	-2.09622200	-0.33070400
C	2.31531500	-3.54451200	-0.49923800
C	1.65733000	-2.18980000	-0.20074900
F	2.13029900	-3.83867800	-1.80186600
F	1.74898100	-4.50812400	0.23896700
F	3.62346900	-3.51006300	-0.24721300
H	-1.42394400	-2.61093200	3.49575100
H	0.22321200	-2.65291300	4.15089600
H	-1.07130100	-1.75007600	5.01511600
C	-3.80022700	0.16748900	0.41302700

C	-3.50902400	1.61096700	-0.00914500
C	-1.99183700	1.67484100	-0.20559400
C	-2.42386700	-0.46171200	0.62123700
H	-4.37639800	0.07337800	1.33678800
H	-4.32221900	-0.40843800	-0.35778100
H	-3.77519700	2.34339200	0.75921100
H	-3.99768500	1.91905400	-0.93672100
N	-1.45405700	0.45413900	0.20807500
S	0.81397100	0.46545000	-2.06413600
C	-0.52777900	-0.17040400	-2.99739900
C	-1.52769100	0.71866300	-3.45127500
C	-0.56702700	-1.52500200	-3.39496900
C	-2.53547400	0.25991100	-4.29436600
H	-1.49059000	1.75488600	-3.13239400
C	-1.58814300	-1.97531200	-4.22508900
H	0.19985100	-2.20578300	-3.04438600
C	-2.56922500	-1.08551600	-4.67704100
H	-3.29505900	0.94742500	-4.65452200
H	-1.61778400	-3.01736100	-4.52826800
H	-3.35935000	-1.44118500	-5.33215000
O	-2.20838800	-1.56924600	1.07562300
O	-1.38070100	2.62927700	-0.63951800
<b>20</b>			
Pd	0.51334700	-0.18421400	0.59508200
O	-0.16689800	1.09423000	2.08972900
O	1.09254700	-0.63028500	2.62349000
C	0.26264200	0.75669900	4.44628000
C	0.42201400	0.37832200	2.96631000
F	0.47871600	2.07094700	4.61107700
F	1.11636100	0.07541300	5.21182100
F	-0.99322200	0.47978900	4.84171400

O	1.89734800	-0.39084800	-2.21982000
O	1.40435600	-1.65481100	-0.40322400
C	2.77915500	-2.63165200	-2.04067000
C	1.96299800	-1.41030200	-1.54572900
F	1.97545300	-3.70412600	-2.17776900
F	3.74590900	-2.94013700	-1.15857100
F	3.35046800	-2.38127800	-3.22328000
C	-3.66065600	2.10648800	0.66142500
C	-3.20214200	3.40334000	-0.02429200
C	-1.96738500	3.03186800	-0.83647300
C	-2.65880000	1.03919200	0.24421000
H	-3.65550800	2.16593900	1.75316900
H	-4.66072000	1.78316700	0.35903600
H	-2.92076300	4.18901700	0.68248500
H	-3.94754700	3.83023500	-0.70069200
N	-1.71986200	1.65271200	-0.61154100
S	-0.30098300	0.88693500	-1.28458300
C	-1.05871600	-0.24746900	-2.46098800
C	-1.08033000	0.18345000	-3.79225200
C	-1.57082800	-1.49361500	-2.08663000
C	-1.64006400	-0.64673500	-4.76290100
H	-0.65627900	1.14489500	-4.06283100
C	-2.12255700	-2.31318700	-3.07170400
H	-1.54515700	-1.80912200	-1.05123500
C	-2.15862500	-1.89236300	-4.40318600
H	-1.65954900	-0.32329600	-5.79892600
H	-2.52155500	-3.28399000	-2.79465600
H	-2.58641200	-2.53964800	-5.16291200
O	-2.64346100	-0.12704600	0.56523700
O	-1.30445200	3.74095700	-1.55140100

TS<sub>20-21</sub>

Pd	0.66949800	-0.26301200	-0.69882200
O	1.16743200	1.47878500	0.29576100
O	1.17629600	-0.38909200	1.46494200
C	1.74131600	1.66950400	2.63629900
C	1.35320900	0.85082300	1.39494600
F	2.62115700	2.62498400	2.31472500
F	2.27193800	0.88234300	3.57540700
F	0.63543600	2.25314200	3.13602400
O	2.68648400	-1.99713100	-0.92427500
O	0.47601700	-2.16346400	-1.29008600
C	1.75580700	-4.13946900	-1.57951700
C	1.68437600	-2.64052800	-1.21276200
F	1.44807400	-4.29095500	-2.89066900
F	0.88263200	-4.85936600	-0.86118300
F	2.98239300	-4.62366000	-1.38000200
C	-3.71910700	0.41600500	-0.82603400
C	-3.25747900	1.82954500	-0.44503900
C	-1.78486100	1.89050500	-0.86839700
C	-2.43524800	-0.34131500	-1.18685200
H	-4.23668700	-0.12334700	-0.02896400
H	-4.37237200	0.40420400	-1.70452500
H	-3.30430000	2.01102300	0.63368100
H	-3.80179100	2.63822400	-0.93779900
N	-1.37375000	0.57247600	-1.11134500
S	0.33720800	0.71917400	-2.77813600
C	-0.50003000	-0.17618700	-4.03085600
C	-1.30522400	0.60395400	-4.89128700
C	-0.32505700	-1.55192700	-4.28150900
C	-1.90090800	0.01770300	-6.00258500
H	-1.44033300	1.66121100	-4.68531200

C	-0.93929300	-2.12467800	-5.38918000
H	0.25821300	-2.16106900	-3.60648600
C	-1.72067800	-1.34661700	-6.25054200
H	-2.50936300	0.62006700	-6.66987500
H	-0.80921000	-3.18501200	-5.58066600
H	-2.19296300	-1.80563800	-7.11398900
O	-2.35753000	-1.50961600	-1.49102800
O	-1.11110100	2.88757700	-0.98055800
<b>21</b>			
Pd	0.23745200	-0.04719100	0.29601700
O	0.94104700	1.62060600	1.19465700
O	0.31124000	0.16855500	2.75300500
C	1.21054400	2.30954300	3.47361500
C	0.79326900	1.25772300	2.42679600
F	2.34926100	2.91816100	3.11714300
F	1.37833200	1.74242500	4.67076400
F	0.23953400	3.23785200	3.56889500
O	1.90107400	-1.42362100	0.31792500
O	-0.07862200	-1.96167100	-0.47317200
C	1.62768100	-3.66865100	-0.59596700
C	1.12661300	-2.27092300	-0.20344600
F	1.78929500	-3.69947400	-1.93662900
F	0.73483400	-4.60261400	-0.25466500
F	2.79674800	-3.93940800	-0.01696100
C	-3.87514000	0.82250200	0.85089300
C	-3.46220800	2.18342700	0.27292800
C	-1.98279200	2.03759100	-0.11303900
C	-2.58406200	0.00598600	0.87818400
H	-4.28264700	0.87203900	1.86400500
H	-4.60673600	0.29346500	0.23255500
H	-3.53964900	3.00058500	0.99643500

H	-4.02666100	2.48249900	-0.61421400
N	-1.57639500	0.76558400	0.27712900
S	0.91903500	0.63593000	-1.87828400
C	-0.32631300	0.23832000	-3.02870600
C	-1.21321900	1.25105600	-3.46779900
C	-0.39104800	-1.05197200	-3.60828600
C	-2.12765400	0.97669800	-4.47817900
H	-1.16409000	2.22722000	-2.99774000
C	-1.31854700	-1.31510300	-4.60785400
H	0.28551500	-1.82425300	-3.26118400
C	-2.18291900	-0.30273800	-5.04428500
H	-2.80046200	1.75446500	-4.82623200
H	-1.36971100	-2.30349300	-5.05356800
H	-2.90235400	-0.51300400	-5.83053800
O	-2.43275300	-1.11002600	1.33143500
O	-1.31244700	2.88352500	-0.66833200
<b>4'</b>			
Pd	0.25913400	0.35746700	0.32588800
C	3.57683600	-1.62265600	2.66589900
C	2.53033800	-0.59596100	2.31298700
O	2.22047100	-0.40085100	1.12073600
O	2.00453700	0.01780200	3.33117400
H	1.39453900	0.81217600	3.07936100
O	0.61671100	2.35873200	0.69513200
O	0.73714500	2.16238200	2.95563300
C	0.63993800	4.34033100	1.96317500
C	0.67883600	2.79316900	1.88594500
F	0.97267600	4.78607400	3.18204300
F	-0.60498700	4.77516200	1.68230400
F	1.48511300	4.89069200	1.07228100
H	4.47749900	-1.43459800	2.07508900

