

# Substituent's Effects of PNP Ligands in Ru(II)-Catalyzed Hydrogenation of CO<sub>2</sub> to Formate: Theoretical Analysis Considering Steric Hindrance and Promotion of Hydrogen Bonding

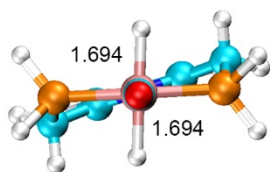
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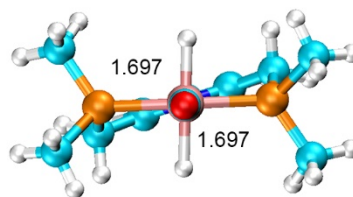
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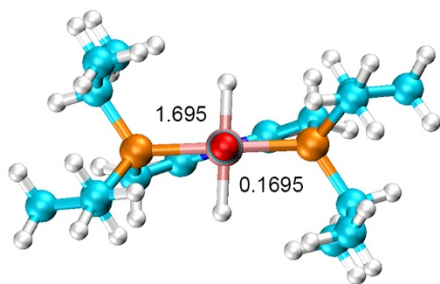
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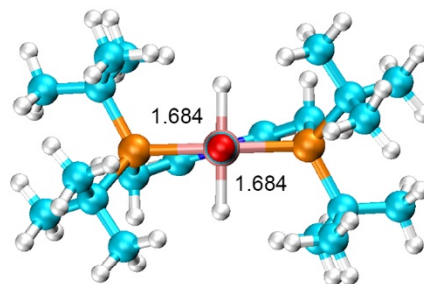
Complex A-1, R = Hydrogen



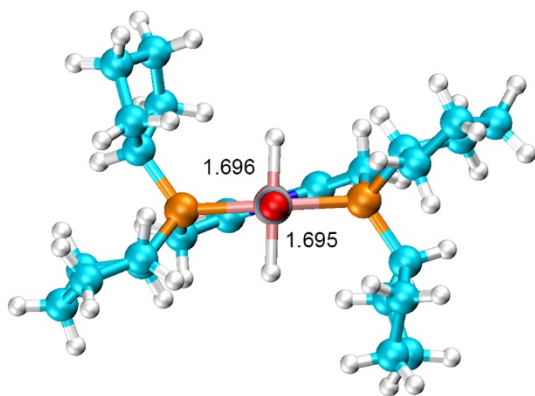
Complex B-1, R = Methyl



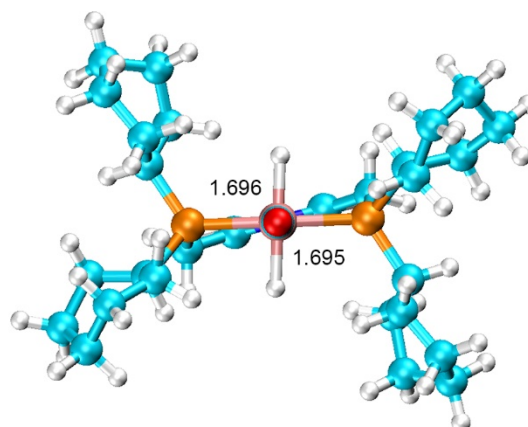
Complex C-1, R = *iso*-Propyl



Complex D-1, R = *tert*-Butyl

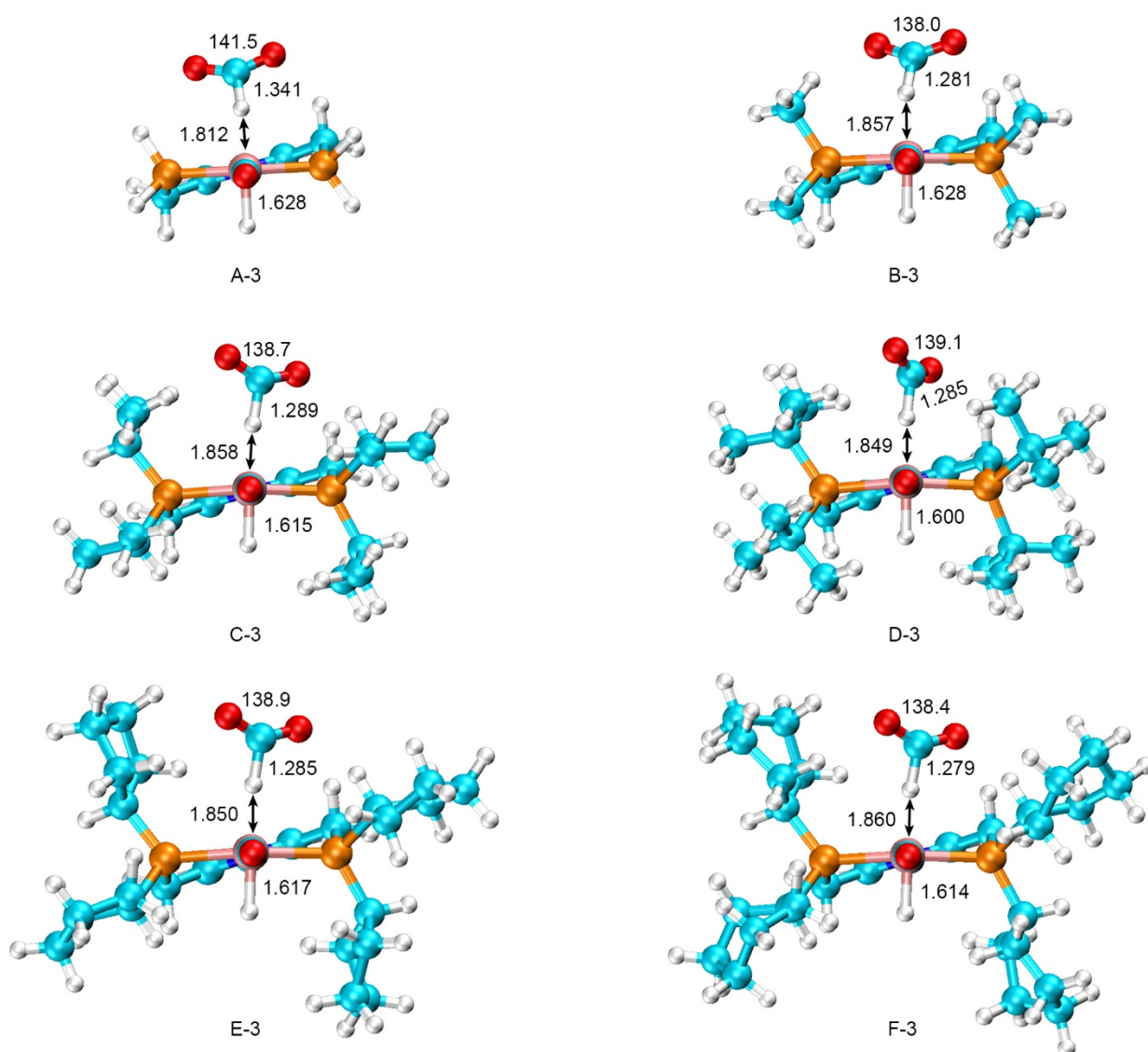


Complex E-1, R = Cyclopentyl

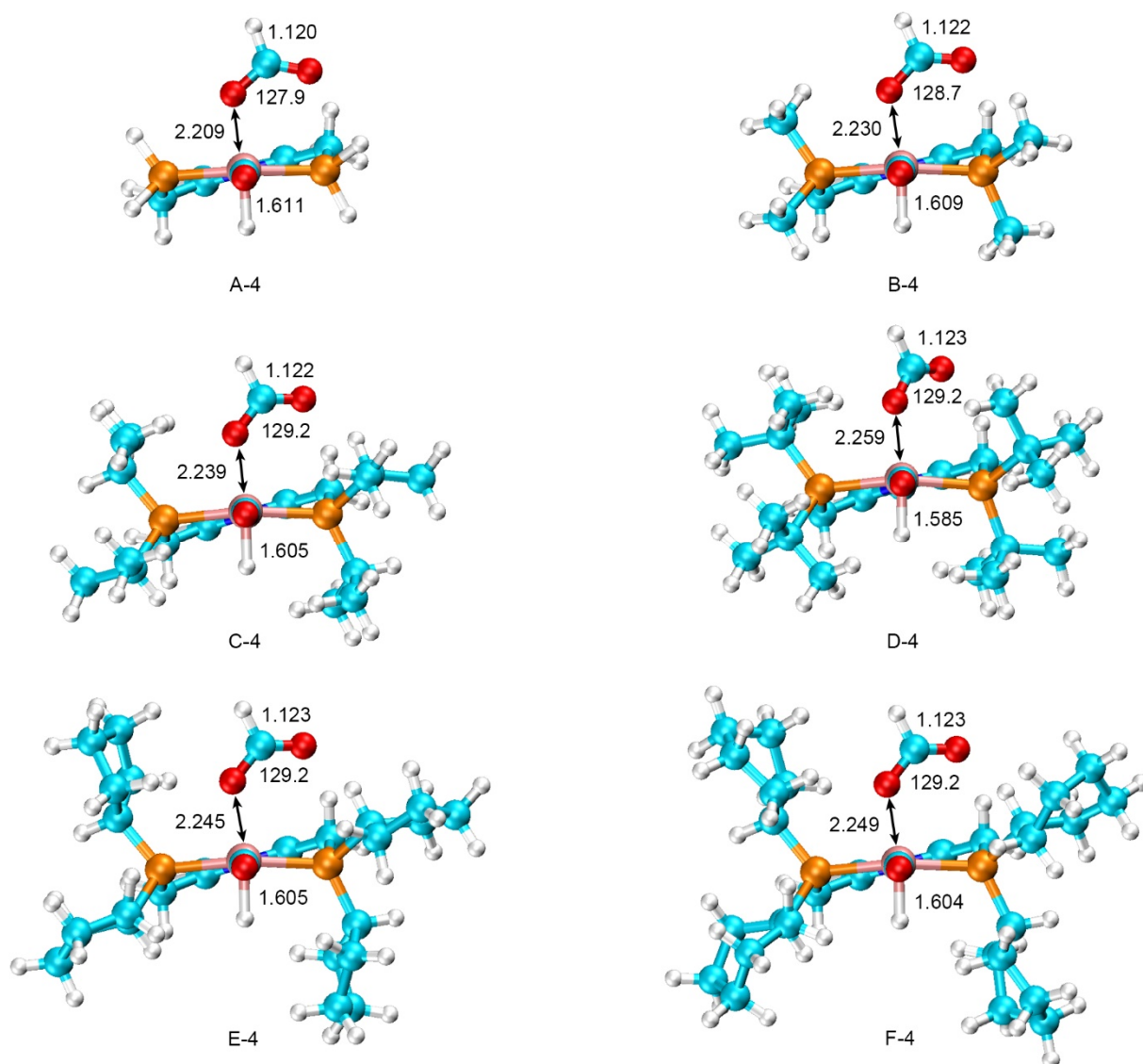


Complex F-1, R = Cyclohexyl

**Figure S1.** Optimized geometries of six Ru-PNP complexes with different substituents. The distances of Ru-H bond are in Å.



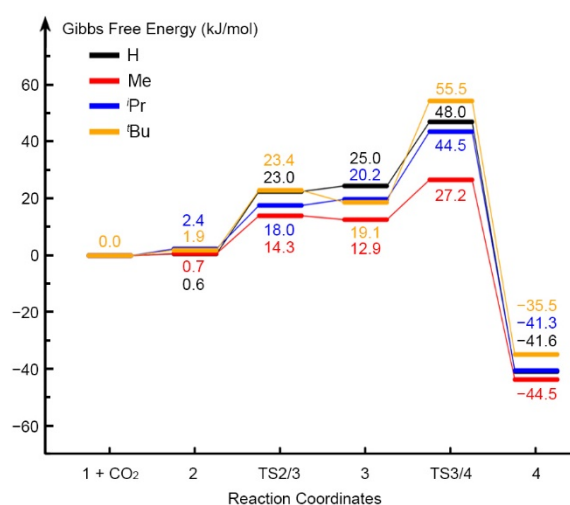
**Figure S2.** Optimized geometries of the products in hydride addition step on six Ru-PNP complexes. Pink balls: Ru; Orange: P; red: O; blue: N; Cyan: C; white: H; All distance are in Å and the O-C-O bond angles are in degree (°).



**Figure S3.** Optimized geometries of the products in  $\text{HCOO}^-$  rotation step on six Ru-PNP complexes. Pink balls: Ru; Orange: P; red: O; blue: N; Cyan: C; white: H; All distances are in Å and the O-C-O bond angles are in degree (°).

**Table S1.** The binding energy and binding free energy for CO<sub>2</sub> coordination on Ru-PNP complexes with different substituents calculated with B3LYP-D3(BJ) functional.

Complex code	Substituent type	Binding energy (kJ/mol)	Binding free energy (kJ/mol)
A	Hydrogen (H)	−34.8	0.6
B	Methyl (Me)	−34.4	0.7
C	<i>iso</i> -Propyl ( <sup>i</sup> Pr)	−31.3	2.4
D	<i>tert</i> -Butyl ( <sup>t</sup> Bu)	−32.1	1.9



**Figure S4.** Free energy profiles for the total reaction of CO<sub>2</sub> hydrogenation on R-substituted (R = H, Me, iPr, tBu) complexes calculated with B3LYP-D3(BJ) functional.

It can be seen from Figure S4 that the total barriers are all decreased, compared with the results obtained with B3LYP functional. One reason for this decrease is the increase of binding energy for CO<sub>2</sub> coordination on the Ru-PNP complexes (see Table S1). But the order of total barrier does not change, still be <sup>t</sup>Bu > <sup>i</sup>Pr > Me > H.

**Table S2.** Cartesian coordinates for optimized geometries of all the species in gas phase.

<b>A-1</b>				H	-4.43769100	-0.57821600	1.23594300
				H	-4.88227900	1.79715500	0.55423500
				H	-3.03857200	3.09111700	-0.55497500
				C	-2.14622900	-1.99971300	0.81877500
				C	-0.49628200	2.23106500	-1.04077000
Ru	-1.04512900	-0.00019200	0.00061800	H	-2.43837300	-2.60465300	-0.05774700
P	-0.69573400	2.24770800	0.29005100	H	-2.74636100	-2.33590900	1.67700900
P	-0.69378300	-2.24788600	-0.29272000	H	-0.85598700	3.01063700	-1.72820600
N	1.14791900	0.00021100	0.00066800	H	0.05442800	2.72565900	-0.22198100
C	1.83628500	1.16166600	-0.15625900	H	-0.18083300	-1.69685800	-1.64628000
C	3.23355900	1.19037400	-0.14372300	C	2.19614700	-1.53168700	-0.74693700
C	3.94403700	0.00072600	0.00024900	O	3.23544400	-2.01520200	-0.93866900
C	3.23404500	-1.18921600	0.14419200	H	1.15809000	0.22067300	0.79612500
C	1.83679800	-1.16103700	0.15708000	H	-0.14765400	-2.30404900	2.43438000
H	3.75210200	2.14252300	-0.26446400	H	0.43241200	1.12272600	-3.19282600
H	5.03590000	0.00091800	0.00021900	H	1.90307000	1.93940100	-1.85893000
H	3.75298100	-2.14120600	0.26456100	H	-0.26664500	-3.72854500	0.83574400
C	1.03893400	2.41823200	-0.40069900	C	2.63966300	2.17056300	1.87056600
C	1.03982300	-2.41808100	0.40050900	O	2.26689700	2.92992800	1.06104500
H	0.88856500	2.52520000	-1.48951600	O	3.03775300	1.45878700	2.70285000
H	1.57600600	3.30860700	-0.04209200	<b>A-3</b>			
H	1.57833300	-3.30814200	0.04338500				
H	0.88670500	-2.52437300	1.48898400				
H	-0.98529800	0.35573900	-1.65457200	Ru	-1.04573300	0.06197900	-0.37409600
C	-2.89297100	-0.00110100	0.00088300	P	-0.69218400	2.30063600	0.06900100
O	-4.05512500	-0.00051900	0.00037700	P	-0.69800200	-2.18565000	-0.82716300
H	-0.98470300	-0.35628500	1.65544600	N	1.14973400	0.05934300	-0.40295700
H	-0.58694600	2.92516900	1.54782600	C	1.83927100	1.22980300	-0.44508000
H	-0.58277800	-2.92167100	-1.55210100	C	3.23607100	1.25362900	-0.44230000
H	-1.35917300	-3.29386900	0.41217500	C	3.94249600	0.05391700	-0.42799500
H	-1.36074300	3.29180400	-0.41807600	C	3.23213300	-1.14315400	-0.39770900
<b>A-2</b>				C	1.83562600	-1.11546900	-0.36516600
				H	3.75711800	2.21147200	-0.46425700
				H	5.03426400	0.05197800	-0.43619000
Ru	0.54622200	-0.75840600	-0.44186200	H	3.74969600	-2.10268100	-0.37156700
P	-0.30799500	-2.31393300	1.01120800	C	1.05845600	2.51740600	-0.55109900
P	0.76896500	1.07792100	-1.80189900	C	1.05022300	-2.39192400	-0.20668700
N	-1.41349200	0.16215000	-0.08616900	H	0.95693800	2.77977400	-1.61882700
C	-2.41224900	-0.54911400	0.50031700	H	1.59059000	3.34182100	-0.05497000
C	-3.66259600	0.02079600	0.75585400	H	1.57829400	-3.25002800	-0.64533900
C	-3.90827700	1.33775900	0.37399200	H	0.91716000	-2.56141000	0.87800100
C	-2.88742700	2.05656300	-0.24374000	H	-1.04322900	0.40831600	-1.96457600
C	-1.64412600	1.45172400	-0.44953000	C	-2.89745500	0.07567200	-0.42646800