H	3.81513800	-1.59377400	3.72865400
H	3.20129400	-2.61458400	2.39533200
C	-3.90882500	1.12374600	-0.13431100
C	-2.67924100	0.64955500	0.33887400
C	-1.50231000	0.95517300	-0.35247300
C	-1.55398900	1.74778700	-1.50403700
C	-2.78716500	2.21064000	-1.97471200
C	-3.96570400	1.89891800	-1.29299500
H	-4.81934100	0.88657800	0.41016300
H	-2.65104900	0.05314200	1.24727500
H	-0.64020500	2.01366200	-2.02721600
H	-2.82139400	2.82590800	-2.87036000
H	-4.92099300	2.26574600	-1.65784100
C	3.17160200	-2.41893300	-2.41218600
C	3.35199400	-3.53837400	-1.37577000
C	2.15621000	-3.42991700	-0.43750200
C	1.84321200	-1.75477600	-2.07633800
H	3.95052300	-1.65288400	-2.35874100
H	3.13800100	-2.77466700	-3.44542300
H	4.26651700	-3.44617600	-0.78454300
H	3.35284600	-4.54006400	-1.81586300
N	1.30800400	-2.42577300	-0.95404500
S	-0.10584600	-1.91767400	-0.07776900
C	-1.43195500	-2.43889200	-1.17162900
C	-2.16989200	-3.55403300	-0.75540100
C	-1.74058500	-1.76752400	-2.36065400
C	-3.22965200	-4.00462700	-1.54370100
H	-1.91448200	-4.06019500	0.17017500
C	-2.79673200	-2.23501000	-3.14107600
H	-1.16410500	-0.90231000	-2.66021600
C	-3.54026300	-3.34666600	-2.73477300

H	-3.80756100	-4.86722500	-1.22655700
H	-3.04533200	-1.72098700	-4.06444100
H	-4.36572300	-3.69794100	-3.34698400
O	1.31964000	-0.82684100	-2.64601000
O	1.94582700	-4.06839300	0.56658000
<b>TS<sub>4-5</sub></b>			
Pd	0.26549500	0.53692700	0.50837400
C	3.33693600	-1.24646100	3.39800600
C	2.30420600	-0.28226500	2.87956000
O	2.17643300	-0.06527200	1.66836000
O	1.58828000	0.30589000	3.81193200
H	1.04131300	1.05885900	3.41880000
O	0.82149800	2.53912500	0.68449700
O	0.39949200	2.43730300	2.90823500
C	0.92753900	4.55433000	1.90017600
C	0.69830700	3.02283300	1.85383400
F	1.00752500	5.00564400	3.15870800
F	-0.09493300	5.18678700	1.29072900
F	2.06508500	4.88846700	1.26300400
H	3.57007800	-1.97630300	2.62265600
H	4.24598700	-0.68780500	3.64712000
H	2.98492500	-1.73440500	4.30886400
C	-3.79433500	1.62100400	0.77943000
C	-2.54634400	1.00938400	0.95846900
C	-1.54040600	1.23620700	0.01387300
C	-1.75419300	2.04679700	-1.09873900
C	-3.01082100	2.64220100	-1.26327400
C	-4.02874200	2.43204400	-0.33061500
H	-4.57707300	1.45182500	1.51392700
H	-2.37614300	0.38371300	1.82810600
H	-0.96266100	2.20590300	-1.81886700



H	-3.18257100	3.28189600	-2.12485200
H	-4.99902000	2.90074900	-0.46709400
C	2.75143100	-0.32041300	-3.09798600
C	3.54875400	-1.20121500	-2.12911500
C	2.56643500	-1.50486600	-0.99146300
C	1.52023100	0.11054900	-2.29433500
H	3.27804100	0.56782000	-3.45432800
H	2.40333900	-0.87131200	-3.97830000
H	4.40296100	-0.67139100	-1.69426100
H	3.91904100	-2.13840500	-2.55009600
N	1.49949000	-0.61265600	-1.10502000
S	-0.17495700	-1.68637000	0.32130000
C	-1.08002400	-2.31048100	-1.05196400
C	-0.75734600	-3.63200800	-1.43090600
C	-2.10961900	-1.62049100	-1.72008100
C	-1.46571000	-4.25453800	-2.45332600
H	0.05010800	-4.14827800	-0.92141100
C	-2.79991200	-2.25210000	-2.75042000
H	-2.35658800	-0.60692500	-1.43400900
C	-2.48567000	-3.56495900	-3.11627500
H	-1.21784300	-5.27214200	-2.73931800
H	-3.59187100	-1.71847300	-3.26693500
H	-3.03558500	-4.04993600	-3.91746000
O	0.70655000	0.93863300	-2.65205700
O	2.70758000	-2.38145700	-0.16458200
<b>5'</b>			
Pd	0.35146300	0.18275300	0.15189200
C	3.60670400	-1.59325400	2.82567300
C	2.41061800	-0.79938900	2.38593100
O	2.28943500	-0.38061000	1.23085300
O	1.50738700	-0.62106300	3.33603400

H	0.76444100	-0.06223700	2.99434200
O	0.99231500	2.55808700	0.90348000
O	-0.21370100	1.03798200	2.00991900
C	0.12002100	3.14011500	3.08965500
C	0.35079700	2.20499100	1.88702000
F	0.54430600	2.54533400	4.22352800
F	-1.19662100	3.39701200	3.21889900
F	0.76829200	4.29686000	2.94772000
H	3.36225400	-2.65681800	2.72770700
H	4.45362000	-1.37244900	2.17653300
H	3.84776200	-1.39122700	3.87049700
C	-3.38366100	2.02436500	-0.77847000
C	-2.24626400	1.54832500	-0.11409000
C	-1.34326800	0.74513600	-0.81066400
C	-1.58431600	0.36974600	-2.13116300
C	-2.72340400	0.85424800	-2.77941000
C	-3.62253400	1.68491100	-2.10895100
H	-4.08218900	2.65690900	-0.23770500
H	-2.09650200	1.79777600	0.92772700
H	-0.90616900	-0.28855500	-2.65709600
H	-2.90105900	0.57546600	-3.81449200
H	-4.50681300	2.05705600	-2.61796200
C	2.66336500	-0.03517700	-3.41779100
C	2.86626700	-1.48032300	-2.95055900
C	1.97212200	-1.63343100	-1.71186100
C	1.68916400	0.55730400	-2.40002800
H	3.57793700	0.56386000	-3.41965200
H	2.22270400	0.04625100	-4.41621800
H	3.89536600	-1.70561700	-2.65662600
H	2.57172700	-2.23099800	-3.68994700
N	1.27697500	-0.44709500	-1.52363500

S	-0.75715300	-1.77397000	0.81924800
C	-1.61026600	-2.66583000	-0.43166600
C	-0.98366200	-3.73772800	-1.09985100
C	-2.97984000	-2.40721600	-0.65432900
C	-1.72426300	-4.54011300	-1.96453700
H	0.07393100	-3.90750900	-0.93709200
C	-3.70961100	-3.21735100	-1.51751800
H	-3.45032300	-1.57533800	-0.14176600
C	-3.08287900	-4.28322200	-2.17313500
H	-1.24313800	-5.36921800	-2.47505900
H	-4.76479800	-3.02073900	-1.68177400
H	-3.65551100	-4.91391000	-2.84744800
O	1.31846300	1.71495200	-2.34770300
O	1.90674400	-2.64140400	-1.03107100
<b>TS4-6'</b>			
Pd	-0.06554600	0.01855400	-0.14541000
C	4.12884600	0.08045400	1.10804600
C	2.82569900	-0.49972600	0.64609300
O	2.05591600	0.16022000	-0.06223900
O	2.58347400	-1.71897600	1.08488200
H	1.77295600	-2.11164000	0.67191100
O	-0.02777000	2.05640300	0.09875100
O	0.72096200	1.70254500	2.21115300
C	0.51777500	3.95312900	1.37514100
C	0.40521000	2.41072800	1.26101000
F	0.91079400	4.33085700	2.60004500
F	-0.66794900	4.54537400	1.11982100
F	1.41623100	4.42921300	0.48708600
H	4.53509400	0.72649500	0.32867600
H	3.91752800	0.70200400	1.98544600
H	4.83889600	-0.69964600	1.38266100