O	-4.05467600	0.08875600	-0.48079500	Ru	-1.03456100	0.08491100	-0.40586200
H	-1.02203300	-0.27846100	1.40505700	P	-0.68644800	2.29759300	0.12455200
H	-0.63457800	2.75901800	1.41435000	P	-0.68526300	-2.13466400	-0.94395000
H	-0.66176000	-2.72147900	-2.14935400	N	1.16054300	0.08189100	-0.40619400
H	-1.35477800	-3.26964700	-0.17797600	C	1.85071200	1.25289200	-0.40720300
H	-1.34630300	3.40104700	-0.55506300	C	3.24767500	1.27639600	-0.38511600
C	-0.18194900	-0.39066200	2.44481000	C	3.95436800	0.07654300	-0.39376700
O	0.11997200	0.71535800	2.85353000	C	3.24314800	-1.12072800	-0.40810300
O	0.01049100	-1.57565200	2.66479600	C	1.84613900	-1.09326000	-0.39642500
A-4				H	3.76869500	2.23454800	-0.37522100
				H	5.04615700	0.07439900	-0.38716300
				H	3.76039100	-2.08090700	-0.40510100
Ru	-0.89122100	0.32027900	-0.31008800	C	1.06595000	2.53954400	-0.48784100
P	-0.34587100	2.44528900	0.39151100	C	1.05515900	-2.37380100	-0.30355500
P	-0.73363600	-1.85249900	-1.13385900	H	0.96003900	2.81781500	-1.55116300
N	1.29173800	0.06232700	-0.20728300	H	1.59534400	3.35804400	0.02104400
C	2.09919600	1.14018000	-0.01643200	H	1.58909600	-3.21076400	-0.77555200
C	3.48107700	1.00232200	0.13119600	H	0.91338200	-2.60457200	0.76730300
C	4.05617000	-0.26381000	0.04109800	H	-1.00219500	0.53203600	-1.99476400
C	3.23142200	-1.35885300	-0.19433300	C	-2.88485300	0.09850000	-0.45643900
C	1.84780800	-1.17547700	-0.30470200	O	-4.04351600	0.11064900	-0.50107100
H	4.09600000	1.88769500	0.29772900	H	-0.99896600	-0.36678300	1.29319300
H	5.13542900	-0.39251600	0.14616000	H	-0.62671800	2.74691100	1.47578300
H	3.64452300	-2.36482800	-0.27793300	H	-0.61990400	-2.63634400	-2.27984900
C	1.47431100	2.51575300	-0.03923600	H	-1.34920200	-3.24404600	-0.34534000
C	0.94510700	-2.36755400	-0.49925000	H	-1.33727900	3.41889500	-0.46588600
H	1.50981100	2.89305200	-1.07647700	C	-0.19557700	-0.54279200	2.59763200
H	2.04193700	3.21952900	0.58660400	O	-0.01409600	0.56117400	3.02839900
H	1.43470300	-3.13025900	-1.12219000	O	-0.04521600	-1.73085600	2.70515400
H	0.70584800	-2.80589800	0.48442900	A-TS3/4			
H	-0.72578200	0.82536800	-1.83084300				
C	-2.70974900	0.55772900	-0.52744000				
O	-3.84539000	0.71961000	-0.69886600	Ru	-0.98879400	0.18402800	-0.32337000
H	-1.16724700	-1.43959800	3.39799100	P	-0.54787000	2.36811900	0.31390800
H	-0.36010600	2.80683500	1.77354400	P	-0.69914200	-2.05554600	-0.94372800
H	-0.58719600	-2.02406800	-2.54645700	N	1.21574000	0.08035400	-0.29846600
H	-1.54052500	-2.98337300	-0.85490200	C	1.95356300	1.21692000	-0.21989100
H	-0.80127300	3.67713000	-0.16064300	C	3.34918200	1.18232300	-0.18913000
C	-1.07580400	-1.39723100	2.28269900	C	4.00574600	-0.04335300	-0.26850300
O	-1.13032200	-2.45247600	1.63547100	C	3.24656800	-1.20591100	-0.35359700
O	-0.91418500	-0.20561300	1.83482800	C	1.85100000	-1.12108800	-0.34383900
A-TS2/3				H	3.90907800	2.11523000	-0.11389500
				H	5.09650000	-0.09114400	-0.25744900
				H	3.72254800	-2.18597500	-0.39856000



C	1.23716700	2.54670700	-0.20928800	H	-4.46803200	-0.96743800	-1.01374900
C	1.01608600	-2.37094600	-0.29187200	H	-3.06211300	-1.46914400	-2.02984200
H	1.20044900	2.93925100	-1.24060600	C	-3.21753400	-0.36774300	1.65428300
H	1.78432500	3.28000300	0.40052100	H	-4.24848600	-0.00652900	1.50464000
H	1.52133200	-3.22259300	-0.76757000	H	-3.24190800	-1.36003400	2.13068000
H	0.81469600	-2.59678300	0.77667900	H	-2.67270400	0.31290900	2.32497600
H	-0.87613700	0.60594100	-1.83512700	C	3.21744400	-0.36832500	-1.65431000
C	-2.82209500	0.30392600	-0.54406700	H	4.24857700	-0.00762200	-1.50467100
O	-3.96043900	0.39268000	-0.73912300	H	3.24131100	-1.36054300	-2.13088400
H	-1.80496400	-0.44828000	1.77750800	H	2.67289500	0.31270400	-2.32484900
H	-0.55484000	2.73947700	1.68502900	C	3.46702300	-1.42941400	1.00858600
H	-0.63735200	-2.43936100	-2.31603700	H	3.54900100	-2.45990100	0.62972200
H	-1.43668600	-3.14793200	-0.41669700	H	4.46770000	-0.96774500	1.01427600
H	-1.11705900	3.53855100	-0.26735100	H	3.06157700	-1.47033100	2.02965200
C	-0.76327900	-0.82257900	2.13381400				
O	-0.64181000	-2.06436200	2.18056200	<b>B-2</b>			
O	0.05680200	0.10284400	2.36564400				
<b>B-1</b>				Ru	-0.12458600	-0.84968800	-0.41332500
				P	-2.37616200	-0.46259600	-0.09692100
				P	2.13969900	-0.57436800	-0.75774400
Ru	-0.00007600	-0.83572200	-0.00000400	N	-0.07644900	1.33675200	-0.47391100
P	2.27834200	-0.50113500	-0.06113000	C	-1.22808800	2.04602700	-0.61531200
P	-2.27841800	-0.50070200	0.06112300	C	-1.22667500	3.44391600	-0.63749500
N	0.00013400	1.34839200	0.00000700	C	-0.01843900	4.13214700	-0.55084900
C	1.14020500	2.03650500	0.27635400	C	1.16043200	3.39990700	-0.42775500
C	1.16902900	3.43412100	0.26615300	C	1.10474900	2.00387500	-0.37424700
C	0.00040300	4.14474500	0.00001400	H	-2.17128300	3.97956500	-0.74270800
C	-1.16836000	3.43434600	-0.26612700	H	0.00427800	5.22355000	-0.57981400
C	-1.13980600	2.03672400	-0.27632500	H	2.12673400	3.90081100	-0.35244500
H	2.10357700	3.95286300	0.48492100	C	-2.50437100	1.26753900	-0.80853900
H	0.00050900	5.23675200	0.00000600	C	2.34988800	1.18527200	-0.14583700
H	-2.10280500	3.95326900	-0.48490900	H	-2.64231000	1.10617500	-1.89288900
C	2.36176300	1.23365500	0.64645300	H	-3.37520700	1.83321000	-0.44020700
C	-2.36152100	1.23411300	-0.64644300	H	3.23815700	1.69219900	-0.55602500
H	2.35410100	1.08386900	1.74099000	H	2.49698200	1.08081200	0.94378600
H	3.28621000	1.77419100	0.38686100	H	-0.46012200	-0.82397800	-2.07322700
H	-3.28585800	1.77482900	-0.38683900	C	-0.16123400	-2.68983800	-0.37055300
H	-2.35389300	1.08435300	-1.74098400	O	-0.18276200	-3.85531400	-0.34231300
H	0.16019100	-0.77276500	1.68825900	H	0.20942800	-0.76363800	1.24604300
C	-0.00024700	-2.67723900	-0.00012400	C	0.87991500	0.12997000	3.62508800
O	-0.00054500	-3.84337900	0.00013200	O	-0.23281200	0.14180000	3.97575800
H	-0.16030900	-0.77267200	-1.68826300	O	2.01309200	0.14866800	3.33491800
C	-3.46721500	-1.42880600	-1.00861500	C	-3.11978800	-0.31570400	1.59410000
H	-3.54873400	-2.45949600	-0.63020600	H	-4.13725400	0.10841100	1.57006600

H	-3.15524100	-1.32082000	2.04288500	H	-3.32500700	-1.59248900	1.80266700
H	-2.46185700	0.30286000	2.22130800	H	-2.56901200	-0.01648800	2.17047700
C	-3.69991300	-1.36758000	-1.01801200	C	-3.48617500	-1.54110900	-1.25972600
H	-3.75515800	-2.39694700	-0.63146300	H	-3.50505400	-2.58602700	-0.91410300
H	-4.68537700	-0.88749100	-0.90391100	H	-4.51036700	-1.13605400	-1.23223700
H	-3.42052200	-1.41435000	-2.08032000	H	-3.10257900	-1.52561700	-2.29020900
C	3.42944200	-1.48668700	0.20216500	C	3.50543400	-1.31123800	0.55655900
H	3.41883300	-2.54251000	-0.10953300	H	3.56533900	-2.37010300	0.26237800
H	4.43693100	-1.07192100	0.03654400	H	4.50048700	-0.84824300	0.45990400
H	3.17122900	-1.43524700	1.26935800	H	3.14510600	-1.23277500	1.59347600
C	2.86411200	-0.54896500	-2.46330100	C	3.02146500	-0.46172300	-2.18736500
H	3.91667000	-0.22097900	-2.47074400	H	4.05718200	-0.08619300	-2.16696200
H	2.79351700	-1.56381600	-2.88454500	H	3.01472400	-1.49053900	-2.57887700
H	2.25513200	0.11707500	-3.09214200	H	2.40943700	0.16110600	-2.85620600

### B-3

Ru	-0.03302200	-0.84498400	-0.27140500
P	-2.34378500	-0.58306300	-0.16998700
P	2.26073800	-0.46456700	-0.50328700
N	-0.07723600	1.33552900	-0.38065400
C	-1.25515300	1.98600600	-0.57630300
C	-1.32208500	3.38126100	-0.59206000
C	-0.15467000	4.12591000	-0.44309900
C	1.05249700	3.45480600	-0.26991500
C	1.06617200	2.05756000	-0.22324300
H	-2.28577300	3.87122700	-0.73637300
H	-0.18603300	5.21724900	-0.46133400
H	1.98632400	4.00346300	-0.14201600
C	-2.48785900	1.15798700	-0.84492200
C	2.34328600	1.31163300	0.07103400
H	-2.58422100	1.03438800	-1.93874900
H	-3.39350500	1.67614200	-0.49288000
H	3.21954500	1.85529600	-0.31557500
H	2.44046000	1.22644700	1.16893400
H	-0.19336100	-0.91331200	-1.87792300
C	0.01884000	-2.69049100	-0.25929700
O	0.05249700	-3.85184600	-0.27952400
H	0.10796600	-0.75390400	1.57802600
C	0.37348900	0.01319200	2.56844500
O	-0.63089600	0.60006400	2.95235200
O	1.56361500	-0.05366600	2.86829300
C	-3.21287400	-0.55336700	1.45466900
H	-4.20825200	-0.08751300	1.37545700

### B-4

Ru	-0.08798500	-0.77494900	-0.24677200
P	-2.39316200	-0.51507700	-0.09560300
P	2.18195600	-0.35138000	-0.62919200
N	-0.12813200	1.41518800	-0.19713700
C	-1.30986900	2.08048800	-0.30036100
C	-1.37568300	3.47136300	-0.18834300
C	-0.20073400	4.20037300	-0.01133300
C	1.00994300	3.51802500	0.05142400
C	1.02452600	2.11996500	-0.03042700
H	-2.34183900	3.97264500	-0.26063400
H	-0.22993600	5.28911000	0.06974200
H	1.95033500	4.05433600	0.18446700
C	-2.54900900	1.27756900	-0.61847500
C	2.31610200	1.35897100	0.10697600
H	-2.65980100	1.24747200	-1.71749000
H	-3.45019500	1.76577500	-0.21471100
H	3.16362400	1.94463600	-0.28319700
H	2.48244000	1.14071500	1.17856800
H	-0.25701100	-0.71767300	-1.84588800
C	-0.04002000	-2.60825200	-0.40464000
O	-0.01419600	-3.76350000	-0.54119600
H	0.51091800	-0.64527700	3.87919000
C	0.84055200	-0.56645000	2.80955800
O	2.04144300	-0.37307200	2.57236400
O	-0.12980300	-0.68869300	1.98119800
C	-3.23372700	-0.59770800	1.54626900
H	-4.24064800	-0.15168000	1.51783200

H	-3.30832100	-1.65511800	1.84335700	H	-3.29823000	-1.59719900	1.78419700
H	-2.59268800	-0.09349300	2.28230200	H	-2.64898300	0.01433800	2.15197400
C	-3.58047400	-1.37044100	-1.22223900	C	-3.49446200	-1.50416000	-1.28792900
H	-3.61670200	-2.43637300	-0.94969900	H	-3.51786200	-2.55371500	-0.95649000
H	-4.59480000	-0.94616600	-1.15092900	H	-4.51641700	-1.09365300	-1.25158700
H	-3.21260900	-1.29267900	-2.25571400	H	-3.11118900	-1.47746900	-2.31803000
C	3.62119700	-1.26911800	0.06517900	C	3.51872400	-1.31551600	0.40441700
H	3.64252500	-2.27503900	-0.38190700	H	3.57571700	-2.35918500	0.05913600
H	4.56754400	-0.75275000	-0.16304500	H	4.50907000	-0.84426300	0.29810700
H	3.47096100	-1.34319100	1.14990800	H	3.20376000	-1.30327900	1.45744600
C	2.67571000	-0.12334600	-2.40027000	C	2.99204000	-0.34336700	-2.27010300
H	3.70172600	0.26922200	-2.49037200	H	4.02484000	0.04050900	-2.24047700
H	2.61235200	-1.09548100	-2.91313200	H	2.98975200	-1.35306800	-2.70900700
H	1.96782100	0.56279400	-2.88765200	H	2.36721500	0.30148300	-2.90535000

#### B-TS2/3

Ru	-0.03825100	-0.82560700	-0.33296800
P	-2.33593300	-0.56861900	-0.19310800
P	2.23366000	-0.43567000	-0.58465300
N	-0.09016100	1.35872600	-0.36515700
C	-1.26779800	2.01359700	-0.54633200
C	-1.33562200	3.40960300	-0.52412800
C	-0.16925600	4.15150000	-0.35289900
C	1.03852400	3.47545700	-0.19665200
C	1.05183500	2.07748700	-0.18972400
H	-2.29934500	3.90244300	-0.65943400
H	-0.20089900	5.24297300	-0.34331100
H	1.97285600	4.02084400	-0.05712700
C	-2.49365900	1.18494000	-0.83889100
C	2.32836700	1.31625400	0.06989100
H	-2.57187300	1.07226200	-1.93533200
H	-3.40721400	1.69364100	-0.49268000
H	3.20422600	1.87520900	-0.29631200
H	2.43991900	1.18970400	1.16111700
H	-0.25670800	-0.81459200	-1.97908500
C	0.01515100	-2.66818200	-0.34086000
O	0.05020900	-3.83168500	-0.35623600
H	0.18554500	-0.73475800	1.39799600
C	0.47951400	-0.07991100	2.91674800
O	-0.59828200	0.26958900	3.28277800
O	1.65973300	-0.20611600	3.04828100
C	-3.23594900	-0.55913300	1.42103500
H	-4.25364200	-0.14799900	1.32133400

#### B-TS3/4

Ru	-0.05276800	-0.82400600	-0.25061900
P	-2.37084400	-0.57407000	-0.09267700
P	2.24083800	-0.38382600	-0.54247400
N	-0.11771200	1.36376200	-0.30826300
C	-1.30216400	2.00776700	-0.46836700
C	-1.38406400	3.40130800	-0.43396700
C	-0.22208600	4.15116300	-0.26482400
C	0.99136800	3.48670100	-0.11867900
C	1.01792900	2.08831400	-0.12148600
H	-2.35358100	3.88698000	-0.55123400
H	-0.26405800	5.24216800	-0.24333900
H	1.91993000	4.03875300	0.03031500
C	-2.53377800	1.17665500	-0.73522900
C	2.29595500	1.34349700	0.15673000
H	-2.65322500	1.07209300	-1.82877900
H	-3.43632600	1.68144200	-0.35675100
H	3.17701500	1.91923300	-0.16671100
H	2.35745300	1.16896400	1.25130600
H	-0.21736900	-0.83664600	-1.81307500
C	0.01583400	-2.66501800	-0.35637800
O	0.05680300	-3.81955300	-0.48048400
H	0.26980400	-1.46046000	2.05387100
C	0.58185400	-0.41123000	2.43746700
O	-0.34773800	0.43654000	2.43703600
O	1.78555000	-0.29172600	2.74639800
C	-3.18131700	-0.58555700	1.56079300
H	-4.16819500	-0.09656500	1.53775800

H	-3.30094600	-1.63369800	1.87786000	C	-2.87347900	1.00073500	2.41533200
H	-2.48353300	-0.08720800	2.25269900	C	-3.35852600	-1.04666800	-1.40046900
C	-3.53686700	-1.51513600	-1.17267200	C	-3.35327200	-2.57759100	-1.28631100
H	-3.54969000	-2.56594600	-0.84521000	C	-4.78934000	-0.50617500	-1.53286200
H	-4.55971600	-1.10990900	-1.11549000	H	2.79094700	-0.78537900	2.31120100
H	-3.18051900	-1.48202500	-2.21272800	H	4.38660200	0.08641800	-1.17134600
C	3.56573000	-1.28240000	0.36201600	H	-4.38646600	0.08722000	1.17156200
H	3.62619000	-2.31268700	-0.02044700	H	-2.79132100	-0.78436200	-2.31117600
H	4.54089600	-0.78595800	0.23458500	H	3.81077400	-3.01649200	2.18918500
H	3.26773100	-1.28497200	1.42281400	H	3.94490100	-2.92726600	0.42404100
C	2.88219000	-0.23510800	-2.26971800	H	2.33762000	-2.98532600	1.19144400
H	3.90780300	0.16708100	-2.28310300	H	4.82434600	0.58819800	1.64962900
H	2.87749100	-1.23123400	-2.73827900	H	5.40902900	-0.77514500	0.66243500
H	2.21827400	0.42112400	-2.85143100	H	5.27457100	-0.94587000	2.42160300
<b>C-1</b>				H	1.81261600	0.86234000	-2.67633100
				H	3.46173200	0.98600400	-3.34834500
				H	2.99371900	2.00065000	-1.96807900
				H	3.71234800	-2.29677300	-1.61331500
Ru	-0.00004400	-0.50975500	0.00000400	H	2.25765100	-1.73166100	-2.47107900
P	2.29775400	-0.18710100	0.08891800	H	3.88062700	-1.42016200	-3.15025000
P	-2.29777500	-0.18677800	-0.08876000	H	-3.81096700	-3.01560500	-2.18977100
N	0.00003900	1.68068700	0.00018900	H	-2.33736800	-2.98462600	-1.19268100
C	1.12722700	2.36965400	0.31889900	H	-3.94431500	-2.92714200	-0.42452600
C	1.15650000	3.76779100	0.31195600	H	-4.82486800	0.58863900	-1.64867900
C	0.00046700	4.47921000	-0.00038800	H	-5.40908900	-0.77519900	-0.66190000
C	-1.15577800	3.76801800	-0.31239700	H	-5.27495300	-0.94519800	-2.42115900
C	-1.12692300	2.36985300	-0.31872000	H	-3.71362400	-2.29634600	1.61279400
H	2.08233200	4.28558900	0.56702300	H	-3.88116200	-1.42019100	3.15006400
H	0.00064200	5.57125100	-0.00062000	H	-2.25847400	-1.73250200	2.47061600
H	-2.08147600	4.28596900	-0.56764100	H	-1.81209700	0.86158800	2.67676300
C	2.33888600	1.57725100	0.73714900	H	-3.46116100	0.98559600	3.34892200
C	-2.33891000	1.57771200	-0.73658800	H	-2.99283300	2.00055100	1.96901200
H	2.30560300	1.46536200	1.83543400	C	0.00006900	-2.34274500	-0.00033200
H	3.26325700	2.12172300	0.49025500	O	-0.00059100	-3.51202200	-0.00065700
H	-3.26308700	2.12220400	-0.48895300	H	-0.06620600	-0.44312400	-1.69282000
H	-2.30632900	1.46628600	-1.83492200	<b>C-2</b>			
H	0.06625500	-0.44383300	1.69282400				
C	3.35837700	-1.04726500	1.40051400				
C	3.35341700	-2.57816200	1.28570800				
C	4.78906400	-0.50657500	1.53338100	Ru	-0.05824300	-0.47484400	-0.36540100
C	3.34873800	-0.12415000	-1.48435000	P	2.24547500	-0.14645600	-0.39637000
C	3.29805900	-1.47436400	-2.21474400	P	-2.35929100	-0.13996900	-0.35810900
C	2.87401900	1.00104600	-2.41475200	N	-0.04368400	1.70409400	-0.15940700
C	-3.34869700	-0.12393700	1.48453600	C	1.09475200	2.35592800	0.19481700
C	-3.29873900	-1.47441200	2.21446800	C	1.12066500	3.74544200	0.35378500

C	-0.04629600	4.48221600	0.16641400	H	-4.83826600	0.81730200	-1.92575000
C	-1.21014300	3.80813200	-0.19672200	H	-5.48156700	-0.55300500	-0.98533300
C	-1.17918100	2.42083500	-0.36830500	H	-5.34265800	-0.67219000	-2.74806400
H	2.05394400	4.23435300	0.63697300	H	-3.62603000	-2.40990400	1.20428800
H	-0.04795500	5.56639000	0.29747100	H	-3.91630000	-1.64087800	2.78110500
H	-2.14266400	4.34878500	-0.36498600	H	-2.25067600	-1.81264800	2.16464900
C	2.32558300	1.52771000	0.45743700	H	-1.89607100	0.76199500	2.46971000
C	-2.39423300	1.67424900	-0.85265300	H	-3.53846400	0.76700200	3.15679300
H	2.35277900	1.28532900	1.53408800	H	-3.13189700	1.89010800	1.84200800
H	3.23530200	2.10341100	0.22508500	C	-0.07086700	-2.30128500	-0.52817700
H	-3.31747500	2.20029400	-0.56598900	O	-0.08099800	-3.46586500	-0.62993700
H	-2.35478800	1.64988500	-1.95629100	H	-0.20215500	-0.25982900	-2.03671000
H	0.07269000	-0.56260200	1.32526200	C	0.69064700	-0.52831200	3.96100400
C	3.41807900	-1.14575600	0.70271200	O	1.71014200	0.00992200	3.76040500
C	3.37177300	-2.65547600	0.42739400	O	-0.31353400	-1.06057700	4.22175500
C	4.86336800	-0.62997400	0.74100400				
C	3.16847600	0.13794500	-2.02406400	<b>C-3</b>			
C	3.13090100	-1.12334400	-2.89972200				
C	2.58256400	1.33357200	-2.78847800	Ru	-0.01852200	-0.48971100	-0.18158000
C	-3.39617900	-0.21390200	1.22372500	P	2.31249300	-0.16856800	-0.24468600
C	-3.29145400	-1.60298000	1.87258200	P	-2.34460400	-0.16231900	-0.32817200
C	-2.96346100	0.87005600	2.22100300	N	0.00041000	1.69474100	-0.20333000
C	-3.43839800	-0.88289000	-1.72385500	C	1.14346400	2.37116500	0.09033900
C	-3.49808500	-2.41672200	-1.68526600	C	1.16846800	3.76991000	0.12348100
C	-4.84580300	-0.28098600	-1.84380800	C	0.00242400	4.48605100	-0.12943800
H	2.95823200	-0.97774100	1.69117800	C	-1.16172000	3.78644200	-0.44085300
H	4.21508600	0.36746000	-1.75724000	C	-1.13208400	2.39049700	-0.49083100
H	-4.44317300	-0.02568400	0.92750700	H	2.10021200	4.28156600	0.36728600
H	-2.84949200	-0.59838500	-2.61362000	H	0.00099400	5.57739400	-0.09060900
H	3.91798000	-3.19212300	1.22203400	H	-2.09097400	4.31262400	-0.66284000
H	3.85464400	-2.91600500	-0.52805000	C	2.37141700	1.57439900	0.43765900
H	2.34338200	-3.04076500	0.40530100	C	-2.34096100	1.61310900	-0.94538600
H	4.92595500	0.44715500	0.96261600	H	2.34961300	1.40717700	1.53123000
H	5.38852800	-0.81178500	-0.21101300	H	3.28561700	2.12782200	0.17617500
H	5.42835000	-1.15902800	1.52739500	H	-3.26658300	2.15973500	-0.71252000
H	1.51495700	1.16795500	-3.00502600	H	-2.28505200	1.52551400	-2.04514400
H	3.11250700	1.45755700	-3.74824500	H	0.09088100	-0.41764200	1.67130500
H	2.68120200	2.28045200	-2.23469500	C	3.45588300	-1.06725200	0.95875800
H	3.62621700	-1.98325500	-2.42506200	C	3.44782900	-2.59368900	0.79634700
H	2.08897500	-1.40809400	-3.11813100	C	4.88867400	-0.51728900	0.99791900
H	3.64293900	-0.93258900	-3.85824400	C	3.19625500	-0.09249100	-1.90944700
H	-3.95222300	-2.79105800	-2.61860200	C	3.08817400	-1.43289900	-2.65199200
H	-2.50265000	-2.87149700	-1.58982300	C	2.66191800	1.05103600	-2.78367500
H	-4.12456500	-2.78011600	-0.85465600	C	-3.50972100	-0.17291000	1.15798400

C	-3.39561600	-1.50503300	1.91888500	P	2.36885100	-0.21018600	0.24568500
C	-3.25336200	1.00611200	2.10826900	N	0.03137100	1.66887700	0.22810000
C	-3.28924300	-1.00698600	-1.73635500	C	-1.11129200	2.37001200	-0.00149700
C	-3.37601600	-2.53261500	-1.58696100	C	-1.12011000	3.77051900	0.03952100
C	-4.67117100	-0.40563600	-2.02968600	C	0.05705100	4.46014400	0.30947200
H	2.95854200	-0.82300000	1.91293900	C	1.21724600	3.73299800	0.57209100
H	4.25682700	0.10820400	-1.67778300	C	1.17195600	2.33715100	0.54696500
H	-4.52524100	-0.07226400	0.73554000	H	-2.05098100	4.30368500	-0.15748500
H	-2.62026600	-0.79267400	-2.58864700	H	0.07017500	5.55209100	0.32707000
H	3.95400800	-3.05300700	1.66189500	H	2.15355000	4.23719100	0.81489700
H	3.99097900	-2.91960700	-0.10557100	C	-2.36177900	1.60892900	-0.34253400
H	2.43003100	-3.00558500	0.75168300	C	2.37210100	1.52468600	0.96562000
H	4.92295300	0.56996200	1.16842000	H	-2.39344400	1.49586300	-1.44379500
H	5.44392000	-0.73802700	0.07088000	H	-3.25535100	2.15422500	-0.00244000
H	5.44125100	-0.99166500	1.82631900	H	3.30408700	2.07788500	0.77780400
H	1.58712500	0.92021300	-2.98835200	H	2.30199000	1.37333400	2.05777700
H	3.19200700	1.05623200	-3.75102100	H	-0.05175800	-0.04208600	-4.12413000
H	2.80744000	2.04097400	-2.32422700	C	-3.55697500	-0.99017900	-0.90438700
H	3.52381600	-2.26737700	-2.08410900	C	-3.48703300	-2.52345000	-0.89543800
H	2.03437700	-1.67843800	-2.85922100	C	-4.99513600	-0.49173300	-0.70871700
H	3.62107700	-1.37205600	-3.61600600	C	-3.04812500	-0.15545700	1.95605600
H	-3.74657200	-2.97326100	-2.52795000	C	-2.95788200	-1.53718200	2.62075700
H	-2.40233200	-2.98992600	-1.36419200	C	-2.41637700	0.91586300	2.85592000
H	-4.08262600	-2.82408300	-0.79379100	C	3.52917700	-0.11757500	-1.24441500
H	-4.64247500	0.68436300	-2.18212500	C	3.39986700	-1.38974300	-2.09887700
H	-5.38824400	-0.61704000	-1.22019100	C	3.26270300	1.13205300	-2.09759600
H	-5.08356400	-0.85360700	-2.94967600	C	3.31423300	-1.14309800	1.59311100
H	-3.53888600	-2.38083100	1.26922300	C	3.40386700	-2.65359000	1.33274500
H	-4.16854000	-1.54437200	2.70516800	C	4.69352700	-0.56094600	1.93296700
H	-2.41359000	-1.57847500	2.41086900	H	-3.18522100	-0.64288100	-1.88207900
H	-2.25642400	0.93222400	2.56590000	H	-4.11167400	0.10060600	1.80817300
H	-3.98790600	0.97280800	2.93038900	H	4.55280300	-0.05367200	-0.83395400
H	-3.35843500	1.98603900	1.61672100	H	2.64188800	-0.99260300	2.45658000
C	-0.02618200	-2.33001300	-0.22162100	H	-4.11671700	-2.92074800	-1.70962400
O	-0.03168300	-3.49304500	-0.27085600	H	-3.86239200	-2.95839500	0.04516700
H	-0.07037900	-0.48538800	-1.79571800	H	-2.46455400	-2.89227000	-1.05677000
C	0.30548500	-0.23056700	2.92802500	H	-5.07216000	0.60697700	-0.72971300
O	1.37256900	0.35158600	3.11640500	H	-5.43450600	-0.84766000	0.23815900
O	-0.61754800	-0.68418600	3.58256200	H	-5.63135400	-0.87604200	-1.52405100
<b>C-4</b>				H	-1.33914600	0.73009300	2.99034800
				H	-2.89209200	0.89166700	3.85111400
				H	-2.54326100	1.93381600	2.45595300
Ru	0.03900900	-0.51433500	0.05582900	H	-3.47277700	-2.31837100	2.04270200
P	-2.28550000	-0.17293000	0.22692900	H	-1.90636900	-1.84260400	2.74168600