C	-3.84331500	0.46044300	1.37145400
C	-2.68650000	-0.27426400	1.13596500
C	-2.15681700	-0.37169300	-0.17437200
C	-2.83528600	0.25506300	-1.24483800
C	-3.99327900	0.98493800	-1.00197700
C	-4.49237000	1.08832200	0.30254500
H	-4.24106400	0.54459400	2.37788600
H	-2.18251400	-0.77720600	1.95647800
H	-2.44858400	0.16883500	-2.25458400
H	-4.50777300	1.47791800	-1.82114400
H	-5.39866200	1.65865500	0.48554800
C	2.29912200	-4.86742900	-1.51978400
C	1.58509100	-5.62152300	-0.39222600
C	0.56920900	-4.61222200	0.16424300
C	1.73795200	-3.44066600	-1.44710600
H	3.38726100	-4.83036800	-1.41891300
H	2.08288000	-5.26933300	-2.51482800
H	2.25582000	-5.92217400	0.41878600
H	1.05222700	-6.51926500	-0.71691000
N	0.78662000	-3.36462700	-0.43115800
S	-0.95018800	-2.03532400	-0.40092200
C	-1.31589300	-2.40561000	-2.12422300
C	-2.24449700	-3.42557200	-2.36326800
C	-0.70090200	-1.72604500	-3.18111700
C	-2.57231500	-3.75466300	-3.67875700
H	-2.69956600	-3.95292200	-1.53060900
C	-1.03663000	-2.06796300	-4.49207900
H	0.04260200	-0.96432400	-2.97681400
C	-1.97134500	-3.07549000	-4.74133700
H	-3.29526800	-4.54157500	-3.87128000
H	-0.55970700	-1.54839200	-5.31750300

H	-2.22803800	-3.33480200	-5.76419200
O	2.08297600	-2.51056000	-2.15606700
O	-0.28549900	-4.85336900	0.99443300
<b>6'</b>			
Pd	-0.14816100	0.92932800	0.56565200
C	3.82926400	-0.50829600	0.00988600
C	2.30821700	-0.53823800	0.11076000
O	1.80823000	0.67085900	0.22034200
O	1.68164300	-1.59730300	0.09433600
O	0.28443800	2.88544500	0.89408700
O	-0.53744500	2.70670300	3.00379400
C	0.34511100	4.81303600	2.23445800
C	-0.01341900	3.31229200	2.07556300
F	0.14200700	5.23423400	3.49029400
F	-0.42918600	5.56186200	1.41689400
F	1.63087700	5.04831700	1.91713200
H	4.14936600	0.23686400	-0.72207200
H	4.24503000	-0.21580400	0.97893900
H	4.19877600	-1.49721700	-0.26238200
C	-3.29634600	1.91745600	1.48999300
C	-2.42523200	0.80883700	1.42736500
C	-2.39182400	0.02430700	0.24597100
C	-3.24075500	0.32633800	-0.83652400
C	-4.11024600	1.40075600	-0.72948700
C	-4.12966300	2.20858900	0.42353600
H	-3.29408100	2.52416000	2.38862300
H	-1.89374000	0.51335500	2.32850900
H	-3.20644400	-0.27276600	-1.73892000
H	-4.77542900	1.62960300	-1.55696800
H	-4.80454800	3.05700300	0.47468700
S	-1.03840600	-1.17376200	0.21810700

C	-0.98084300	-1.68850700	-1.50437700
C	-1.54054300	-2.92987400	-1.82006400
C	-0.36550200	-0.90164000	-2.48301600
C	-1.50059100	-3.37907900	-3.14145000
H	-1.99353600	-3.54023900	-1.04501500
C	-0.33103500	-1.36280400	-3.79831300
H	0.08653900	0.04716800	-2.21319200
C	-0.89842500	-2.59691900	-4.12789600
H	-1.93343000	-4.34199000	-3.39423800
H	0.14759000	-0.75988800	-4.56382100
H	-0.86349200	-2.95169600	-5.15351600
$7_{en}$			
Pd	-0.27645300	0.73772400	0.30763400
O	0.12489200	2.76604300	0.84591300
O	1.87582100	1.44309500	0.50087500
C	2.31107000	3.76922200	0.97804100
C	1.37577300	2.56385600	0.77539000
F	3.48564500	3.38396300	1.50131300
F	1.76618700	4.68688600	1.78758600
F	2.55347500	4.34886100	-0.21598000
C	-4.37628700	-0.10495300	1.21868300
C	-2.98504600	-0.22481400	1.11631500
C	-2.25250800	0.73593200	0.40908800
C	-2.91359000	1.81453700	-0.19137500
C	-4.30433000	1.92157100	-0.09018600
C	-5.03770200	0.96325500	0.61284500
H	-4.93708700	-0.85035600	1.77667000
H	-2.48696400	-1.05713600	1.60711000
H	-2.35115700	2.57955600	-0.71919400
H	-4.81074500	2.76260500	-0.55667800
H	-6.11730200	1.05249100	0.69237200

C	3.56722700	-1.22198400	-1.60331900
C	3.69417700	-2.40225200	-0.62626000
C	2.30190600	-2.61604000	-0.04387600
C	2.08700900	-0.87507500	-1.64539000
H	4.09520500	-0.32799600	-1.25791300
H	3.91678700	-1.44082100	-2.61524300
H	4.38878900	-2.21734100	0.19708900
H	4.00779000	-3.33177400	-1.11086600
N	1.43975800	-1.69442000	-0.68768400
S	-0.21239500	-1.51112000	-0.19331900
C	-1.11685100	-2.00555300	-1.66737400
C	-1.49523300	-3.35135200	-1.74753300
C	-1.46417100	-1.09203200	-2.66773700
C	-2.22180700	-3.78858800	-2.85524400
H	-1.22586500	-4.04161100	-0.95413600
C	-2.19529000	-1.54276300	-3.76615300
H	-1.15584200	-0.05724200	-2.58547000
C	-2.57147800	-2.88519500	-3.86089500
H	-2.51977600	-4.83010500	-2.92642400
H	-2.47028500	-0.84259800	-4.54885900
H	-3.14252200	-3.22685300	-4.71914300
O	1.52941300	-0.06511400	-2.34556200
O	1.95808600	-3.41254600	0.79422500

**TS<sub>7-9en</sub>**

Pd	-0.08167900	0.19450800	0.41100500
O	0.53152200	2.13751700	0.92215500
O	2.03787600	0.67470500	1.68251000
C	2.49897200	3.03211800	1.94010100
C	1.63043800	1.83388100	1.50649900
F	3.39768700	2.67616600	2.86701300
F	1.75197100	4.03147500	2.43564900

F	3.16939200	3.50331000	0.86484100
C	-4.20911400	1.12006600	0.53046500
C	-2.97442300	0.49050300	0.74107300
C	-1.89140700	0.86548700	-0.05739800
C	-2.01129700	1.81688100	-1.06918400
C	-3.25630900	2.42378100	-1.26771700
C	-4.35163200	2.07929800	-0.47136500
H	-5.05576500	0.84508700	1.15363700
H	-2.87425400	-0.25678300	1.52018500
H	-1.15893900	2.07805000	-1.68509700
H	-3.36027400	3.17465100	-2.04622000
H	-5.31328100	2.55722600	-0.63324800
C	2.82399500	-0.42299400	-2.81111600
C	3.57066900	-1.20125900	-1.71683700
C	2.48618400	-1.58719600	-0.70433600
C	1.45741800	-0.11097000	-2.19526600
H	3.30319800	0.50981900	-3.11706300
H	2.66030700	-1.01986000	-3.71484400
H	4.30304300	-0.57974000	-1.19136200
H	4.08428400	-2.10228600	-2.05890500
N	1.35318300	-0.82163700	-1.00423600
S	-0.43274300	-2.01921600	0.06757800
C	-1.16906800	-2.56090700	-1.43593600
C	-0.92192000	-3.90954600	-1.77264100
C	-1.99693000	-1.77120400	-2.25659700
C	-1.51160300	-4.46105000	-2.90560000
H	-0.27034800	-4.50711900	-1.14276900
C	-2.56347000	-2.33223300	-3.39658500
H	-2.18372600	-0.73617600	-2.00247700
C	-2.32953400	-3.67313400	-3.72067200
H	-1.32559400	-5.50036800	-3.15809200