H	-3.42166000	-1.50437500	3.62141800	C	3.18577600	0.11599000	-1.91845900
H	3.77294500	-3.16285900	2.23908700	C	3.13808500	-1.15650700	-2.77738500
H	2.43073600	-3.09278800	1.07361600	C	2.60390200	1.30651400	-2.69379600
H	4.11319300	-2.88424500	0.52178800	C	-3.49537300	-0.17346300	1.14023600
H	4.65968700	0.51348800	2.17094800	C	-3.50991600	-1.57887000	1.76206300
H	5.41107100	-0.70396900	1.10873100	C	-3.11156500	0.87610700	2.19330000
H	5.10922000	-1.07825900	2.81433400	C	-3.31270000	-0.85589700	-1.79832000
H	3.59946600	-2.30747200	-1.52614800	C	-3.33917300	-2.39109200	-1.80109400
H	4.12421000	-1.35354100	-2.93049200	C	-4.72351700	-0.28078300	-1.98954400
H	2.38500100	-1.45497300	-2.51833400	H	3.00891600	-0.95895700	1.81420300
H	2.22862900	1.12780800	-2.47156000	H	4.23547800	0.34346000	-1.66243500
H	3.94217700	1.13313600	-2.96705000	H	-4.50228500	0.06896300	0.75635000
H	3.43925100	2.06946000	-1.54728900	H	-2.67976400	-0.53770200	-2.64551300
C	0.02691200	-2.34906600	0.01897900	H	3.96670300	-3.17453500	1.36174500
O	0.02294100	-3.51471200	0.02533200	H	3.90663700	-2.91601800	-0.39134100
H	0.05830000	-0.60733500	1.65778400	H	2.39471300	-3.03774800	0.54260700
C	-0.53363100	0.04228000	-3.11393500	H	4.96690200	0.46456900	1.06968800
O	0.25614800	-0.28863700	-2.16145900	H	5.43049200	-0.79902700	-0.10010900
O	-1.70921500	0.43277900	-3.05805500	H	5.47620200	-1.13615600	1.64033500
C-TS2/3				H	1.53730100	1.14349800	-2.91650000
				H	3.13872200	1.42146200	-3.65184600
				H	2.70185100	2.25740600	-2.14727700
Ru	-0.02849700	-0.46570500	-0.23662100	H	3.62616800	-2.01371800	-2.29114300
P	2.29015800	-0.14284600	-0.27458300	H	2.09483900	-1.43708200	-2.99428700
P	-2.33904900	-0.11401800	-0.35360400	H	3.65256700	-0.98176700	-3.73750100
N	-0.00130900	1.71743600	-0.08580200	H	-3.73172100	-2.74919500	-2.76800100
C	1.13683600	2.36524500	0.27777500	H	-2.34094400	-2.82739600	-1.66175100
C	1.16692300	3.75637000	0.42311700	H	-4.00109400	-2.79088100	-1.01666300
C	0.00771300	4.49668700	0.20766400	H	-4.73837800	0.81992000	-2.02681200
C	-1.15242800	3.82733900	-0.17575500	H	-5.40724000	-0.60255800	-1.18733600
C	-1.12626800	2.43857800	-0.33299000	H	-5.14865300	-0.64567200	-2.94003100
H	2.09725900	4.24298000	0.71890200	H	-3.82966000	-2.35320300	1.04948900
H	0.00946000	5.58182400	0.33028800	H	-4.21210700	-1.60109800	2.61278900
H	-2.07674600	4.37257900	-0.37142900	H	-2.51257000	-1.84476100	2.14321600
C	2.36142700	1.53632100	0.56304600	H	-2.09803700	0.69485300	2.57959400
C	-2.33167800	1.69919300	-0.85269300	H	-3.80635300	0.81044200	3.04742900
H	2.36267100	1.29491400	1.63981900	H	-3.16207100	1.90658400	1.80808600
H	3.27610200	2.10724300	0.33999700	C	-0.04479700	-2.29718600	-0.37739000
H	-3.25896900	2.23068600	-0.59108400	O	-0.05456500	-3.45958700	-0.47303800
H	-2.26399200	1.68193600	-1.95504200	H	-0.10443700	-0.31463700	-1.88351900
H	0.06305700	-0.51706100	1.51409800	C	0.36698900	-0.62343800	3.14559200
C	3.46420000	-1.13546600	0.82578400	O	1.36318300	0.02187000	3.30057700
C	3.42140700	-2.64729000	0.56070700	O	-0.52805100	-1.29618300	3.54733300
C	4.90762500	-0.61352100	0.85259900				

<b>C-TS3/4</b>				H	3.09314300	0.85558800	-3.78813500
				H	2.74560100	1.91493300	-2.40574900
Ru	-0.00852000	-0.56206800	-0.05732600	H	3.43077100	-2.38227700	-1.94776200
P	2.32723900	-0.17952200	-0.18688100	H	1.95177600	-1.81011400	-2.75128400
P	-2.35336400	-0.28045400	-0.24675300	H	3.54070900	-1.57020100	-3.52542800
N	-0.02143900	1.60424600	-0.34427700	H	-3.86173900	-3.43456900	-1.78356300
C	1.08917800	2.33812600	-0.07652000	H	-2.53245100	-3.25315700	-0.61707700
C	1.06864800	3.73514700	-0.15622400	H	-4.19959400	-2.82050300	-0.15403800
C	-0.11217500	4.38668500	-0.49621900	H	-4.44442800	0.20896500	-2.49554100
C	-1.24296700	3.62489000	-0.78601200	H	-5.33402500	-0.69681700	-1.24511200
C	-1.16522500	2.23260300	-0.72064300	H	-4.98615500	-1.45030200	-2.81133800
H	1.97466700	4.29691700	0.07358400	H	-3.10196000	-2.16969500	1.90211900
H	-0.15149000	5.47710000	-0.54116800	H	-4.01553500	-1.16476600	3.05229100
H	-2.18212200	4.09946900	-1.07244600	H	-2.27685000	-0.84808100	2.78384800
C	2.33534200	1.61402400	0.35738600	H	-2.66234300	1.59412800	2.18833900
C	-2.33125200	1.37251500	-1.13437100	H	-4.36203500	1.28793600	2.62969400
H	2.32551500	1.54690600	1.46407500	H	-3.99864300	2.03723100	1.06628300
H	3.23559900	2.16500900	0.04609400	C	0.01951400	-2.39893900	0.05131700
H	-3.27548300	1.92952200	-1.05961300	O	0.03677300	-3.56278800	0.06813100
H	-2.19190100	1.10606500	-2.19747100	H	-0.03404200	-0.74197300	-1.61797300
H	0.27441400	-0.95188000	2.24209300	C	0.43126200	0.12727400	2.64516900
C	3.53180100	-0.96652400	1.02679200	O	1.56701300	0.36206900	3.10468200
C	3.61934400	-2.49393400	0.90250900	O	-0.57127900	0.87220300	2.51497900
C	4.92624400	-0.32555200	1.03136900				
C	3.14266300	-0.19431700	-1.88933000	<b>D-1</b>			
C	3.00979200	-1.57120800	-2.55847600				
C	2.58800800	0.90310400	-2.80863400	Ru	-0.00000800	-0.46865000	-0.00005000
C	-3.56603000	-0.12398400	1.20093800	P	-2.31995200	-0.14801100	-0.08475800
C	-3.21465000	-1.14707200	2.29397500	P	2.31993900	-0.14803600	0.08472000
C	-3.64226300	1.29046800	1.79315900	N	-0.00002400	1.71515800	0.00012800
C	-3.25558200	-1.36872100	-1.50247300	C	-1.12602000	2.40297200	-0.32433500
C	-3.46552600	-2.79641000	-0.97594300	C	-1.15397900	3.80130800	-0.32084900
C	-4.57164200	-0.78337700	-2.03652200	C	0.00004600	4.51214700	0.00020600
H	3.02407300	-0.71947700	1.97796300	C	1.15403800	3.80123200	0.32123000
H	4.21160200	0.01261700	-1.70480400	C	1.12601500	2.40289900	0.32464400
H	-4.54808400	-0.38127900	0.76576400	H	-2.07758500	4.31974200	-0.58254900
H	-2.52695400	-1.41327500	-2.33086600	H	0.00007500	5.60421900	0.00023600
H	4.14568800	-2.89803800	1.78343800	H	2.07766200	4.31961600	0.58295900
H	4.18939800	-2.81044900	0.01334500	C	-2.34097900	1.61341100	-0.74388700
H	2.62958600	-2.97075000	0.86345300	C	2.34094300	1.61326600	0.74415200
H	4.89253900	0.76314500	1.18983000	H	-2.30085800	1.49718800	-1.84023500
H	5.48228200	-0.52249500	0.09885700	H	-3.26306600	2.16724800	-0.51066900
H	5.51995900	-0.75232300	1.85721100	H	3.26302900	2.16717800	0.51109400
H	1.50838900	0.76715100	-2.98193100	H	2.30077900	1.49687500	1.84047800



H	0.00022300	-0.37848000	-1.68181500	C	-2.99779400	-1.33204000	2.39924000
C	0.00001800	-2.30063200	-0.00012400	C	-2.60951800	1.13077100	2.40014600
O	0.00003600	-3.47114600	-0.00005700	C	-4.76734200	0.23336200	1.52148200
H	-0.00022000	-0.37891200	1.68162600	H	-3.44701000	-2.21269600	1.91860100
C	3.42365200	-1.07818900	1.38071200	H	-1.91871200	-1.51112600	2.51143700
C	4.68669000	-0.29711200	1.79689100	H	-3.44225500	-1.24155800	3.40606900
C	2.57782300	-1.31350100	2.64836700	H	-2.84909700	2.11526400	1.96774400
C	3.82044300	-2.45477500	0.81304000	H	-3.00472200	1.12467400	3.43085900
H	5.37713500	-0.10712400	0.96647600	H	-1.51679000	1.01449600	2.45211600
H	4.44088900	0.66773900	2.26746300	H	-5.16710400	0.38483500	2.53982500
H	5.23664900	-0.88750900	2.55084500	H	-5.00453200	1.14170900	0.94464900
H	1.68939500	-1.92259800	2.44307800	H	-5.31890800	-0.60975200	1.08216600
H	3.20547400	-1.83311400	3.39371500				
H	2.22697200	-0.37409300	3.10193600	<b>D-2</b>			
H	4.30607000	-3.04690900	1.60812600				
H	2.94266400	-3.02211500	0.46740800	Ru	-0.01645900	-0.49861200	0.33485000
H	4.53530200	-2.37825100	-0.01877100	P	-2.33347100	-0.44503800	-0.03004700
C	3.25504400	-0.02968000	-1.61459100	P	2.31206300	-0.32932300	0.07241000
C	2.60970600	1.13132000	-2.39980500	N	0.00864000	0.49811600	-1.60418600
C	4.76742500	0.23348700	-1.52137400	C	-1.10242700	0.50705000	-2.38632200
C	2.99769900	-1.33158000	-2.39944000	C	-1.11845900	1.16126500	-3.62195400
H	1.51697200	1.01518600	-2.45185700	C	0.03339600	1.79970100	-4.07690800
H	2.84938100	2.11565700	-1.96708800	C	1.17469100	1.76901000	-3.27914600
H	3.00499600	1.12545500	-3.43047700	C	1.13592400	1.11657800	-2.04253700
H	5.31901900	-0.60982000	-1.08246400	H	-2.02989000	1.15370500	-4.22154500
H	5.16707900	0.38537300	-2.53968900	H	0.04188200	2.31173700	-5.04148800
H	5.00469300	1.14159300	-0.94419200	H	2.09657200	2.25635400	-3.59960400
H	3.44229500	-1.24099900	-3.40620500	C	-2.30698000	-0.26051000	-1.90307400
H	3.44668400	-2.21240200	-1.91890400	C	2.33831300	1.11651000	-1.13277000
H	1.91859500	-1.51041700	-2.51186100	H	-2.21588600	-1.29504900	-2.27596400
C	-3.42373200	-1.07792400	-1.38091400	H	-3.23203700	0.15871900	-2.32703100
C	-4.68679300	-0.29680700	-1.79691000	H	3.26542600	1.20189000	-1.71989800
C	-2.57787500	-1.31290800	-2.64860000	H	2.26996900	2.01197600	-0.49205400
C	-3.82044200	-2.45462100	-0.81348800	H	-0.02720800	-1.94985500	-0.51096200
H	-5.37735400	-0.10720200	-0.96649000	C	-0.03692700	-1.33488500	1.96709100
H	-4.44105000	0.66820700	-2.26717300	O	-0.05064400	-1.86931100	3.00799900
H	-5.23666000	-0.88699200	-2.55111700	H	0.00407500	1.04157500	1.03435800
H	-1.68942900	-1.92201800	-2.44347000	C	3.45812800	0.29045000	1.50669600
H	-3.20551500	-1.83229400	-3.39412500	C	4.74429300	0.99059000	1.02353800
H	-2.22708000	-0.37334600	-3.10192100	C	2.66392700	1.30983700	2.34800000
H	-4.30608500	-3.04664300	-1.60865100	C	3.81427800	-0.90115800	2.41666100
H	-2.94263700	-3.02200600	-0.46799500	H	5.41230800	0.33494000	0.45292900
H	-4.53527300	-2.37828800	0.01836500	H	4.52606800	1.87834300	0.40970600
C	-3.25501500	-0.02993800	1.61466800	H	5.30781000	1.34405600	1.90507400

H	1.73671600	0.88531600	2.75171900	H	-5.37144600	0.36684700	0.84914600
H	3.30216400	1.64011200	3.18634800	C	0.15750800	4.02927800	1.44265700
H	2.39482400	2.20165500	1.76384100	O	0.93084500	4.08714900	0.56730500
H	4.32507400	-0.52536200	3.32012700	O	-0.61148700	4.00766000	2.31894200
H	2.91601000	-1.44531600	2.74660900				
H	4.49475400	-1.61539300	1.93158800	<b>D-3</b>			
C	3.19170100	-1.77194200	-0.88909200				
C	2.53444400	-1.85530700	-2.28281700	Ru	-0.00757100	-0.49364900	-0.00059100
C	4.70784900	-1.60474500	-1.08678000	P	-2.34800300	-0.20147300	-0.29529500
C	2.90518000	-3.09465000	-0.15043600	P	2.34504400	-0.17746200	-0.14294800
H	1.44019300	-1.92990900	-2.20496500	N	0.01869100	1.63852700	-0.42418600
H	2.79349000	-0.99515000	-2.92003400	C	-1.09514800	2.26160800	-0.89248800
H	2.90337900	-2.76152400	-2.79376500	C	-1.12852600	3.64509500	-1.07934800
H	5.26897000	-1.67578700	-0.14450300	C	0.01229000	4.39981700	-0.81019500
H	5.07353900	-2.41616100	-1.74067100	C	1.16193800	3.74930200	-0.37359000
H	4.96995800	-0.65347600	-1.57674800	C	1.14211200	2.36321100	-0.18506300
H	3.31355100	-3.93393400	-0.74067100	H	-2.04140000	4.11741300	-1.44429800
H	3.37093100	-3.13373800	0.84451400	H	0.00578700	5.48311100	-0.94811000
H	1.82258200	-3.24602500	-0.03327300	H	2.07563600	4.30521200	-0.16081900
C	-3.42119500	-2.03040600	0.21316400	C	-2.27404600	1.40080400	-1.27324600
C	-4.66036400	-2.08245700	-0.70425400	C	2.36263600	1.64017000	0.32186200
C	-2.55489200	-3.26653000	-0.10275300	H	-2.13191900	1.08529400	-2.32090700
C	-3.85683100	-2.12479500	1.68886200	H	-3.20895800	1.97855600	-1.23480300
H	-5.36205600	-1.25658900	-0.53866800	H	3.28089400	2.17221200	0.03110700
H	-4.38600100	-2.09276200	-1.77074900	H	2.28164900	1.64574600	1.42383700
H	-5.20751900	-3.02109300	-0.50743500	H	0.00174200	-0.78763300	-1.57321400
H	-1.68947500	-3.34476300	0.56598200	C	-0.01892400	-2.30745700	0.31969800
H	-3.18114300	-4.16829700	0.01587400	O	-0.02399900	-3.45854000	0.49652300
H	-2.16854600	-3.25906300	-1.13314100	H	-0.00904600	-0.03955600	1.79122400
H	-4.33776600	-3.10347300	1.86069000	C	3.58141900	-0.97632600	1.11467900
H	-2.99755700	-2.05441300	2.37316900	C	4.84699700	-0.12596200	1.34604800
H	-4.58667900	-1.35068500	1.96622600	C	2.85701000	-1.11304900	2.46780800
C	-3.31027100	1.11900600	0.58061800	C	3.96996300	-2.38812000	0.63547000
C	-3.07889200	1.26841400	2.09748800	H	5.46038100	0.00361800	0.44604500
C	-2.67713600	2.33554600	-0.12609800	H	4.60452200	0.86908400	1.74910300
C	-4.81877000	1.12724000	0.27970600	H	5.47479100	-0.63106700	2.10051900
H	-3.51873300	0.44172400	2.67348100	H	1.95054400	-1.72832100	2.40098500
H	-2.00521300	1.31814700	2.32673400	H	3.54455700	-1.59878100	3.18130900
H	-3.54948000	2.20430800	2.44588900	H	2.57694700	-0.13918800	2.89067100
H	-2.93900700	2.38006100	-1.19494500	H	4.53855500	-2.89019300	1.43676600
H	-3.05512500	3.25967600	0.34381300	H	3.08459600	-3.00767900	0.42435600
H	-1.58218600	2.32381100	-0.02874300	H	4.60975900	-2.37643900	-0.25841200
H	-5.23282800	2.10935600	0.56936600	C	3.07971400	-0.25255400	-1.93621000
H	-5.03828300	0.98850300	-0.79108300	C	2.33506800	0.78845400	-2.79800300

C	4.58409800	0.06243900	-2.01257000	P	-2.37071700	-0.22675900	-0.19679800
C	2.80575400	-1.64688200	-2.53485500	P	2.32225900	-0.20588900	-0.10489300
H	1.24724400	0.63542200	-2.77224900	N	0.01037300	1.59281200	-0.54272000
H	2.55436600	1.82199300	-2.48934800	C	-1.10405700	2.15510100	-1.08010800
H	2.66948300	0.68184300	-3.84432800	C	-1.12614900	3.49710600	-1.46711000
H	5.20530300	-0.70986400	-1.53898900	C	0.03198400	4.26354700	-1.34299600
H	4.88404700	0.11329500	-3.07381900	C	1.18785300	3.66209000	-0.85635900
H	4.83270100	1.03502600	-1.55918400	C	1.15584100	2.31897200	-0.46206600
H	3.15849700	-1.66485000	-3.58081700	H	-2.04126500	3.92441800	-1.87919400
H	3.32679500	-2.45045400	-1.99729500	H	0.03528600	5.31489800	-1.63886300
H	1.72989600	-1.87300200	-2.53191300	H	2.11779900	4.22409100	-0.76366300
C	-3.29221700	-1.38626600	-1.50716200	C	-2.29271100	1.26213900	-1.34430400
C	-4.50436800	-0.72015800	-2.19178100	C	2.38158100	1.65431900	0.09976500
C	-2.32496100	-1.83765100	-2.62077800	H	-2.16146100	0.83868000	-2.35492400
C	-3.74613300	-2.64147400	-0.73670900	H	-3.22476400	1.84621800	-1.36302200
H	-5.28114000	-0.40113600	-1.48805300	H	3.29687100	2.12751400	-0.28548000
H	-4.21125500	0.14962400	-2.80035700	H	2.31156100	1.80250100	1.19675300
H	-4.96540300	-1.44971200	-2.87999900	H	-0.01130900	-0.91413200	-1.36595600
H	-1.48294400	-2.42062900	-2.22869000	C	-0.02838000	-2.25829600	0.60391300
H	-2.88610100	-2.46976900	-3.33045500	O	-0.03034900	-3.39937200	0.84513100
H	-1.90855700	-0.99173900	-3.18943400	H	-0.19278000	1.10207700	4.08467200
H	-4.15725000	-3.37434400	-1.45226300	C	3.60698200	-0.86291900	1.18488800
H	-2.90780500	-3.12592600	-0.21335600	C	4.87282300	0.01139400	1.27496400
H	-4.53379600	-2.42469500	-0.00186400	C	2.92307600	-0.85268500	2.56604500
C	-3.45924800	0.22241300	1.23119300	C	3.98564600	-2.31932000	0.85407600
C	-3.26574400	-0.88192500	2.29109600	H	5.44992900	0.04482900	0.34207100
C	-2.95427000	1.56538400	1.80128600	H	4.63419600	1.04282100	1.57444700
C	-4.95756000	0.38637000	0.91992400	H	5.53410400	-0.40438800	2.05532600
H	-3.55683900	-1.87522900	1.92008000	H	2.00727100	-1.45894400	2.57842000
H	-2.23115900	-0.92679300	2.65845100	H	3.62815500	-1.27474700	3.30338700
H	-3.90960300	-0.65400600	3.15855000	H	2.66086200	0.16315400	2.88826400
H	-3.24955700	2.41712200	1.16803400	H	4.58773000	-2.72461400	1.68540900
H	-3.41267700	1.72176900	2.79216900	H	3.09619700	-2.96043000	0.75170800
H	-1.86680900	1.59925000	1.94174900	H	4.59000200	-2.41259600	-0.05940200
H	-5.46548700	0.73931200	1.83414600	C	2.97790000	-0.53321800	-1.90247600
H	-5.15014800	1.13610700	0.13577000	C	2.22261500	0.40291900	-2.86913900
H	-5.44005800	-0.55705100	0.62847600	C	4.48428500	-0.26395000	-2.07742800
C	0.10965700	0.47618400	2.96269900	C	2.66060500	-1.98694400	-2.30913800
O	0.65090500	1.57974900	2.91004700	H	1.13401000	0.28165000	-2.78512400
O	-0.35305400	-0.28478800	3.79468000	H	2.47410500	1.46259200	-2.71012600
				H	2.51492300	0.14983300	-3.90299300
<b>D-4</b>				H	5.11236000	-0.97296300	-1.52129100
				H	4.74311900	-0.37127900	-3.14547500
Ru	-0.02415500	-0.47746800	0.15760400	H	4.76613200	0.75766000	-1.77746300

H	2.99416500	-2.15069200	-3.34887500	H	-2.03877000	4.01932800	-1.72096300
H	3.17149000	-2.72668200	-1.67873100	H	0.01984300	5.40787500	-1.34979300
H	1.58039800	-2.18467800	-2.26171700	H	2.09303700	4.27777200	-0.50052800
C	-3.29027300	-1.54612400	-1.27703400	C	-2.28035700	1.32459600	-1.35598600
C	-4.49576200	-0.97555100	-2.05244000	C	2.37214600	1.65192800	0.17212400
C	-2.30357800	-2.12107500	-2.31417200	H	-2.14982900	0.95078800	-2.38591300
C	-3.75141600	-2.70676800	-0.37264600	H	-3.21468300	1.90492700	-1.33846400
H	-5.28104500	-0.57084700	-1.40426700	H	3.28676900	2.14977100	-0.18448300
H	-4.19810700	-0.18986400	-2.76425100	H	2.34015500	1.74778600	1.27014600
H	-4.94919500	-1.78735000	-2.64762200	H	-0.01483700	-0.85602300	-1.58933000
H	-1.46306900	-2.64280300	-1.84092200	C	-0.02784900	-2.27853700	0.45858700
H	-2.84867600	-2.84153400	-2.94825100	O	-0.03844200	-3.41357100	0.73118100
H	-1.88583100	-1.34739600	-2.97683800	H	0.00553500	0.03009200	1.68407300
H	-4.14352600	-3.52169200	-1.00545800	C	3.57022600	-0.89997200	1.16763100
H	-2.92160000	-3.12024600	0.22047400	C	4.85903200	-0.06607000	1.31234900
H	-4.55655700	-2.41360100	0.31565900	C	2.86034500	-0.89788700	2.53499000
C	-3.51724200	0.35846900	1.24954400	C	3.91748600	-2.35907600	0.81470100
C	-3.31566800	-0.61229700	2.43214500	H	5.47793000	-0.05178700	0.40743700
C	-3.02436200	1.76023900	1.66767800	H	4.64546400	0.97428000	1.60205200
C	-5.01367100	0.46999100	0.91240700	H	5.47164200	-0.50261300	2.12049300
H	-3.63937800	-1.63593300	2.19327200	H	1.92530100	-1.47140100	2.52511900
H	-2.26059300	-0.63200800	2.73976100	H	3.53734500	-1.34909200	3.28065100
H	-3.92486800	-0.26624600	3.28606400	H	2.63189700	0.12115500	2.87681800
H	-3.27907800	2.52982100	0.92212800	H	4.48839300	-2.80228500	1.64871800
H	-3.52592400	2.04313800	2.60916400	H	3.01374000	-2.97155400	0.67170200
H	-1.94336700	1.77843600	1.84767200	H	4.54095800	-2.44290000	-0.08677400
H	-5.53404800	0.90983100	1.78145600	C	3.08328300	-0.40999600	-1.92656000
H	-5.20777400	1.13192800	0.05337800	C	2.35572500	0.57598900	-2.86442800
H	-5.48315300	-0.50417500	0.71693200	C	4.59259600	-0.12661400	-2.02397200
C	0.25960500	1.09313200	3.05707400	C	2.78874000	-1.84026000	-2.42238400
O	-0.21237100	0.16314700	2.31540400	H	1.26507300	0.45120100	-2.81309300
O	1.12129500	1.94631900	2.79231900	H	2.60738800	1.62590100	-2.64788800
<b>D-TS2/3</b>				H	2.67384500	0.37336600	-3.90175600
				H	5.20066900	-0.87487000	-1.49725400
				H	4.89225200	-0.15729100	-3.08621500
				H	4.85980800	0.87138000	-1.64146800
Ru	-0.01017600	-0.49687800	0.01089800	H	3.13576800	-1.93863700	-3.46605800
P	-2.33816300	-0.22499900	-0.29222200	H	3.30383200	-2.60920100	-1.83033800
P	2.33083100	-0.19832400	-0.14732400	H	1.70986000	-2.04989400	-2.39597500
N	0.01896400	1.60994600	-0.54110400	C	-3.31120200	-1.46817900	-1.42163700
C	-1.09546100	2.20378700	-1.04309100	C	-4.52536500	-0.83271500	-2.13084000
C	-1.12436200	3.57110700	-1.32996500	C	-2.36483600	-1.99970900	-2.51725300
C	0.02192800	4.33811700	-1.13019000	C	-3.76746900	-2.67105900	-0.57217400
C	1.17296900	3.71368100	-0.65845500	H	-5.28841400	-0.45564900	-1.44079300
C	1.14707000	2.34555600	-0.36799100				

H	-4.22981300	-0.01008700	-2.80066000	H	2.24996200	1.38826200	1.68493100
H	-5.00617200	-1.59956300	-2.76297300	H	-0.01251100	-0.60888300	-1.52737500
H	-1.51739500	-2.55531600	-2.09838800	C	-0.04743700	-2.31822700	0.12881800
H	-2.94138000	-2.67649300	-3.17183800	O	-0.05531400	-3.47951000	0.14586700
H	-1.95296800	-1.19731000	-3.14809600	H	-0.31382000	0.70358400	2.06237400
H	-4.18876200	-3.44358900	-1.23853500	C	3.65712400	-1.13399700	0.84342500
H	-2.92773100	-3.12851100	-0.02706400	C	4.87154100	-0.26133800	1.21820000
H	-4.54938100	-2.40683400	0.15360800	C	3.00622600	-1.63806800	2.14545500
C	-3.44441300	0.28294900	1.21646700	C	4.11152900	-2.36745500	0.03998600
C	-3.24014900	-0.76299300	2.33095900	H	5.40141300	0.15352900	0.35039800
C	-2.92618500	1.64996200	1.71137500	H	4.58516900	0.56579300	1.88431300
C	-4.94661200	0.43787800	0.92164500	H	5.59104300	-0.88595500	1.77528200
H	-3.58292400	-1.76409000	2.03254800	H	2.15021300	-2.29809600	1.95427000
H	-2.18794200	-0.83204500	2.63580400	H	3.76488700	-2.22017300	2.69750100
H	-3.82714000	-0.46307200	3.21662400	H	2.65779100	-0.82382000	2.79469400
H	-3.21951800	2.47061800	1.03732100	H	4.74784700	-2.98907200	0.69232600
H	-3.37123100	1.86428400	2.69784600	H	3.25827000	-2.99104600	-0.26940300
H	-1.83543800	1.67292900	1.82755700	H	4.70531100	-2.11787200	-0.84995200
H	-5.44207700	0.83438200	1.82525900	C	2.94456100	0.10165500	-1.99322700
H	-5.14726200	1.15129000	0.10645400	C	2.12043200	1.22823400	-2.65078300
H	-5.43649400	-0.51550900	0.67968100	C	4.42979500	0.49687400	-2.09467900
C	0.14442000	0.79753900	3.16774400	C	2.68690100	-1.18995300	-2.79651300
O	0.60378200	1.86937200	2.89986000	H	1.04205300	1.02303800	-2.61329500
O	-0.26804000	-0.01964600	3.92699200	H	2.30807400	2.21060900	-2.19252900
<b>D-TS3/4</b>				H	2.41577300	1.30208000	-3.71153100
				H	5.10957100	-0.29686400	-1.75821500
				H	4.67140000	0.70592400	-3.15150000
Ru	-0.03570500	-0.47381400	0.02288300	H	4.65673800	1.41141400	-1.52436800
P	-2.38583400	-0.13907100	-0.25498500	H	2.95908100	-1.01600900	-3.85223700
P	2.32941400	-0.13954300	-0.16355600	H	3.27867200	-2.04269900	-2.44088500
N	0.00026200	1.69482500	-0.15358800	H	1.62461700	-1.47305800	-2.76376400
C	-1.11053200	2.37555300	-0.53984400	C	-3.27690300	-1.17850300	-1.62797000
C	-1.14004400	3.77222300	-0.53606600	C	-4.48484700	-0.45453500	-2.25805600
C	0.00033000	4.47823600	-0.15443700	C	-2.27065900	-1.46801800	-2.76046800
C	1.14770500	3.77288200	0.19730900	C	-3.71774100	-2.53002600	-1.03178300
C	1.12853900	2.37349900	0.18871100	H	-5.28521300	-0.23837400	-1.54223500
H	-2.04875400	4.29408000	-0.83851100	H	-4.19475900	0.48923000	-2.74616500
H	-0.00441600	5.57023100	-0.13950700	H	-4.91257900	-1.10124500	-3.04354200
H	2.05920500	4.29368800	0.49239000	H	-1.42746000	-2.07883500	-2.41645500
C	-2.28821800	1.57242100	-1.03721600	H	-2.79522300	-2.01946300	-3.55955000
C	2.34273100	1.57696200	0.59241200	H	-1.86181500	-0.54959600	-3.21046900
H	-2.13168500	1.38425900	-2.11315400	H	-4.09439600	-3.17533800	-1.84406200
H	-3.22003600	2.14945300	-0.94664800	H	-2.88000700	-3.05755200	-0.55149500
H	3.26237900	2.15060000	0.40623500	H	-4.52666400	-2.42731700	-0.29536000

C	-3.54915900	0.07923800	1.28052900	H	4.37463600	0.57089600	-1.03713200
C	-3.30452700	-1.12273600	2.21662600	C	4.01722900	-0.88139800	-3.44310000
C	-3.13440500	1.37420500	2.00897700	H	2.67137800	-1.78598900	-1.99764200
C	-5.04820000	0.19998200	0.95336800	H	4.37486400	-1.82127400	-1.47224900
H	-3.58293500	-2.07771400	1.74617700	C	3.05184500	0.25543400	-3.81655600
H	-2.25162500	-1.18414300	2.53712500	H	3.34784600	2.03020200	-2.52833300
H	-3.93480100	-1.00494100	3.11560700	H	1.75596400	1.24844600	-2.36346700
H	-3.38724500	2.27867600	1.43308600	H	5.06284600	-0.52469700	-3.46808600
H	-3.68794500	1.42924200	2.96157000	H	3.94911500	-1.74688400	-4.12117200
H	-2.06514700	1.39672500	2.25602100	H	3.43000900	0.88437200	-4.63756800
H	-5.59035200	0.40058400	1.89366700	H	2.09217500	-0.17397100	-4.14789700
H	-5.27073200	1.03544400	0.27041700	C	3.28673400	-0.63517200	1.52641200
H	-5.47231100	-0.72081400	0.53067000	C	3.33626600	-2.19337800	1.48954100
C	0.29361000	0.09404200	2.83004700	C	4.75266000	-0.19634000	1.72630200
O	-0.10887700	-1.08341400	2.97433500	H	2.71423900	-0.34112300	2.42258100
O	1.24648000	0.71627400	3.34637400	C	4.71618500	-2.58305200	2.09251100
<b>E-1</b>				H	3.23306400	-2.58710900	0.46854500
				H	2.49591000	-2.61013800	2.06187700
				C	5.30123200	-1.27879500	2.66869800
				H	4.84664900	0.82399500	2.13110400
Ru	0.00120700	-0.24034200	0.00452400	H	5.30834100	-0.22761400	0.77283400
P	2.28141100	0.14810800	0.15560900	H	4.63479600	-3.37800000	2.84941000
P	-2.29265400	0.02078800	-0.16858600	H	5.38111000	-2.96635600	1.30016400
N	-0.05088400	1.94184900	-0.14434700	H	4.91838000	-1.10517100	3.68983000
C	1.04511900	2.68085100	0.17295400	H	6.40120000	-1.28663500	2.72758000
C	1.04030800	4.07537000	0.06938800	C	-3.38042100	0.19019700	1.35288700
C	-0.11893100	4.73147300	-0.33843700	C	-3.30038100	-1.04653700	2.30600200
C	-1.24343200	3.96985100	-0.64881200	C	-2.99866400	1.40276400	2.23621800
C	-1.18054000	2.57595900	-0.55820800	H	-4.42074500	0.32179300	1.01026900
H	1.94095600	4.63478700	0.32664200	C	-3.07922100	-0.47518600	3.73004200
H	-0.14557700	5.82065300	-0.41345500	H	-2.47520100	-1.72040500	2.03107700
H	-2.16934000	4.44411800	-0.97749500	H	-4.23408900	-1.62787700	2.24872700
C	2.25314800	1.94861300	0.69836100	C	-3.49019000	1.00236500	3.63485800
C	-2.34928000	1.71921000	-0.97232000	H	-3.43543200	2.34718000	1.87460600
H	2.16789100	1.90194200	1.79872600	H	-1.90122900	1.51472600	2.25863400
H	3.17838000	2.49676100	0.46122100	H	-3.63741400	-1.03043400	4.49988600
H	-3.30162600	2.25176700	-0.82507400	H	-2.00911700	-0.53858700	3.98620200
H	-2.24860700	1.51108500	-2.05264600	H	-4.58918700	1.10354100	3.69435300
H	0.01596400	-0.06832700	1.69114500	H	-3.05775900	1.62435200	4.43493700
C	0.03257300	-2.07288700	0.10475000	C	-3.28685900	-0.98907800	-1.39078900
O	0.04245100	-3.24019300	0.15989200	C	-3.49960200	-2.47079800	-1.01348600
H	-0.02023900	-0.28229800	-1.69065600	C	-4.70030900	-0.47710800	-1.79250600
C	3.39757400	0.16857100	-1.35473800	H	-2.63270600	-0.97166600	-2.27923500
C	3.61836100	-1.21903700	-1.99886800	C	-4.53985200	-2.92833900	-2.04646200
C	2.83053400	1.05800600	-2.50524200				