H	-3.19724100	-1.72175700	-4.03237700
H	-2.78469200	-4.10274100	-4.60812200
O	0.61137400	0.62878500	-2.66023100
O	2.58867300	-2.40498300	0.18057300
<b>TS<sub>7-10en</sub></b>			
Pd	0.77636800	-0.89767300	-1.09318300
O	3.15300600	-3.03978300	-0.87122100
O	2.81780100	-0.81091300	-1.19506300
C	3.52061800	-1.88886500	-1.06859700
C	5.03436200	-1.57658000	-1.20188900
F	5.42450300	-0.69356200	-0.25914400
F	5.30531300	-1.03799600	-2.40940900
F	5.78130800	-2.68141200	-1.06629300
C	0.88582100	1.45819600	0.59798400
C	1.03569200	2.82614800	0.82448400
C	0.72801800	3.74741900	-0.18472800
C	0.26270300	3.30754500	-1.42504100
C	0.09894000	1.93919500	-1.66622700
C	0.49164600	1.03158800	-0.67755600
H	1.12324200	0.73948100	1.37555900
H	1.39104100	3.17273600	1.79059000
H	0.83009400	4.81142600	0.00744400
H	0.00421400	4.02338400	-2.20003500
H	-0.29708400	1.59907600	-2.61778800
C	0.30886100	-5.18948900	-1.31781300
C	0.66897100	-4.94273400	0.15666300
C	0.36122100	-3.46696400	0.39488500
C	0.01694700	-3.80274700	-1.89777800
H	1.11378000	-5.64674900	-1.89777000
H	-0.58528500	-5.80834600	-1.44719400
H	1.73905900	-5.06902100	0.34299400

H	0.11802600	-5.55781800	0.87223100
N	0.11830100	-2.87623000	-0.85311800
S	-1.50081700	-1.04246500	-0.85849400
C	-2.30229600	-0.96334600	-2.41238800
C	-3.70113900	-1.16472900	-2.41297000
C	-1.63289900	-0.69622700	-3.62601800
C	-4.41419300	-1.07044300	-3.60229800
H	-4.21127100	-1.38596300	-1.48062300
C	-2.35627100	-0.62121700	-4.80907300
H	-0.55426900	-0.58683500	-3.62811800
C	-3.74501000	-0.80023000	-4.80064200
H	-5.48985300	-1.21624100	-3.59875500
H	-1.83823500	-0.42846100	-5.74322300
H	-4.30373200	-0.73570900	-5.72939500
O	-0.23967500	-3.53392100	-3.05259800
O	0.34758300	-2.87362900	1.45213700
<b>9<sub>en</sub></b>			
Pd	0.19161100	-0.09163700	0.47902200
O	0.35154900	1.65442400	1.79005200
O	1.81030700	0.01166400	2.10666200
C	1.96297000	1.92974000	3.56138300
C	1.34775800	1.14466900	2.38949300
F	1.38027000	1.52271000	4.71089200
F	1.76272000	3.24650800	3.43513000
F	3.27946200	1.70208200	3.65635800
C	-3.35605300	1.85579200	-0.57262900
C	-2.19910500	1.38727000	0.06356900
C	-1.40051200	0.45709700	-0.60438400
C	-1.69727800	0.01730100	-1.89141100
C	-2.84965000	0.50836900	-2.51395800
C	-3.68015900	1.41973400	-1.85706700

H	-3.98726300	2.57555700	-0.05909600
H	-1.92686400	1.76184300	1.04493000
H	-1.06146400	-0.69997900	-2.39656500
H	-3.09499900	0.16903200	-3.51665300
H	-4.57295900	1.79445600	-2.34905700
C	3.22020000	1.43012700	-2.23259700
C	2.75596400	0.18469200	-2.99532500
C	1.69262700	-0.45733700	-2.10178000
C	2.33972400	1.47954700	-0.98143300
H	4.26525700	1.38124600	-1.91329700
H	3.09420800	2.36470200	-2.78571300
H	3.54486500	-0.55036000	-3.17597300
H	2.29618900	0.41027400	-3.96230200
N	1.49703400	0.35446800	-0.99821300
S	-0.04362900	-2.32937100	0.32031700
C	-1.34230900	-3.02246300	-0.64445700
C	-1.01991200	-3.88361300	-1.71104400
C	-2.68990400	-2.82920700	-0.28137700
C	-2.03551100	-4.54005800	-2.40055700
H	0.01867800	-4.00943700	-1.99420200
C	-3.69597100	-3.49819700	-0.97098000
H	-2.93097400	-2.16355700	0.54033300
C	-3.37108700	-4.35154700	-2.03080000
H	-1.78714100	-5.20037800	-3.22591600
H	-4.73338700	-3.35455600	-0.68468200
H	-4.15971700	-4.86992000	-2.56844900
O	2.38176700	2.33456600	-0.12647800
O	1.12768100	-1.51024300	-2.34888000
<b>10<sub>en</sub></b>			
Pd	-0.20437100	0.10492900	0.67077000
O	2.56923300	-1.95064500	0.51901800

O	1.79501600	0.20094300	0.65249800
C	2.68585000	-0.74226500	0.59387300
C	4.10358000	-0.10233300	0.64329900
F	4.28392700	0.56252900	1.80551300
F	4.27133000	0.78015000	-0.36410700
F	5.06283700	-1.02987200	0.54490700
C	-0.50524300	2.42821500	1.68168300
C	0.46917400	3.43573900	1.57382400
C	0.53755200	4.22136700	0.43233400
C	-0.37094100	4.01882800	-0.61992100
C	-1.33166300	3.01974900	-0.55034800
C	-1.39364600	2.21464400	0.60185100
H	-0.61947300	1.88462700	2.61579100
H	1.15915300	3.59191100	2.39615000
H	1.29152700	4.99762500	0.35160300
H	-0.31601800	4.64147200	-1.50765900
H	-2.01665500	2.84764900	-1.37236900
C	0.09946100	-3.98732400	-0.49495700
C	-0.03629500	-4.12985300	1.02916000
C	-0.26731600	-2.70296400	1.53229700
C	-0.13816500	-2.50207400	-0.76835400
H	1.10250200	-4.23023700	-0.85571000
H	-0.61464900	-4.58589400	-1.06783300
H	0.86345300	-4.51949400	1.51146500
H	-0.87621300	-4.75995500	1.33773500
N	-0.35135500	-1.86396900	0.43284400
S	-2.46888500	0.77044600	0.77999900
C	-3.31413500	0.62370700	-0.80182100
C	-4.61508700	1.14068200	-0.87461800
C	-2.72428100	-0.02663900	-1.89230000
C	-5.32744600	1.02401300	-2.06761600

H	-5.06267600	1.62378100	-0.01141300
C	-3.45637100	-0.13749400	-3.07676300
H	-1.72727200	-0.45886200	-1.82711700
C	-4.74744500	0.38644200	-3.16734500
H	-6.33417100	1.42489000	-2.13388500
H	-3.00891500	-0.64481500	-3.92574000
H	-5.30708400	0.29134400	-4.09315800
O	-0.15482100	-1.96380000	-1.86811200
O	-0.37721700	-2.34900200	2.69326900
<b>8'</b>			
Pd	0.31748000	0.08913300	0.04406300
O	2.47487300	-0.67922000	1.97432000
O	2.34904700	0.21050400	-0.11106300
C	2.95589100	-0.24835200	0.93252200
C	4.49510500	-0.19838000	0.75438000
F	4.91739800	1.07616800	0.62026200
F	4.87633000	-0.87730900	-0.34853400
F	5.13276800	-0.73448900	1.80557700
C	0.74914100	2.34193400	1.84937200
C	0.72053900	3.68007100	2.25578400
C	0.22762200	4.67003200	1.40287100
C	-0.23821600	4.32047200	0.13544900
C	-0.21989300	2.98305400	-0.28017900
C	0.27027600	1.99610500	0.58072600
H	1.15836900	1.57960300	2.50504600
H	1.09599500	3.94584000	3.24059100
H	0.21272900	5.70822800	1.72227000
H	-0.61545200	5.08494900	-0.53918200
H	-0.57873300	2.72859400	-1.27348200
C	-1.23027700	-4.12324400	-0.09664900
C	-2.71651400	-4.16030400	0.30808100