H	-3.92454200	-2.56043800	0.00122800	H	5.37272300	2.99973400	-0.45019000
H	-2.56656000	-3.05173300	-1.03436400	H	4.16207400	3.97058200	-1.30677800
C	-5.53613400	-1.75270400	-2.11071600	H	4.35510100	3.82045500	1.51510900
H	-4.63736700	0.20041800	-2.65804300	H	2.85133500	4.23301200	0.67773500
H	-5.17597100	0.09682700	-0.98144300	C	3.27112600	-1.76540900	-0.76821900
H	-4.04747600	-3.06695700	-3.02496300	C	3.31007000	-1.61420100	-2.31907400
H	-5.02062600	-3.88350900	-1.78383300	C	4.73466800	-2.03453400	-0.36040600
H	-6.04701700	-1.68672900	-3.08366700	H	2.67833300	-2.66631700	-0.53482200
H	-6.32148800	-1.88690700	-1.34839300	C	4.66103800	-2.24205000	-2.76739700
E-2				H	3.24888300	-0.56159700	-2.63139000
				H	2.44271100	-2.11585000	-2.77015300
				C	5.24389700	-2.91774100	-1.51022400
Ru	0.01626300	-0.24008200	-0.25183400	H	4.82674800	-2.50995500	0.62919900
P	2.30113000	-0.43148400	0.11578200	H	5.31799200	-1.09761700	-0.33390200
P	-2.28098300	-0.14047800	0.04389200	H	4.53918200	-2.94678800	-3.60398400
N	-0.02380800	-0.21490600	1.93360000	H	5.34859800	-1.45282300	-3.11530300
C	1.07545400	-0.57757800	2.64648100	H	4.83441200	-3.93713000	-1.39838400
C	1.08559900	-0.53257000	4.04399000	H	6.34155500	-3.00641400	-1.53614100
C	-0.06313200	-0.14000200	4.72778500	C	-3.30603500	-1.70770200	0.18786700
C	-1.19432000	0.20604700	3.99203200	C	-3.23571600	-2.61652600	-1.08187500
C	-1.14747600	0.17156600	2.59468800	C	-2.86562700	-2.62203700	1.35615500
H	1.98868900	-0.82211900	4.58327900	H	-4.35266000	-1.40462900	0.36177400
H	-0.07746500	-0.10759900	5.81932100	C	-2.99974600	-4.05941100	-0.56276700
H	-2.11382100	0.51783800	4.48950300	H	-2.41950100	-2.31324200	-1.75445700
C	2.26635500	-1.08987600	1.87734900	H	-4.17555100	-2.54423800	-1.65127600
C	-2.33035600	0.60638400	1.76742200	C	-3.36083100	-4.01165900	0.93007200
H	2.14819000	-2.18221600	1.76234400	H	-3.26703000	-2.29537100	2.32850500
H	3.19992500	-0.91378100	2.43429500	H	-1.76423800	-2.63657800	1.42206800
H	-3.27388600	0.42572700	2.30560200	H	-3.57867500	-4.81014300	-1.12284500
H	-2.24681800	1.69373200	1.59450200	H	-1.93350900	-4.31698200	-0.67062900
H	0.04234400	-1.92998100	-0.16839400	H	-4.45528200	-4.08221200	1.06633600
C	0.02975700	-0.23460000	-2.08751300	H	-2.90262400	-4.82710000	1.51240900
O	0.02572700	-0.21989100	-3.25588600	C	-3.34061700	1.06604600	-0.91548400
H	-0.00384800	1.45493500	-0.19497500	C	-3.56381500	0.71908900	-2.40264400
C	3.45822800	1.04158400	0.24571200	C	-4.75969900	1.39724600	-0.37254900
C	3.64174300	1.83974100	-1.06009600	H	-2.72940300	1.98234400	-0.88119100
C	2.96534700	2.11672100	1.24478100	C	-4.63738500	1.73492300	-2.81877300
H	4.44159000	0.66218600	0.57666400	H	-3.96320100	-0.30393100	-2.51118800
C	4.28738800	3.15145600	-0.58203700	H	-2.64089800	0.77907000	-2.99716200
H	2.65143100	2.03705500	-1.50515900	C	-5.61676700	1.74919800	-1.62589100
H	4.25297400	1.31540000	-1.81072100	H	-4.71640500	2.23006100	0.34582400
C	3.61903800	3.45211700	0.78338400	H	-5.20376800	0.54301600	0.16278600
H	3.21759200	1.86198600	2.28583800	H	-4.17201900	2.72837800	-2.94326800
H	1.86818900	2.19165200	1.17455300	H	-5.12722500	1.48192800	-3.77192800

H	-6.13375100	2.71538700	-1.52055000	C	-3.16392800	1.84662400	-0.63178700
H	-6.39854800	0.98579700	-1.77360000	C	-3.26094900	1.79544500	-2.19024000
C	-0.49104200	4.11599500	-0.17753300	C	-4.58850700	2.19753300	-0.14869600
O	0.50984400	4.33864900	-0.73379000	H	-2.49582300	2.68188300	-0.36224200
O	-1.50487500	3.95479600	0.38339300	C	-4.62701900	2.44408800	-2.54562700
<b>E-3</b>				H	-3.19965100	0.76926000	-2.57906100
				H	-2.41752300	2.34139100	-2.63619100
				C	-5.10150800	3.13336000	-1.25381500
Ru	0.01502600	0.15219700	-0.24255000	H	-4.60065200	2.65571400	0.85298600
P	-2.29073100	0.38301800	0.13973000	H	-5.22785800	1.29901200	-0.10921200
P	2.34159700	0.01988500	0.06489900	H	-4.55342200	3.13866400	-3.39602100
N	0.04583100	-0.06360400	1.92885700	H	-5.35233000	1.66397000	-2.83254000
C	-1.04671600	0.26381100	2.66908100	H	-4.62555000	4.12460700	-1.14989000
C	-1.06355400	0.08718400	4.05514700	H	-6.19152500	3.28676700	-1.21894000
C	0.07313200	-0.40040300	4.69740300	C	3.33009500	1.57890900	0.36849000
C	1.19983100	-0.70184600	3.93701600	C	3.28494800	2.59015000	-0.82334900
C	1.16186800	-0.53460000	2.54870900	C	2.85288700	2.38695600	1.59936700
H	-1.96001400	0.34707200	4.61944500	H	4.37418500	1.26850000	0.54155300
H	0.08106000	-0.54029200	5.78047300	C	3.00802000	3.97973400	-0.19230600
H	2.10734700	-1.08536200	4.40462100	H	2.50244900	2.33015800	-1.55164100
C	-2.21763000	0.88581300	1.95104300	H	4.24478500	2.57978900	-1.36227800
C	2.33012900	-0.91960100	1.68422000	C	3.33637800	3.81315200	1.29984900
H	-2.06387000	1.97952800	1.93490300	H	3.23856700	1.98333400	2.54857900
H	-3.15694600	0.69556800	2.49191400	H	1.75079200	2.38083500	1.64802600
H	3.27669600	-0.86741900	2.24261200	H	3.58494600	4.78399200	-0.67404000
H	2.16589800	-1.96267700	1.34777600	H	1.94027600	4.23053600	-0.30461600
H	0.04947100	1.75839700	-0.05853600	H	4.42629400	3.88517700	1.46582200
C	0.00702400	0.40160300	-2.06954800	H	2.85497800	4.57197900	1.93690000
O	0.01074100	0.58351600	-3.21838200	C	3.39298000	-1.08731000	-1.00622700
H	-0.00803900	-1.69341300	-0.37180200	C	3.62035200	-0.60985400	-2.45619900
C	-3.51243000	-1.03433700	0.12880200	C	4.80972500	-1.45794500	-0.47861800
C	-3.69476500	-1.74300700	-1.23029800	H	2.78580300	-2.00645000	-1.04073900
C	-3.13700100	-2.18238700	1.11009100	C	4.71652400	-1.56877800	-2.94432300
H	-4.48381500	-0.61153300	0.44008300	H	4.00028900	0.42624700	-2.48025000
C	-4.39842600	-3.04974300	-0.83137300	H	2.70447300	-0.64252300	-3.06409000
H	-2.70900700	-1.97762700	-1.66266200	C	5.68797600	-1.65537800	-1.74975300
H	-4.27396600	-1.14886900	-1.95404700	H	4.76071600	-2.36924900	0.13599300
C	-3.66304200	-3.49101400	0.45052000	H	5.23782600	-0.66876100	0.16045900
H	-3.57423800	-2.00637800	2.10561000	H	4.27130800	-2.55770000	-3.14786900
H	-2.04636000	-2.24612400	1.23899900	H	5.20534800	-1.23011000	-3.87097200
H	-5.46489300	-2.84973400	-0.62157600	H	6.24397200	-2.60493900	-1.72898200
H	-4.35529400	-3.80953700	-1.62635000	H	6.43698400	-0.84883700	-1.81839800
H	-4.31525800	-4.06279800	1.12860900	C	0.13700400	-2.96459300	-0.49207000
H	-2.80818900	-4.12580300	0.17969200	O	-0.79007300	-3.43462700	-1.13026300



O	1.16113300	-3.34671700	0.07184600	C	-4.59232600	2.98520900	-1.86581400
<b>E-4</b>				H	-3.12788300	1.40836100	-2.33171500
				H	-2.38335000	2.94557400	-1.92714000
				C	-5.07418300	3.33064900	-0.44603800
Ru	-0.01606900	0.08705100	-0.24746100	H	-4.59846400	2.32469600	1.47285600
P	-2.31554600	0.26484300	0.18933200	H	-5.23133700	1.26799300	0.19212500
P	2.31300800	-0.01844000	0.05478800	H	-4.52396300	3.86678600	-2.52104600
N	0.02427400	-0.61951500	1.82586400	H	-5.31016300	2.29157700	-2.33623300
C	-1.07964400	-0.51164600	2.61295200	H	-4.58903900	4.25748100	-0.09156800
C	-1.09507300	-1.00818800	3.91880800	H	-6.16305200	3.48328300	-0.38118700
C	0.05920600	-1.58609200	4.44526300	C	3.18765000	1.49986300	0.72377300
C	1.20092300	-1.64765500	3.65291900	C	3.07828100	2.75935900	-0.19621600
C	1.16153400	-1.16397700	2.33900300	C	2.68212900	1.97032800	2.10870500
H	-2.00271900	-0.91934700	4.51720800	H	4.25076900	1.22512300	0.82711600
H	0.06969800	-1.97417100	5.46614400	C	2.74115400	3.94668000	0.74322700
H	2.12611000	-2.08218200	4.03337600	H	2.30241900	2.64017700	-0.96651200
C	-2.26795600	0.24314700	2.06764700	H	4.03166700	2.92570500	-0.72116700
C	2.36352900	-1.27058600	1.44421100	C	3.09124600	3.44961600	2.15480500
H	-2.15512100	1.30107000	2.36509200	H	3.09835100	1.37655200	2.93739400
H	-3.20384200	-0.12020900	2.51889900	H	1.58276600	1.89787200	2.15453300
H	3.29628500	-1.26136700	2.02820800	H	3.27433700	4.86919400	0.46606500
H	2.28450400	-2.22331500	0.88308000	H	1.66159500	4.16512300	0.69071400
H	0.06766700	1.58677800	0.31664600	H	4.17798700	3.53556800	2.33510300
C	-0.00827300	0.79020100	-1.94518600	H	2.57976300	4.01232700	2.95203100
O	0.00771100	1.26080500	-3.01082200	C	3.47316400	-0.75869200	-1.20555200
H	-0.18970500	-3.90230800	-1.56803000	C	3.66253500	0.06073200	-2.50011400
C	-3.56578600	-1.06499300	-0.22711400	C	4.91376200	-1.12421100	-0.73809600
C	-3.69482700	-1.37779500	-1.73478800	H	2.94380000	-1.68906100	-1.46157800
C	-3.26183900	-2.44151600	0.44356300	C	4.86804200	-0.63255300	-3.15267400
H	-4.54237300	-0.70581200	0.14031300	H	3.92027800	1.11100000	-2.27993100
C	-4.36351200	-2.76048700	-1.74038100	H	2.76220900	0.06683300	-3.13175600
H	-2.69147100	-1.44309200	-2.18483400	C	5.82814000	-0.87347500	-1.97205100
H	-4.27598700	-0.61920300	-2.28186000	H	4.94607800	-2.17435000	-0.41031400
C	-3.63557500	-3.51717500	-0.61489600	H	5.25198900	-0.51813000	0.11788300
H	-3.84828500	-2.55371900	1.36929900	H	4.54654500	-1.59551500	-3.58611100
H	-2.19877000	-2.53367200	0.70260100	H	5.32255700	-0.04060600	-3.96260500
H	-5.43802400	-2.65602600	-1.50412300	H	6.52405900	-1.70663900	-2.15493600
H	-4.29071700	-3.26696800	-2.71554800	H	6.44419000	0.02674400	-1.80717800
H	-4.24504000	-4.32977300	-0.19008900	C	0.33939900	-3.04034500	-1.07970900
H	-2.71411100	-3.96932300	-1.01251400	O	-0.40515900	-2.00682300	-0.95729600
C	-3.15383600	1.90134700	-0.15681400	O	1.52010500	-3.20088000	-0.73491100
C	-3.22237600	2.28247300	-1.67175300				
C	-4.58085700	2.13790100	0.38746600	<b>E-TS2/3</b>			
H	-2.47607700	2.61576800	0.34009000				

Ru	-0.01220500	-0.13685100	-0.24505300	H	4.65599000	-2.64535200	0.66560900
P	2.27921300	-0.40196200	0.12436900	H	5.24332700	-1.26355600	-0.28740000
P	-2.32255900	-0.03623500	0.06191300	H	4.40759200	-3.03875400	-3.57874100
N	-0.05160700	-0.07694800	1.93777500	H	5.27863500	-1.59265300	-3.05202900
C	1.03862100	-0.45566700	2.65582400	H	4.59887500	-4.06357700	-1.37071200
C	1.05398300	-0.37534600	4.05141700	H	6.16193500	-3.22610400	-1.48385200
C	-0.08226100	0.06697800	4.72580600	C	-3.31782100	-1.61088700	0.26965300
C	-1.20786000	0.42023400	3.98533100	C	-3.27302100	-2.55069600	-0.97857300
C	-1.16699300	0.34850500	2.58917000	C	-2.84346800	-2.49194000	1.45005900
H	1.94953600	-0.67608100	4.59682700	H	-4.36205300	-1.31146700	0.46156600
H	-0.09193700	0.13005800	5.81604100	C	-3.01909400	-3.97907200	-0.42822900
H	-2.11758700	0.76695000	4.47721400	H	-2.47666400	-2.26012100	-1.67987400
C	2.20752400	-1.02994200	1.89688400	H	-4.22648800	-2.49614100	-1.52635600
C	-2.34361400	0.77892100	1.75219900	C	-3.34285400	-3.89371400	1.07176600
H	2.04442300	-2.11840700	1.80170800	H	-3.22215500	-2.14051800	2.42274800
H	3.14706000	-0.88479000	2.45199600	H	-1.74106200	-2.49949800	1.49154700
H	-3.28839800	0.64627900	2.30175700	H	-3.60988300	-4.74507600	-0.95386700
H	-2.22624800	1.85301800	1.52438000	H	-1.95558700	-4.23896100	-0.55689000
H	-0.02796100	-1.79332300	-0.14925800	H	-4.43315000	-3.96434100	1.23674700
C	-0.00197300	-0.20628400	-2.08285200	H	-2.86745600	-4.69237500	1.66323700
O	-0.00756100	-0.25268900	-3.24774700	C	-3.39470600	1.12720200	-0.93163900
H	-0.00183700	1.61205000	-0.22439500	C	-3.61522400	0.74092700	-2.40943200
C	3.52126500	0.99709100	0.23179000	C	-4.81770100	1.44804500	-0.39376000
C	3.76583400	1.76906300	-1.08192500	H	-2.80073100	2.05483000	-0.91621700
C	3.11729200	2.10160300	1.24766300	C	-4.69619800	1.74008800	-2.84742100
H	4.47587100	0.54916000	0.55909000	H	-4.00638800	-0.28761100	-2.49475600
C	4.47036100	3.04527100	-0.59675200	H	-2.69411300	0.79645400	-3.00739300
H	2.80122000	2.02775600	-1.54817300	C	-5.67396100	1.77981900	-1.65333600
H	4.36445800	1.20213500	-1.81165400	H	-4.78443000	2.28679300	0.31787600
C	3.71004400	3.42989000	0.69058500	H	-5.25519800	0.59293700	0.14589500
H	3.48943300	1.86801200	2.25737300	H	-4.23579700	2.73183200	-2.99738200
H	2.02125800	2.17690400	1.31158300	H	-5.18623800	1.45997100	-3.79274400
H	5.52729400	2.81951700	-0.36831400	H	-6.18457800	2.75090300	-1.56539300
H	4.46210800	3.84714500	-1.35083400	H	-6.46044100	1.01843600	-1.78512400
H	4.36337100	3.93071300	1.42168100	C	-0.17234000	3.27300500	-0.37113600
H	2.89307600	4.12377300	0.44589600	O	0.76824200	3.58896600	-1.02700700
C	3.16311100	-1.80395400	-0.74434600	O	-1.16940400	3.50661900	0.24598400
C	3.22052300	-1.66626400	-2.29740400				
C	4.60390300	-2.16249500	-0.32324800	<b>E-TS3/4</b>			
H	2.51436100	-2.66436100	-0.50794400				
C	4.54726700	-2.35276200	-2.72959400	Ru	-0.02321700	0.02496700	-0.21382300
H	3.20277200	-0.61540800	-2.62051800	P	-2.32980800	0.28985800	0.13374900
H	2.33850300	-2.13914800	-2.75140200	P	2.32269100	0.03641000	0.07678000
C	5.07161300	-3.07064400	-1.47111900	N	0.03171000	0.17030600	1.96696300

C	-1.06990300	0.55674100	2.66292300	H	-4.62386700	3.90500300	-1.50493200
C	-1.06098400	0.61548700	4.05974800	H	-6.18904300	3.06774400	-1.58338600
C	0.10813600	0.30344000	4.75060000	C	3.20780100	1.68398900	0.13191900
C	1.24018900	-0.06774500	4.02980200	C	3.11798300	2.49188200	-1.20457000
C	1.17845200	-0.14180500	2.63412500	C	2.69231500	2.65251800	1.22381400
H	-1.96419100	0.91730700	4.59161800	H	4.26583900	1.45939600	0.34553500
H	0.13610400	0.34959500	5.84140600	C	2.76858800	3.94739400	-0.79878700
H	2.17066900	-0.32339500	4.53783100	H	2.35657200	2.08165600	-1.88425200
C	-2.29272400	0.98286100	1.88417400	H	4.08034400	2.44569400	-1.73676600
C	2.35272900	-0.62595500	1.82801800	C	3.10614500	4.03483900	0.69780800
H	-2.25224700	2.08006000	1.76335200	H	3.09907200	2.42390400	2.22111300
H	-3.20977900	0.75880600	2.45025400	H	1.59223900	2.60444600	1.28759100
H	3.30080400	-0.45264600	2.35863100	H	3.30210400	4.69432000	-1.40635300
H	2.22381300	-1.71754300	1.65871800	H	1.68909700	4.12376800	-0.94022300
H	0.02342500	1.59358100	-0.29139200	H	4.19171100	4.18266500	0.83981100
C	-0.04600600	-0.00378800	-2.06199600	H	2.59097600	4.86182900	1.21173300
O	-0.05252700	0.03080100	-3.22166300	C	3.43510800	-1.15109400	-0.82973500
H	-0.21070100	-2.08158500	0.86599000	C	3.60385300	-0.89732500	-2.34196400
C	-3.54197000	-1.13274600	0.22482500	C	4.88096700	-1.33948900	-0.29013100
C	-3.66629500	-1.94445500	-1.08802400	H	2.88721000	-2.10029800	-0.70390800
C	-3.19634900	-2.18909100	1.32431000	C	4.73443000	-1.87295500	-2.70061100
H	-4.52185000	-0.68701600	0.46534100	H	3.93086400	0.13792800	-2.54369600
C	-4.22622300	-3.29219700	-0.60930200	H	2.67761000	-1.07572000	-2.90682900
H	-2.66543700	-2.10424900	-1.52064400	C	5.73515300	-1.72791500	-1.53468300
H	-4.30731100	-1.44966900	-1.83417600	H	4.90109600	-2.11942500	0.48578300
C	-3.40242900	-3.57442200	0.65668700	H	5.28166200	-0.42158000	0.17089400
H	-3.85684600	-2.05208700	2.19552000	H	4.32951700	-2.89845700	-2.73121300
H	-2.16144400	-2.09350200	1.68681500	H	5.18838400	-1.66655500	-3.68238600
H	-5.30021800	-3.19456400	-0.36491700	H	6.31739100	-2.64693800	-1.36823900
H	-4.12816400	-4.08351600	-1.36818900	H	6.46006700	-0.92751500	-1.75848400
H	-3.88381900	-4.29652000	1.33399600	C	0.31003100	-2.73840900	0.06479100
H	-2.42495900	-3.98222100	0.35941600	O	-0.33320200	-2.82373900	-1.00689800
C	-3.19334900	1.66557500	-0.79548600	O	1.40755300	-3.22131000	0.41834300
C	-3.24968500	1.47647900	-2.34323500				
C	-4.63301300	2.04433500	-0.38654800	<b>F-1</b>			
H	-2.54368200	2.53290200	-0.58517200				
C	-4.57928900	2.14259400	-2.79726000	Ru	-0.00073900	0.00596700	-0.13590100
H	-3.22489200	0.41640100	-2.63233400	P	2.29398900	-0.17191900	0.15259800
H	-2.37150300	1.94146200	-2.81290700	P	-2.28986000	0.17969100	0.20096300
C	-5.09928700	2.91013900	-1.56699800	N	0.01775300	-0.01979900	2.05418600
H	-4.68315300	2.56268700	0.58416700	C	1.14670600	-0.36583100	2.72817700
H	-5.27361400	1.14837400	-0.31794400	C	1.19267800	-0.36747600	4.12575000
H	-4.44410000	2.79300500	-3.67447000	C	0.05102500	-0.03817800	4.85262200
H	-5.31021900	1.36844100	-3.08467400	C	-1.10753900	0.29935900	4.15722900

C	-1.09505600	0.31589300	2.75880000	C	-3.51684200	-2.01134600	-1.14172200
H	2.11960100	-0.64321500	4.63077200	C	-2.88895700	-2.36509100	1.29233400
H	0.06402300	-0.04475400	5.94460700	H	-2.51862600	-2.38635300	-1.42116700
H	-2.02215900	0.56845300	4.68770300	H	-3.79569000	-1.28120000	-1.91650600
C	2.33799500	-0.81247700	1.92058600	C	-4.55124500	-3.16155300	-1.13354400
C	-2.30772300	0.77071600	1.98705300	C	-3.24786100	-3.82441400	0.93290600
H	2.27055600	-1.90933700	1.81008000	H	-3.31573400	-2.11462500	2.27858000
H	3.27672900	-0.59498600	2.45196000	H	-1.79255500	-2.28512000	1.37482300
H	-3.23125200	0.51544300	2.52945000	H	-4.29904000	-3.86709600	-1.94344900
H	-2.26408400	1.87185500	1.91375100	H	-5.55344500	-2.76633900	-1.37329200
H	-0.00793700	-1.68853300	-0.09016800	C	-4.60098700	-3.90667400	0.22006900
C	-0.00441400	0.02046200	-1.97037300	H	-2.46677600	-4.24768700	0.27705000
O	0.00440700	0.02354200	-3.13942500	H	-3.24690000	-4.44021000	1.84755900
H	0.00575800	1.69942000	-0.03663300	H	-4.90346200	-4.95590500	0.06817700
C	3.26793700	2.15234000	-1.14938700	H	-5.37368500	-3.45759000	0.87060600
C	3.06185000	2.27774700	1.37090800	C	-3.40510700	-1.34373100	0.24100700
H	2.24458100	2.55711500	-1.19944200	H	-4.40769200	-0.99248300	0.54189600
H	3.37525000	1.49999800	-2.02855300	C	3.39635100	1.35751100	0.16471400
C	4.31329200	3.28945800	-1.21518600	H	4.43832700	1.00373800	0.25926100
C	3.38590200	3.76370200	1.09241400	C	3.27788200	-1.52158600	-0.72093500
H	3.62636600	1.93649600	2.25540600	H	2.58445500	-2.37263400	-0.60128000
H	1.98978800	2.19540600	1.61447900	C	-4.79008500	1.59424600	-0.28030500
H	3.94460800	4.06741400	-1.90536300	C	-3.08444700	1.57976000	-2.17269100
H	5.25359600	2.91238500	-1.65342800	C	-5.41451300	2.93534700	-0.73692500
C	4.60206600	3.90773800	0.17270800	H	-5.31053900	0.75587300	-0.77354500
H	2.51573200	4.25023500	0.61823400	H	-4.95506600	1.46145300	0.80174700
H	3.54996000	4.29093500	2.04680600	H	-2.98794000	0.56569400	-2.58955700
H	4.89182300	4.96626800	0.06808800	H	-2.12438700	2.07632100	-2.37899600
H	5.46549800	3.40092100	0.64129200	C	-4.23239300	2.31846100	-2.89644800
C	3.44723600	-1.29861800	-2.23546300	C	-4.77752000	3.46805900	-2.04237900
C	4.64047200	-1.88780300	-0.07434700	H	-6.49999200	2.79264500	-0.87471200
H	4.22229500	-0.53159100	-2.40514800	H	-5.30250900	3.68820100	0.06209300
H	2.52104800	-0.91612000	-2.68775500	H	-3.87504900	2.68920300	-3.87082500
C	3.86301900	-2.61677700	-2.93131800	H	-5.05536800	1.61602300	-3.12185700
C	5.57106400	-2.63982900	-1.05716900	H	-5.51234600	4.06424500	-2.60765500
H	4.46175100	-2.51678700	0.81386500	H	-3.94639600	4.15534700	-1.80263000
H	5.16144700	-0.98522500	0.28771300	C	-3.29267500	1.53921000	-0.63299500
H	4.38710600	-2.37247900	-3.87088600	H	-2.81301900	2.44130000	-0.21385200
H	2.96092800	-3.18225300	-3.21851300				
C	4.76444100	-3.49914400	-2.03639600	<b>F-2</b>			
H	6.17647800	-1.91470100	-1.62962600				
H	6.28902200	-3.25557600	-0.49070100	Ru	-0.00516800	0.15073600	-0.10798000
H	5.43486200	-4.11561400	-2.65721800	P	2.29412100	0.09195300	0.22793400
H	4.14581100	-4.20974800	-1.45909000	P	-2.29703500	0.46429600	0.16866300

N	0.00996200	0.62255400	2.03200800	C	5.00438400	-3.42385800	-1.29327900
C	1.12507400	0.39684900	2.77513000	H	6.28913000	-1.69441600	-1.11106100
C	1.16177700	0.68493300	4.14299100	H	6.45223200	-2.82709500	0.23033500
C	0.02575300	1.19221800	4.76956900	H	5.73775100	-4.07944200	-1.79058900
C	-1.11512200	1.41872000	4.00304600	H	4.41314300	-4.07570500	-0.62592900
C	-1.09225600	1.14207800	2.63238700	C	-3.79602800	-1.85318400	-0.58888000
H	2.07633400	0.49469600	4.70651600	C	-2.98059100	-1.73007600	1.81587400
H	0.03065000	1.41165700	5.83938600	H	-2.86699800	-2.38159100	-0.85292400
H	-2.02165700	1.82674000	4.45240700	H	-4.09104100	-1.28177900	-1.48208000
C	2.30823600	-0.22483300	2.08256200	C	-4.91252200	-2.86856700	-0.24575300
C	-2.26938100	1.47646800	1.75542500	C	-3.47416200	-3.19399800	1.81225600
H	2.20422800	-1.32197800	2.15737500	H	-3.30627300	-1.23496100	2.74685100
H	3.24852600	0.05340700	2.58220700	H	-1.87766700	-1.72711900	1.81178800
H	-3.20903000	1.43035600	2.32776900	H	-4.79452900	-3.75163700	-0.89623700
H	-2.14133100	2.51795300	1.41075400	H	-5.89926600	-2.43769300	-0.48866700
H	-0.00130100	-1.48982300	0.33253300	C	-4.89024200	-3.30005600	1.23907200
C	0.00304800	-0.26611200	-1.89455500	H	-2.79236500	-3.81372500	1.20494100
O	0.02365600	-0.54347300	-3.03017500	H	-3.43316100	-3.59946300	2.83687600
H	-0.00706900	1.81811500	-0.40021100	H	-5.28233400	-4.32501700	1.34459300
C	3.22535000	2.19084300	-1.44633600	H	-5.56319300	-2.65323900	1.83142000
C	2.97276600	2.75052300	1.00307200	C	-3.50675800	-0.91840800	0.59913900
H	2.20284700	2.58125900	-1.57256700	H	-4.44950100	-0.41700200	0.88144700
H	3.33901100	1.39714100	-2.19893300	C	3.34601100	1.63818900	-0.01268000
C	4.27085000	3.30196400	-1.69833600	H	4.39490400	1.33629100	0.15659400
C	3.33649100	4.16556800	0.49060600	C	3.35445700	-1.34459700	-0.36993800
H	3.48797600	2.55814000	1.95948000	H	2.69345200	-2.19485000	-0.13486400
H	1.88918300	2.71948100	1.20295300	C	-4.71614800	1.86409200	-0.65649100
H	3.90091900	3.96117800	-2.50221900	C	-3.03418500	1.28360400	-2.47957900
H	5.21038200	2.85961500	-2.07252600	C	-5.25951000	3.09114800	-1.42842100
C	4.56292000	4.13242300	-0.42701100	H	-5.29126300	0.96484700	-0.93455600
H	2.48287000	4.58798600	-0.06796700	H	-4.88006300	2.00962000	0.42402500
H	3.50469700	4.83799800	1.34796300	H	-3.00613600	0.19430000	-2.63642800
H	4.87646400	5.15355800	-0.69971700	H	-2.04746100	1.65463700	-2.79467300
H	5.41154100	3.69097500	0.12670600	C	-4.14070100	1.89673300	-3.36733100
C	3.57849500	-1.36954800	-1.89384300	C	-4.60279700	3.25143300	-2.81992600
C	4.69999500	-1.53829200	0.38075000	H	-6.35307700	2.98840600	-1.53420800
H	4.32627800	-0.60562300	-2.16739100	H	-5.09294500	4.00635800	-0.83479100
H	2.65595800	-1.11249800	-2.43432000	H	-3.77038600	1.99664300	-4.40051100
C	4.07489800	-2.76464300	-2.34075300	H	-5.00915600	1.21524900	-3.42049500
C	5.71486800	-2.36305700	-0.44535800	H	-5.30373300	3.73911300	-3.51687700
H	4.50636000	-2.05177000	1.33742100	H	-3.72719500	3.92130400	-2.74860300
H	5.15644200	-0.56773800	0.63981400	C	-3.22853000	1.63384700	-0.97767100
H	4.60000400	-2.66248300	-3.30561000	H	-2.69133600	2.58029400	-0.79115100
H	3.20800200	-3.41999700	-2.52432000	C	0.09649500	-4.15582800	-0.67029100