C	-3.15375900	-2.70318300	0.41384200
C	-0.87234600	-2.65186400	-0.15754400
H	-0.56587700	-4.61231600	0.62105900
H	-1.03353600	-4.57170600	-1.07486600
H	-2.88617600	-4.64169800	1.27537900
H	-3.35576100	-4.66632900	-0.42011900
N	-2.00989300	-1.91122700	0.13566400
S	-2.00070300	-0.15492000	0.20327000
C	-2.78254200	0.25306500	-1.36750900
C	-4.17090000	0.43618900	-1.37113200
C	-2.02521200	0.42155400	-2.53422700
C	-4.80579000	0.78288200	-2.56421000
H	-4.73952200	0.29267700	-0.45888700
C	-2.67403700	0.76779400	-3.71908800
H	-0.94686600	0.29572800	-2.50295900
C	-4.05990300	0.94815000	-3.73332100
H	-5.88182900	0.92556700	-2.57779000
H	-2.09533300	0.90415700	-4.62741700
H	-4.55865200	1.22296500	-4.65796400
O	0.22277600	-2.16593600	-0.40777600
O	-4.24331700	-2.25766100	0.67172800

**TS<sub>8</sub>-11'**

Pd	0.20773700	0.32807200	-0.26344700
C	0.76804800	3.01718000	0.78402800
C	0.94956300	4.39676100	0.64582900
C	1.16572100	4.96009700	-0.61538900
C	1.20923400	4.14650800	-1.75041900
C	1.02793100	2.76460500	-1.63040300
C	0.74871500	2.22853700	-0.37009900
H	0.63810000	2.57235600	1.76433000
H	0.93896200	5.02630800	1.53130100

H	1.32767900	6.02995600	-0.70950200
H	1.40631400	4.57872700	-2.72760000
H	1.11050900	2.12007800	-2.50092400
C	-0.23974000	-3.89600300	-1.53103000
C	-0.17083800	-4.13272000	-0.01316200
C	-0.37318700	-2.74513700	0.61189800
C	-0.35631500	-2.37530400	-1.68174800
H	0.64710300	-4.23559600	-2.07280500
H	-1.10731700	-4.36489400	-2.00589200
H	0.79943500	-4.51641700	0.31637600
H	-0.93561000	-4.81244700	0.37200000
N	-0.37942600	-1.80324200	-0.41649300
S	-1.94987000	-0.01660100	0.13196100
C	-2.88329700	0.15926600	-1.32857200
C	-4.10672600	-0.54708700	-1.40883800
C	-2.49000800	1.01125100	-2.38537200
C	-4.92246400	-0.39058800	-2.52119000
H	-4.39797100	-1.20338000	-0.59479400
C	-3.30989500	1.14736100	-3.49777700
H	-1.55219100	1.54979000	-2.31519200
C	-4.52251800	0.45143100	-3.56656200
H	-5.86427100	-0.92640100	-2.58293900
H	-3.00885700	1.79715900	-4.31317800
H	-5.15982100	0.56620300	-4.43831300
O	-0.41979200	-1.75168200	-2.72647500
O	-0.50378200	-2.49653400	1.79237800
O	2.58903400	0.36792000	1.53923500
O	2.19246800	-0.06007700	-0.65032900
C	2.92545400	0.03697900	0.41122800
C	4.39968700	-0.33811900	0.11283200
F	4.90841200	0.45193900	-0.85401300

F	4.48246000	-1.61763700	-0.31182100
F	5.17145600	-0.21246300	1.19916600
<b>11'</b>			
Pd	0.26670000	0.02401800	0.57856300
C	0.91779200	2.89660600	0.29276200
C	1.54352100	3.99101000	-0.31719000
C	2.22166400	3.83525200	-1.52635900
C	2.27894600	2.58336000	-2.13841100
C	1.65521700	1.47409000	-1.55297500
C	0.99545300	1.66654300	-0.34764300
H	0.40302300	3.01595300	1.23810900
H	1.49523700	4.96205600	0.16723400
H	2.70430700	4.68931700	-1.99192000
H	2.80295800	2.45363800	-3.08083400
H	1.68714100	0.50982600	-2.04137400
C	-1.20409000	-2.38576400	-2.75785900
C	-1.10427200	-3.25651200	-1.49148800
C	-0.61571100	-2.27638700	-0.44155100
C	-0.72927800	-0.98066900	-2.33729400
H	-0.57775200	-2.73648300	-3.58260100
H	-2.22538900	-2.29576600	-3.13760600
H	-0.39078900	-4.08140700	-1.58097800
H	-2.05928500	-3.68295400	-1.17254800
N	-0.35954500	-1.05656100	-0.99875200
S	-1.81291600	0.97492200	0.93055900
C	-3.07045400	0.11283200	0.03607800
C	-3.68626400	-1.01787400	0.60712400
C	-3.53403800	0.61238100	-1.19578500
C	-4.75181300	-1.63419100	-0.04621800
H	-3.32193000	-1.39676700	1.55608500
C	-4.59970100	-0.01110800	-1.84207700



H	-3.04665400	1.47547400	-1.63573900
C	-5.20911400	-1.13202500	-1.26905600
H	-5.23019300	-2.50103600	0.40024100
H	-4.95554200	0.37757200	-2.79151400
H	-6.04288500	-1.61205800	-1.77351100
O	-0.69531100	0.00102800	-3.04930400
O	-0.46057100	-2.44793600	0.77309500
O	1.12464700	0.69873600	2.35492500
O	2.41792100	-0.62262200	1.13851300
C	2.21689700	0.05746400	2.16657400
C	3.30024400	0.19359600	3.25035500
F	3.86853000	1.41067900	3.15717500
F	4.25059700	-0.73332000	3.09951200
F	2.76354700	0.06854800	4.47309300
<b>TS<sub>8</sub>-12'</b>			
Pd	-0.05188600	-0.24321200	-0.61787200
O	2.28515500	-0.80048300	1.35985400
O	1.96401600	-0.45185700	-0.85923600
C	2.66550800	-0.68473300	0.20259600
C	4.17056400	-0.82452400	-0.14016300
F	4.63274900	0.29609800	-0.73260400
F	4.37042500	-1.85389900	-0.99137600
F	4.90937300	-1.04684300	0.95531900
C	0.41824500	1.86464500	1.30117700
C	0.65415700	3.18075700	1.69980600
C	0.33815100	4.24853800	0.85003500
C	-0.21759500	4.00774900	-0.40679300
C	-0.46828500	2.69513000	-0.82272100
C	-0.08134300	1.64003600	0.01099700
H	0.68413000	1.03011400	1.94150800
H	1.08826300	3.37066300	2.67724200

H	0.50973300	5.26932300	1.17898300
H	-0.47912700	4.83537900	-1.06002300
H	-0.92750400	2.51336800	-1.78895400
C	-1.18548200	-4.33334000	0.38034400
C	-1.35746100	-4.41397200	-1.14524200
C	-1.25277700	-2.96631800	-1.63839400
C	-1.17859400	-2.83566000	0.69635200
H	-1.98098500	-4.81735100	0.95210900
H	-0.23469900	-4.75421100	0.72229700
H	-2.33394800	-4.80582700	-1.44763100
H	-0.59735800	-5.01558100	-1.65008500
N	-1.07029100	-2.14085300	-0.52073900
S	-2.35301600	-0.15247600	-0.44132400
C	-3.06661700	0.12006700	-2.01475800
C	-4.47363600	0.01500400	-2.09945900
C	-2.31972000	0.46212100	-3.16327000
C	-5.11696800	0.27687400	-3.30321800
H	-5.04362700	-0.26334000	-1.21850900
C	-2.97482900	0.70305300	-4.36390500
H	-1.23768000	0.50483800	-3.10405000
C	-4.37051700	0.61859200	-4.43605400
H	-6.19847600	0.20585000	-3.36329500
H	-2.39840700	0.95458900	-5.24853000
H	-4.87546600	0.81417800	-5.37718400
O	-1.25392800	-2.31422100	1.78541800
O	-1.30088800	-2.58790300	-2.78993100
<b>12'</b>			
Pd	-0.01624800	-0.13237000	0.38278700
O	2.11583700	0.22361800	2.58030300
O	2.00180600	-0.24251300	0.35600200
C	2.59570700	-0.06360400	1.49234300

C	4.12869700	-0.24818400	1.33863400
F	4.41876700	-1.48077100	0.87875900
F	4.76008600	-0.08026600	2.50793200
F	4.62755400	0.65055100	0.46405400
C	-0.41389200	1.79089300	1.88209900
C	0.48283500	2.86367600	2.06096700
C	0.37649700	3.99915600	1.27359600
C	-0.62180200	4.08287700	0.28670800
C	-1.49823000	3.03028000	0.06288200
C	-1.39252400	1.88183400	0.86511100
H	-0.39590100	0.96981900	2.59529300
H	1.24738000	2.77165900	2.82380700
H	1.06234400	4.82789200	1.41707000
H	-0.70163900	4.97734700	-0.32397600
H	-2.24333100	3.08303600	-0.72225300
C	0.43531400	-3.53501700	-2.19419400
C	0.25750600	-4.23445100	-0.83779000
C	0.00245900	-3.09491700	0.15646600
C	0.20935300	-2.04891300	-1.89722500
H	1.43935100	-3.65125200	-2.61347000
H	-0.27373700	-3.86155000	-2.96036100
H	1.13905200	-4.79249700	-0.51031100
H	-0.59038700	-4.92544600	-0.81034000
N	-0.01687900	-1.90043400	-0.54717800
S	-2.31122400	0.35436900	0.58917500
C	-3.16701500	0.61111400	-0.97229800
C	-4.52998800	0.92801200	-0.89739600
C	-2.51922300	0.45536200	-2.20334400
C	-5.25078700	1.11285200	-2.07698500
H	-5.01831700	1.02614800	0.06733100
C	-3.25925100	0.64080100	-3.37313500

H	-1.47037000	0.17171500	-2.26018300
C	-4.61501500	0.97053600	-3.31271300
H	-6.30636100	1.36173200	-2.02839500
H	-2.76718500	0.51631000	-4.33269800
H	-5.18017700	1.10893700	-4.22965300
O	0.20932800	-1.14636800	-2.72407800
O	-0.17006300	-3.20884800	1.35634200
<b>TS<sub>8</sub><sup>-13</sup></b>			
Pd	0.25932500	-0.58970300	-0.55637700
O	2.43080000	-0.38295600	1.45167500
O	2.29981100	-0.40032500	-0.81018200
C	2.91088300	-0.34465900	0.32231300
C	4.44250600	-0.19596500	0.14180500
F	4.73403700	0.96557100	-0.48622000
F	4.94489600	-1.20182800	-0.60394700
F	5.08630400	-0.19618600	1.31865700
C	-0.24943700	1.70671800	1.24680800
C	0.13457800	3.00767200	1.56294600
C	0.22099600	3.97001200	0.55279700
C	-0.07517000	3.64087300	-0.77529700
C	-0.45480000	2.34162900	-1.09970900
C	-0.52748300	1.35876400	-0.09231300
H	-0.31255800	0.95462500	2.02669700
H	0.36979200	3.26978100	2.58978700
H	0.51636000	4.98552400	0.80109000
H	-0.00603000	4.39674100	-1.55195200
H	-0.69065000	2.08891800	-2.12799300
C	-1.42352100	-4.61457500	-0.81487300
C	-2.94333700	-4.61144400	-0.56930800
C	-3.30086500	-3.13099500	-0.37708900
C	-1.03137900	-3.14586600	-0.73553500

H	-0.85422200	-5.17261600	-0.06598800
H	-1.13480000	-5.00600300	-1.79473400
H	-3.24194900	-5.16744000	0.32383200
H	-3.52210400	-5.01195200	-1.40630000
N	-2.12338800	-2.38173900	-0.50627500
S	-1.89002900	-0.32279400	-0.23492600
C	-2.76491800	0.08271800	-1.75366800
C	-4.10832800	0.45059700	-1.62938300
C	-2.15178700	0.00105200	-3.01002700
C	-4.83908700	0.75797700	-2.77798900
H	-4.57777500	0.47710600	-0.65201500
C	-2.89496200	0.30571000	-4.14989000
H	-1.11016900	-0.29646900	-3.08721300
C	-4.23483900	0.68749800	-4.03419600
H	-5.88243900	1.04397500	-2.68845900
H	-2.42592300	0.24662300	-5.12737000
H	-4.80804500	0.92574400	-4.92513900
O	0.14001900	-2.73262700	-0.86692700
O	-4.39489000	-2.66223800	-0.15318800
<b>13'</b>			
Pd	0.36557000	-0.01324300	0.34526500
O	2.63206600	0.33572700	2.36750000
O	2.37839700	-0.23284400	0.18353800
C	3.04536100	-0.01170400	1.26705100
C	4.56621400	-0.21118600	1.03555800
F	5.02147600	0.69187900	0.13894500
F	4.82912400	-1.44054000	0.55628700
F	5.25959500	-0.04863900	2.17046200
C	0.21511300	2.07888300	1.51138200
C	1.21576900	3.07525400	1.48597700
C	1.14303500	4.10768500	0.56744700

C	0.07165600	4.16707000	-0.34496300
C	-0.90362900	3.18181800	-0.37338300
C	-0.83717500	2.12751200	0.55752100
H	0.19586600	1.38885600	2.35292800
H	2.02590300	3.00831000	2.20333200
H	1.90513400	4.88023800	0.55314000
H	0.01275300	4.99153600	-1.04959800
H	-1.70510600	3.21665400	-1.10158900
C	-0.92201700	-4.06443700	-0.53911900
C	-2.40883400	-4.40219200	-0.37464000
C	-3.04360200	-3.05561400	0.03349300
C	-0.88900300	-2.58141200	-0.17521800
H	-0.25609000	-4.61887000	0.12881900
H	-0.54174200	-4.20033600	-1.55624900
H	-2.60362100	-5.14385000	0.40559300
H	-2.88273400	-4.76653200	-1.29040500
N	-2.05547100	-2.07006800	0.14802700
S	-1.84510700	0.62861900	0.56035400
C	-2.71104300	0.68906100	-1.01502500
C	-4.10629900	0.64178500	-0.96312800
C	-2.03078100	0.71289800	-2.23780400
C	-4.83057100	0.64790300	-2.15635700
H	-4.61740700	0.57308900	-0.00900900
C	-2.76719200	0.72202900	-3.42136400
H	-0.94567100	0.71014900	-2.26275100
C	-4.16431100	0.69278300	-3.38137800
H	-5.91452400	0.60517900	-2.12345800
H	-2.24764400	0.74087300	-4.37454400
H	-4.73177900	0.69273500	-4.30708500
O	0.23492500	-1.96220400	-0.22037000
O	-4.22926400	-2.86696300	0.22259100

TS<sub>13'-12'</sub>

Pd	0.47419800	0.10931300	-0.13225600
O	2.70077800	0.25510600	2.04680600
O	2.46323000	0.24567100	-0.21776800
C	3.12027800	0.23631000	0.90099000
C	4.64722600	0.19714100	0.62133600
F	4.98243000	-0.94538400	-0.00917700
F	5.34933900	0.26857700	1.75898700
F	5.01917900	1.22996100	-0.16302000
C	-0.01847000	1.66189000	1.65878500
C	0.85994600	2.71188500	2.00888500
C	0.79603300	3.92455000	1.34555200
C	-0.14056400	4.12511300	0.31113400
C	-0.99741500	3.11090800	-0.08218500
C	-0.92938400	1.87382200	0.58952700
H	-0.07746000	0.78525500	2.29772900
H	1.57349000	2.54052300	2.80599800
H	1.46464400	4.73206600	1.62631000
H	-0.18314600	5.08340600	-0.19773100
H	-1.69744100	3.25236200	-0.89735300
C	0.95200800	-3.55748700	-2.16622300
C	0.97658800	-4.54113000	-0.98405800
C	0.70431400	-3.65479200	0.25518600
C	0.71135500	-2.22655900	-1.47144200
H	1.88988100	-3.50981100	-2.72808000
H	0.15297900	-3.75152400	-2.88924400
H	1.94118800	-5.04153200	-0.85816200
H	0.21433000	-5.32298900	-1.04473600
N	0.59074000	-2.32326000	-0.15370800
S	-1.84410100	0.39258600	0.13029000
C	-2.67660400	0.82467100	-1.40586600

C	-3.97968900	1.33043400	-1.31138900
C	-2.06808900	0.60016000	-2.64591900
C	-4.67232800	1.64403700	-2.48055600
H	-4.44442800	1.47520500	-0.34078200
C	-2.78071700	0.91284100	-3.80557300
H	-1.07208000	0.17101600	-2.70063600
C	-4.07253800	1.43665400	-3.72522700
H	-5.68019900	2.04240300	-2.41736600
H	-2.32066100	0.74077400	-4.77370400
H	-4.61729500	1.67620100	-4.63349100
O	0.63179600	-1.10709700	-2.05846600
O	0.59921100	-4.06439200	1.39263900

**TS<sub>12'-14en</sub>**

Pd	0.46363600	0.45960000	-0.60113200
O	2.27973900	1.90117600	1.08257900
O	2.38035400	1.00093600	-0.98414700
C	2.86347500	1.62410200	0.03790500
C	4.33946700	2.03725500	-0.17409000
F	4.83647700	2.64034600	0.91348300
F	4.44289000	2.89234700	-1.21148000
F	5.10164300	0.96022000	-0.44316500
C	-0.77537600	2.28307600	1.10307400
C	-0.61556800	3.66466800	1.27495000
C	-1.46948100	4.55079600	0.62658000
C	-2.48380900	4.06430600	-0.20972800
C	-2.64099600	2.69743100	-0.42025400
C	-1.78098800	1.81171500	0.24004500
H	-0.14086100	1.60227400	1.66537700
H	0.17934100	4.02308600	1.91984400
H	-1.35235800	5.62068100	0.76719700
H	-3.15144600	4.75861300	-0.71116600



H	-3.40861300	2.32507700	-1.08875100
C	1.66359400	-3.35497300	-2.10573800
C	1.52511500	-2.57380300	-3.42191500
C	0.93425400	-1.22034900	-3.01370500
C	1.21955100	-2.37013200	-1.01773900
H	1.02738400	-4.24392700	-2.05777400
H	2.68552300	-3.67749200	-1.88842000
H	0.86731400	-3.04826900	-4.15550400
H	2.48322000	-2.39038800	-3.91778400
N	0.81080900	-1.19930600	-1.63871000
S	-1.75982000	0.02574000	-0.02041300
C	-2.84843900	-0.23985800	-1.42769700
C	-4.13990700	-0.70233000	-1.14303600
C	-2.42421700	-0.03050500	-2.74481800
C	-5.02568600	-0.94021600	-2.19412200
H	-4.44510700	-0.87573400	-0.11567900
C	-3.32263100	-0.27885100	-3.78433400
H	-1.40910900	0.28729700	-2.96634800
C	-4.61726800	-0.72720000	-3.51266300
H	-6.02875100	-1.29667800	-1.98115300
H	-2.99828900	-0.12728700	-4.80914100
H	-5.30654600	-0.91946000	-4.32952100
O	1.20712100	-2.57468700	0.18204100
O	0.60706400	-0.32078800	-3.77252000

**TS<sub>13'-14'</sub>**

Pd	0.42914100	0.23884400	-0.15258300
O	2.21779800	1.80707300	1.31323300
O	2.40799400	0.54348800	-0.53461600
C	2.86337800	1.32524500	0.38113600
C	4.36857400	1.63815600	0.21978000
F	4.60937600	2.18418000	-0.98843700

F	5.09791400	0.51127900	0.32284600
F	4.78892300	2.49727600	1.15734600
C	-0.76831000	2.51141900	1.04276100
C	-0.54656700	3.89368300	1.00515100
C	-1.36155200	4.70641000	0.22368500
C	-2.39705100	4.14024000	-0.53276500
C	-2.60845500	2.76436600	-0.53675500
C	-1.78553600	1.94620000	0.24992100
H	-0.16885600	1.90185500	1.71518300
H	0.25797900	4.31394900	1.59908400
H	-1.20228600	5.78002500	0.20391000
H	-3.04166100	4.77838200	-1.13004900
H	-3.39680900	2.33243000	-1.14155600
C	0.32871400	-3.99813000	-1.07975200
C	-0.84096900	-4.83843300	-0.55189700
C	-1.76827800	-3.79493000	0.10688400
C	-0.04508300	-2.60079500	-0.58809100
H	1.30720000	-4.27831700	-0.67911200
H	0.41637800	-3.99220800	-2.17058400
H	-0.53915500	-5.57526300	0.19854800
H	-1.38783800	-5.37609300	-1.33102300
N	-1.16981800	-2.52880100	0.07905800
S	-1.84646500	0.14138900	0.31995000
C	-2.81534400	-0.29902700	-1.13310900
C	-3.93631800	-1.10631300	-0.91948300
C	-2.44554700	0.10274400	-2.42153400
C	-4.71167100	-1.49163800	-2.01399900
H	-4.16786700	-1.46924300	0.07575500
C	-3.23149700	-0.28843100	-3.50550900
H	-1.55620500	0.70502500	-2.57673900
C	-4.36499400	-1.08016900	-3.30209600

H	-5.57864400	-2.12520800	-1.85594700
H	-2.95164800	0.01970300	-4.50832800
H	-4.97047500	-1.38570300	-4.15017500
O	0.73998500	-1.62228600	-0.87086700
O	-2.86853300	-4.02431700	0.57002400
<b>14'</b>			
Pd	0.89330800	-0.24813500	-0.04109800
O	1.78970400	1.49249200	0.69774000
O	3.04656200	-0.05586900	-0.23983600
C	2.92862100	1.06634700	0.32007400
C	4.16292000	1.96251300	0.50323400
F	4.40731800	2.61647600	-0.64791600
F	5.23798900	1.22708400	0.81190300
F	3.96256400	2.86528600	1.47109400
C	-1.09442700	2.51361200	1.80610200
C	-1.17446500	3.89858800	1.94234400
C	-1.63477300	4.68196300	0.88264000
C	-2.01370300	4.07624200	-0.31704900
C	-1.92894500	2.69183100	-0.46913600
C	-1.46711400	1.91337100	0.59651100
H	-0.74303700	1.90323300	2.63248300
H	-0.88130600	4.36205900	2.87925400
H	-1.70180200	5.76009600	0.99213100
H	-2.37774300	4.68120300	-1.14214900
H	-2.23048500	2.22971600	-1.40161700
C	-0.11930500	-4.30986600	-1.12237500
C	-1.13720900	-5.07476300	-0.26987000
C	-1.66262700	-4.00480000	0.71500200
C	-0.14038300	-2.93476000	-0.46347400
H	0.89525000	-4.71873900	-1.09542600
H	-0.40162100	-4.21801600	-2.17618400

H	-0.69414400	-5.89811200	0.29829700
H	-1.97303800	-5.48846600	-0.84028800
N	-0.96457400	-2.79880900	0.54276700
S	-1.32164100	0.10685900	0.56333400
C	-2.41205000	-0.37288400	-0.78626400
C	-3.67100700	-0.86893900	-0.43304300
C	-2.02318100	-0.28435600	-2.12715500
C	-4.55680700	-1.25810500	-1.43810000
H	-3.94094000	-0.97368200	0.61226600
C	-2.91903100	-0.67707100	-3.12322600
H	-1.03185100	0.07161200	-2.38683800
C	-4.18397500	-1.15955400	-2.78022500
H	-5.53295900	-1.64903100	-1.16848600
H	-2.62302900	-0.61037100	-4.16579900
H	-4.87525200	-1.46793100	-3.55885100
O	0.61993200	-2.00834500	-0.94145300
O	-2.55945400	-4.17823000	1.51447200

**TS<sub>14'</sub>-14en**

Pd	0.34325900	-0.36942600	-0.65321900
O	1.12063600	1.58581200	-1.26987800
O	2.35457400	-0.23965300	-1.21706600
C	2.22755100	1.00170700	-1.44223300
C	3.43347300	1.78609100	-1.98143500
F	3.30226100	3.09484100	-1.72889800
F	3.51374100	1.61545000	-3.31481000
F	4.57107300	1.34930100	-1.42770500
C	-2.71135900	1.12942200	2.11172700
C	-2.81969900	2.22613700	2.96807500
C	-2.25995900	3.45244400	2.60716800
C	-1.58539500	3.58776000	1.39016000
C	-1.46440900	2.50048900	0.52619000

C	-2.03812200	1.27601800	0.89404000
H	-3.13664600	0.16970700	2.38706000
H	-3.33750300	2.11773000	3.91587200
H	-2.34277300	4.30306100	3.27697500
H	-1.14065500	4.53924000	1.11541100
H	-0.91943500	2.59587800	-0.40587300
C	0.10113000	-4.45347200	0.49651200
C	0.50181400	-4.34238600	1.97763700
C	0.63513200	-2.81996600	2.22390100
C	0.10679200	-2.99941500	0.05189900
H	0.80159200	-5.02954600	-0.11579800
H	-0.89308600	-4.88397100	0.33814600
H	1.45823500	-4.82312800	2.20391200
H	-0.23726300	-4.75852600	2.66796000
N	0.40723300	-2.14472000	1.02345600
S	-1.88264700	-0.19768900	-0.12285800
C	-2.67479100	0.23589100	-1.69197000
C	-3.57925500	1.29463200	-1.80690000
C	-2.40817300	-0.60899100	-2.77825200
C	-4.20967700	1.51813300	-3.03256900
H	-3.79014000	1.93791700	-0.96045700
C	-3.04658300	-0.36948500	-3.99441100
H	-1.71381400	-1.43693900	-2.67006400
C	-3.94391900	0.69295900	-4.12595600
H	-4.91018100	2.34242000	-3.12745300
H	-2.83712700	-1.01644900	-4.84078400
H	-4.43542400	0.87549600	-5.07666300
O	-0.14482500	-2.59133300	-1.11766700
O	0.89040700	-2.30907000	3.29544300
<b>14<sub>en</sub></b>			
Pd	0.48233500	-0.53938100	0.06657200

O	1.15436400	1.04122400	-1.19431200
O	2.52420100	-0.58679900	-0.60604500
C	2.30321100	0.49716500	-1.21109600
C	3.44955400	1.21552700	-1.94030200
F	4.42241900	0.36126600	-2.27217100
F	3.96361000	2.15961000	-1.12862000
F	2.99989800	1.81440600	-3.05268600
C	-0.96516600	2.52421600	0.94928400
C	-1.08299600	3.74075300	1.62241800
C	-2.07615300	3.92179200	2.58824100
C	-2.96068400	2.88439000	2.88732000
C	-2.85459700	1.66194000	2.22252800
C	-1.85934300	1.48979300	1.25353600
H	-0.19135200	2.38130700	0.20293900
H	-0.39081400	4.54532200	1.39376900
H	-2.15682200	4.87015400	3.11092900
H	-3.73019600	3.02083700	3.64089100
H	-3.53358600	0.84760200	2.45507800
C	0.80171900	-3.70758400	2.93505400
C	-0.18575400	-4.34977600	1.94921300
C	-0.43309900	-3.27122500	0.88962500
C	1.02856500	-2.29273300	2.38968500
H	0.42296500	-3.63914900	3.95869000
H	1.76648400	-4.22133600	2.98263000
H	-1.14311300	-4.62422900	2.40237700
H	0.20358500	-5.24514800	1.45589700
N	0.31729100	-2.16093100	1.20384500
S	-1.76474800	-0.13439900	0.47861200
C	-2.47002800	0.09824900	-1.17681600
C	-2.57085500	-1.06097100	-1.95767900
C	-2.93025900	1.33110300	-1.64210300

C	-3.13848700	-0.96729600	-3.22746700
H	-2.20138900	-2.00778000	-1.57306400
C	-3.50006100	1.40220400	-2.91546900
H	-2.85040500	2.22219500	-1.03089000
C	-3.60357000	0.25938600	-3.70866500
H	-3.21669800	-1.85998700	-3.84068100
H	-3.85997000	2.35823500	-3.28385200
H	-4.04490700	0.32363200	-4.69868900
O	1.70803800	-1.42121500	2.90009300
O	-1.18338100	-3.37550800	-0.07273100

**TS<sub>14en-15</sub>**

Pd	0.78063500	-0.34859500	-0.53390000
O	1.07603300	1.66934300	-0.87508500
O	1.79448200	0.26426600	-2.41560000
C	1.63798000	1.43888100	-1.99755900
C	2.16766300	2.62417900	-2.81935200
F	3.47384300	2.80222700	-2.55007100
F	1.51244900	3.75125400	-2.51367200
F	2.03146500	2.38494400	-4.12949800
C	-3.08507800	0.55922100	2.11181000
C	-3.22625500	1.34170600	3.26063600
C	-2.55339700	2.55909900	3.36496700
C	-1.72747300	2.99201600	2.32296800
C	-1.56332900	2.21043600	1.18059100
C	-2.25231800	0.99308100	1.07274300
H	-3.61743000	-0.38229800	2.01924600
H	-3.86790200	0.99978700	4.06711000
H	-2.66735900	3.16844800	4.25655300
H	-1.19413400	3.93434500	2.40583900
H	-0.89887000	2.53109300	0.38580700
C	1.86403600	-4.46060700	-0.79608500

C	0.58709200	-4.48393600	-1.64640300
C	0.01963400	-3.06687100	-1.53770500
C	1.87377600	-3.07591000	-0.14815900
H	1.89961400	-5.22631800	-0.01631000
H	2.77800900	-4.56414000	-1.38890400
H	-0.16361200	-5.19076900	-1.27823700
H	0.75526200	-4.71508100	-2.70126600
N	0.73449000	-2.36213900	-0.56118000
S	-2.01646600	-0.11778400	-0.31778200
C	-2.47500900	0.85792900	-1.76310100
C	-3.29399600	1.98874200	-1.67714100
C	-2.03228300	0.39553900	-3.01009500
C	-3.65229200	2.66727600	-2.84343500
H	-3.64845000	2.34135000	-0.71531500
C	-2.40542000	1.08120000	-4.16616300
H	-1.42006100	-0.49829400	-3.06935200
C	-3.20977900	2.22020200	-4.08893900
H	-4.28437700	3.54779400	-2.77193200
H	-2.05898900	0.72119400	-5.13054400
H	-3.49103700	2.75336100	-4.99204200
O	2.70971200	-2.64245600	0.62045700
O	-0.90753900	-2.62003100	-2.18677300
C	0.20108700	-0.92032600	4.00299800
F	0.94523100	-1.85825200	4.60856000
F	-1.07212900	-1.05531600	4.40933100
F	0.64461100	0.28388400	4.35715200
C	0.28515000	-1.10139300	2.47269900
O	0.79314400	-0.24710200	1.76423100
O	-0.24767300	-2.23399100	2.07996100
H	-0.08921900	-2.33715400	1.10097300



Pd	0.72949000	-0.56682300	-0.02016800
O	1.83511100	0.91428800	-0.93919000
O	2.71348100	-1.11308900	-0.99383200
C	2.75419200	0.10078900	-1.29774700
C	3.89589400	0.64200800	-2.17321400
F	4.10328000	1.94601100	-1.94229200
F	3.57117500	0.48700900	-3.47104000
F	5.03336300	-0.02356700	-1.93832700
C	-1.00548900	2.66544100	-1.09712100
C	-1.40093200	3.96257400	-0.77146200
C	-2.73705700	4.24149500	-0.46945000
C	-3.68643600	3.21922900	-0.49844800
C	-3.30409500	1.91883100	-0.83618700
C	-1.96406300	1.64231800	-1.13594800
H	0.03461800	2.44531900	-1.31021300
H	-0.65887200	4.75509200	-0.74346300
H	-3.03589200	5.25346300	-0.21184800
H	-4.72639800	3.43098200	-0.26773600
H	-4.03939000	1.12110700	-0.87313000
C	0.14543400	-4.17830800	2.19237600
C	-0.55396000	-4.56539900	0.88350200
C	-0.50403300	-3.29811700	0.02654100
C	0.45761800	-2.68831400	2.03906100
H	-0.46425600	-4.32853200	3.08776800
H	1.08815800	-4.70991700	2.35298800
H	-1.60048400	-4.85632500	1.01955400
H	-0.06403400	-5.37642000	0.33838100
N	-0.01495900	-2.24390100	0.79679100
S	-1.52517800	-0.06615300	-1.47989400
C	-0.94791400	-0.03727100	-3.19107800
C	-0.25946100	-1.16990300	-3.64679500

C	-1.21712500	1.02555100	-4.05893300
C	0.16781100	-1.22258600	-4.97301600
H	-0.07768800	-1.99934500	-2.97145300
C	-0.77815000	0.95813500	-5.38292000
H	-1.75997500	1.89740100	-3.71282900
C	-0.08399300	-0.16035300	-5.84429200
H	0.70484800	-2.09981200	-5.32183000
H	-0.98482000	1.78783500	-6.05294700
H	0.25750900	-0.20483300	-6.87405400
O	1.01146500	-1.98263700	2.86092800
O	-0.84235300	-3.22133300	-1.14192500
C	-1.49836800	1.54860300	3.43436100
C	-1.05233000	0.61100700	2.34886700
O	-0.06450500	0.82195700	1.64898400
O	-1.82365500	-0.46458000	2.22528200
H	-1.40071800	-1.07997400	1.58188000
H	-2.57988100	1.69553700	3.38699000
H	-1.26322800	1.09783500	4.40411700
H	-0.97494600	2.49876100	3.33949100