O	1.23142500	-4.21091000	-0.39798300	H	4.37307400	-0.01141400	-2.32982100
O	-1.03583600	-4.15738300	-0.95263000	H	2.71276200	-0.44011400	-2.75444500
<b>F-3</b>				C	4.15012800	-2.04309400	-3.09234300
				C	5.75689500	-2.17263700	-1.13282900
				H	4.51677500	-2.36664400	0.64507500
Ru	-0.00488200	0.09933000	-0.17162800	H	5.17136800	-0.74508300	0.39302000
P	2.32645300	-0.02105100	0.15110900	H	4.69402800	-1.67421800	-3.97843400
P	-2.31605000	0.35934800	0.17428300	H	3.29400100	-2.62422800	-3.47267500
N	0.00579400	-0.00427600	2.00936600	C	5.06510300	-2.96258500	-2.24880800
C	1.12214900	-0.42754400	2.66224400	H	6.33774300	-1.34635900	-1.58047600
C	1.15347500	-0.51708400	4.05788600	H	6.48566000	-2.80296400	-0.59736700
C	0.01926500	-0.18650800	4.79425300	H	5.80939900	-3.45607800	-2.89461600
C	-1.11864800	0.24971300	4.11872700	H	4.46889400	-3.77277000	-1.79362100
C	-1.09488200	0.34858000	2.72491000	C	-3.65823400	-1.76588400	-1.17908000
H	2.06273200	-0.86271000	4.55086100	C	-3.16472700	-2.10841200	1.29003900
H	0.02226600	-0.26436400	5.88356900	H	-2.70800600	-2.28149700	-1.38718500
H	-2.02209600	0.52968800	4.66188700	H	-3.81458500	-1.03441500	-1.98706400
C	2.29972200	-0.85163800	1.83125700	C	-4.82569800	-2.78165800	-1.17662500
C	-2.27068900	0.91608900	1.97205200	C	-3.68762700	-3.52509100	0.96082300
H	2.13645400	-1.91259600	1.55454100	H	-3.57707700	-1.77086900	2.25669800
H	3.23789000	-0.77066100	2.39928400	H	-2.07129600	-2.16328200	1.40906600
H	-3.20931600	0.72078800	2.51165300	H	-4.62351700	-3.54225300	-1.94893000
H	-2.14356900	2.01215500	1.92479300	H	-5.76490200	-2.28199800	-1.47255600
H	-0.04173200	-1.75991800	-0.20589000	C	-5.01432300	-3.46399200	0.19803800
C	0.01310100	0.24002700	-2.00944100	H	-2.93472700	-4.04908100	0.35061400
O	0.04000000	0.34489400	-3.16769200	H	-3.79808600	-4.09962900	1.89527800
H	0.03279600	1.70997500	-0.06692700	H	-5.43424200	-4.47453900	0.06614000
C	3.17445100	2.47656700	-0.89811900	H	-5.75386500	-2.90420400	0.80070200
C	2.95705000	2.33959100	1.61894600	C	-3.53632700	-1.07212100	0.19200200
H	2.14397300	2.86655600	-0.90613600	H	-4.51235100	-0.62350500	0.44781700
H	3.29170800	1.91897500	-1.83869100	C	3.32742300	1.55864000	0.33048400
C	4.19616100	3.63651600	-0.84700200	H	4.38318600	1.24184800	0.39546500
C	3.28530500	3.84842400	1.50776500	C	3.38818900	-1.22675500	-0.82113700
H	3.49756600	1.90250300	2.47513800	H	2.73525000	-2.11534700	-0.81758300
H	1.88105000	2.22744100	1.82871500	C	-4.67843800	1.99686000	-0.23504500
H	3.80163600	4.48151600	-1.43645000	C	-3.03473200	1.85277600	-2.17396500
H	5.13600100	3.33202800	-1.33846600	C	-5.18816300	3.39573900	-0.65574500
C	4.49501200	4.09384700	0.59960800	H	-5.28194200	1.21711400	-0.72882100
H	2.41434100	4.38997500	1.09837900	H	-4.82880300	1.85897600	0.84821200
H	3.45831300	4.26413400	2.51388300	H	-3.03801300	0.83756000	-2.59904000
H	4.78455200	5.15720200	0.61266200	H	-2.04519100	2.27315500	-2.40902200
H	5.36145000	3.53770000	1.00094500	C	-4.13753600	2.69318800	-2.85660200
C	3.63075900	-0.82728200	-2.28815900	C	-4.55120700	3.88017200	-1.98020100
C	4.72476700	-1.60966200	-0.12819500	H	-6.28630400	3.35721900	-0.75332800

H	-4.97607700	4.12472500	0.14501000	H	4.85272900	3.54536000	-1.21566300
H	-3.78008500	3.03716300	-3.84048200	C	4.18047400	4.19516000	0.75245300
H	-5.02452700	2.06604200	-3.05750800	H	2.08998100	4.33259000	1.27780100
H	-5.24998400	4.54062100	-2.51858400	H	3.15406000	4.21989100	2.67942800
H	-3.65639100	4.49225200	-1.76711400	H	4.39876200	5.27431900	0.80598700
C	-3.20111800	1.81510600	-0.62857200	H	5.08557500	3.68298900	1.12605900
H	-2.63428300	2.66741400	-0.21290500	C	3.70397400	-0.62507300	-2.29317600
C	0.10384300	-3.03030500	-0.22689100	C	4.83909600	-1.40083400	-0.15497700
O	1.11687200	-3.37292100	0.38278400	H	4.37544200	0.25115600	-2.29088700
O	-0.80916400	-3.55278700	-0.84656000	H	2.76063200	-0.29481300	-2.75342700
F-4				C	4.33170900	-1.75614100	-3.14375900
				C	5.91662300	-1.85976500	-1.16688200
				H	4.68609900	-2.18768200	0.60143300
				H	5.21523000	-0.51531800	0.38671400
Ru	-0.03559100	-0.02059400	-0.18099800	H	4.87133900	-1.30444500	-3.99368300
P	2.29797500	-0.04895600	0.14945400	H	3.53110200	-2.37731800	-3.57834700
P	-2.34392900	0.25434800	0.16907900	C	5.28836900	-2.64978800	-2.32012500
N	-0.01912600	-0.21666500	2.00172800	H	6.44697500	-0.98171700	-1.57764400
C	1.11669600	-0.60630500	2.64189800	H	6.68005400	-2.46159600	-0.64688800
C	1.14264900	-0.76950700	4.03281300	H	6.06866900	-3.07584300	-2.97176100
C	-0.01237100	-0.54618500	4.77490000	H	4.73404600	-3.50750300	-1.90062000
C	-1.16635900	-0.12896500	4.11356600	C	-3.56361300	-1.76532000	-1.41198400
C	-1.13718100	0.04978700	2.72813300	C	-3.31025200	-2.26178800	1.07319300
H	2.06791100	-1.08702700	4.51501200	H	-2.58075000	-2.23643700	-1.56230700
H	-0.01282700	-0.68548400	5.85819000	H	-3.65686400	-0.98381300	-2.18163800
H	-2.08509000	0.07904300	4.66359800	C	-4.70627300	-2.79136000	-1.58844600
C	2.33193800	-0.90779900	1.81405900	C	-3.74661600	-3.66165600	0.58921000
C	-2.33035800	0.63355300	2.01152600	H	-3.85898300	-2.00605700	1.99592000
H	2.26253200	-1.96966100	1.50329800	H	-2.23978700	-2.30055400	1.32140900
H	3.25367400	-0.75453800	2.39427200	H	-4.43001100	-3.48554700	-2.40006700
H	-3.26436700	0.35198100	2.52007100	H	-5.62595700	-2.28015100	-1.92235600
H	-2.24907000	1.73335900	2.07508100	C	-4.99720700	-3.58267800	-0.29149100
H	-0.21884600	-4.21760100	-0.45506000	H	-2.92466200	-4.12206200	0.01506000
C	-0.00831600	0.24646000	-1.99774200	H	-3.91929200	-4.31416100	1.46089700
O	0.02292000	0.43762600	-3.14687000	H	-5.37045400	-4.59102100	-0.53444000
H	0.04905000	1.57036200	0.00777000	H	-5.80476700	-3.08889100	0.27994400
C	2.94773500	2.55988100	-0.79898800	C	-3.57583200	-1.15979900	0.00583600
C	2.77277300	2.30306600	1.71028400	H	-4.57237600	-0.72178200	0.19033500
H	1.89681200	2.88909700	-0.77675700	C	3.17387300	1.60108500	0.38618100
H	3.08186600	2.05075400	-1.76431100	H	4.25014000	1.35832000	0.42765700
C	3.89948200	3.77523700	-0.70935600	C	3.48186200	-1.11095900	-0.84926800
C	2.99878400	3.83380700	1.65852500	H	2.91104000	-2.05234400	-0.89063900
H	3.35560700	1.87072700	2.54066200	C	-4.66204000	1.99187500	-0.08667900
H	1.71055500	2.11063700	1.93030100	C	-3.03542400	1.95057400	-2.04273300
H	3.45266200	4.61732900	-1.26498500				

C	-5.12791000	3.43697300	-0.38989700	C	2.93300900	2.37590000	1.58830100
H	-5.29393400	1.27546000	-0.63805400	H	2.09948100	2.84822100	-0.94022900
H	-4.81323600	1.77231900	0.98301600	H	3.26093700	1.91068100	-1.86402100
H	-3.09007600	0.97464200	-2.54907400	C	4.13954300	3.65618900	-0.90057200
H	-2.02824700	2.34045600	-2.25394400	C	3.22819900	3.88889300	1.45094500
C	-4.10331800	2.89137600	-2.64520100	H	3.49048100	1.96531800	2.44700100
C	-4.47036600	4.01170400	-1.66669300	H	1.86071600	2.24608400	1.80655200
H	-6.22628800	3.44030800	-0.49356500	H	3.73047800	4.48428600	-1.50413200
H	-4.89849500	4.08944100	0.46993800	H	5.08451900	3.35973400	-1.38757400
H	-3.73262300	3.30636200	-3.59629600	C	4.43150100	4.14413800	0.53735400
H	-5.01503600	2.32043200	-2.89722200	H	2.34499800	4.40367500	1.03363100
H	-5.14157100	4.74494800	-2.14243400	H	3.39334300	4.32536300	2.44975400
H	-3.55205600	4.56591600	-1.40167500	H	4.69973000	5.21328800	0.53212900
C	-3.19325900	1.79371200	-0.50453200	H	5.30941100	3.61208800	0.94680100
H	-2.59752200	2.59213200	-0.02684700	C	3.63765700	-0.82601600	-2.26147900
C	0.30941300	-3.26172200	-0.19404300	C	4.74184000	-1.56640200	-0.09407300
O	1.48258000	-3.33280300	0.20283400	H	4.36491600	0.00258100	-2.30873500
O	-0.42833700	-2.22815900	-0.35534800	H	2.71354500	-0.45978200	-2.73210200
<b>F-TS2/3</b>				C	4.18164200	-2.03829900	-3.05415400
				C	5.78650600	-2.12058800	-1.09081300
				H	4.54982800	-2.31795400	0.68905100
Ru	-0.00674500	0.09407000	-0.15844300	H	5.17056000	-0.68791600	0.41794200
P	2.30835700	-0.00753600	0.15816600	H	4.72076600	-1.66712600	-3.94214100
P	-2.30383100	0.35866200	0.17939100	H	3.33782700	-2.63852800	-3.43311800
N	0.00747300	0.00818400	2.02661900	C	5.11245500	-2.93316000	-2.20162100
C	1.12497200	-0.39679900	2.68673400	H	6.35305700	-1.28812300	-1.54502800
C	1.15251500	-0.48602000	4.08230000	H	6.52598400	-2.73229700	-0.54833800
C	0.01053100	-0.17242600	4.81485200	H	5.86725200	-3.41842300	-2.84151700
C	-1.12860500	0.24879700	4.13247900	H	4.53174700	-3.75155600	-1.74016400
C	-1.09927100	0.34846600	2.73825800	C	-3.70054600	-1.72369800	-1.18996900
H	2.06585100	-0.81535500	4.57938800	C	-3.16776900	-2.11723000	1.26194400
H	0.00969600	-0.24958700	5.90421700	H	-2.75538100	-2.23102900	-1.43700000
H	-2.03816100	0.51892600	4.67070700	H	-3.87012500	-0.97462100	-1.97863200
C	2.32307200	-0.79287800	1.86497000	C	-4.87062200	-2.73741100	-1.18846200
C	-2.27550200	0.90757700	1.98037900	C	-3.71531800	-3.52284400	0.92326900
H	2.23732700	-1.87188200	1.64801100	H	-3.55838900	-1.79353200	2.24194900
H	3.25429200	-0.63363100	2.42918300	H	-2.07171500	-2.17790100	1.35832400
H	-3.21580300	0.70766000	2.51584400	H	-4.68103400	-3.49084000	-1.97133700
H	-2.15144400	2.00406700	1.93432400	H	-5.80997700	-2.23049900	-1.47002000
H	-0.02592400	-1.65370200	-0.15652700	C	-5.05124900	-3.43384700	0.17970000
C	0.00409500	0.17034200	-1.99581300	H	-2.98506000	-4.05772300	0.29431700
O	0.02639000	0.21515900	-3.16083600	H	-3.82036300	-4.10948800	1.85087000
H	0.01187000	1.75055400	-0.03991100	H	-5.48937400	-4.43591400	0.04175900
C	3.13724100	2.47911000	-0.93076500	H	-5.77190200	-2.86949000	0.80005200



C	-3.54640300	-1.05770600	0.19069500	H	3.25484900	-0.48200200	2.47039800
H	-4.51432800	-0.60538600	0.46874300	H	-3.27599900	0.54927400	2.52735800
C	3.30759100	1.58032700	0.30951400	H	-2.37540500	1.95036200	1.93302000
H	4.36698000	1.27541500	0.37447700	H	-0.29571500	-2.15402600	0.88497200
C	3.39886900	-1.21290300	-0.79000200	C	-0.04336300	0.01528100	-1.97977600
H	2.76165900	-2.11204100	-0.78758400	O	-0.02813200	0.07018400	-3.13865900
C	-4.66973500	1.99734100	-0.25549600	H	0.00647100	1.56998200	-0.16281200
C	-2.98636400	1.87617100	-2.16167500	C	3.00429000	2.44265700	-1.10139000
C	-5.17010100	3.40215400	-0.66892100	C	2.79082700	2.52436000	1.41783600
H	-5.26550900	1.22476600	-0.77009200	H	1.95895600	2.78997800	-1.14124900
H	-4.84116100	1.84699200	0.82308900	H	3.14386200	1.80806800	-1.98804200
H	-2.98686700	0.86728700	-2.60207600	C	3.97738800	3.64351700	-1.15849700
H	-1.98793400	2.29052800	-2.36730400	C	3.05685800	4.02943300	1.16978200
C	-4.06861100	2.73398200	-2.85569800	H	3.34628300	2.18959300	2.30973900
C	-4.49912100	3.90703100	-1.96867300	H	1.72008900	2.38889200	1.64089000
H	-6.26540800	3.36512900	-0.79618400	H	3.54994100	4.41434800	-1.82200400
H	-4.97953600	4.11946700	0.14766500	H	4.92916000	3.33333600	-1.62246700
H	-3.68663400	3.09429900	-3.82452800	C	4.25543600	4.24295100	0.23951900
H	-4.95368500	2.11502400	-3.08916700	H	2.16471800	4.49586700	0.71577100
H	-5.18209000	4.58015000	-2.51190400	H	3.21138400	4.54116400	2.13377400
H	-3.60730400	4.51093800	-1.72259800	H	4.49812400	5.31471600	0.15519900
C	-3.18522600	1.81920200	-0.62118100	H	5.14506100	3.76448100	0.68746500
H	-2.62576700	2.66627500	-0.18604600	C	3.63078200	-0.92633300	-2.20409500
C	0.15516900	-3.33025700	-0.26165000	C	4.78629700	-1.46424000	-0.00295300
O	1.11845900	-3.54638600	0.41130000	H	4.33196400	-0.08214600	-2.32728400
O	-0.74879600	-3.65634500	-0.96172100	H	2.68839200	-0.62702300	-2.68592400
<b>F-TS3/4</b>				C	4.19512000	-2.18106600	-2.91236700
				C	5.82291900	-2.09114200	-0.96655100
				H	4.62297800	-2.14215700	0.85045000
Ru	-0.04941100	0.00161300	-0.13162800	H	5.20518200	-0.53037600	0.41217000
P	2.30025800	-0.00492300	0.17271100	H	4.72722600	-1.86351100	-3.82539600
P	-2.36158800	0.26731400	0.19087000	H	3.36011500	-2.82069200	-3.24058300
N	-0.02102000	0.08717100	2.05573100	C	5.14118100	-2.99617800	-1.99961800
C	1.12652700	-0.21392300	2.72639000	H	6.37855500	-1.29431600	-1.49326200
C	1.17697100	-0.16992000	4.12388900	H	6.57296800	-2.65240900	-0.38532100
C	0.03269800	0.16005600	4.84460300	H	5.89311600	-3.52669500	-2.60632700
C	-1.13786800	0.45944700	4.15121100	H	4.56885100	-3.77520700	-1.46680300
C	-1.13554800	0.43106400	2.75334800	C	-3.49153400	-1.92560300	-1.20176900
H	2.10970500	-0.41613700	4.63235700	C	-3.28094100	-2.17206300	1.33036700
H	0.05204300	0.18353400	5.93631300	H	-2.48475400	-2.36074700	-1.30867800
H	-2.05196800	0.72855400	4.68207100	H	-3.62047900	-1.22327100	-2.04013800
C	2.31687300	-0.66323600	1.92613300	C	-4.57726100	-3.02060600	-1.28782200
C	-2.36719700	0.84727100	1.98362500	C	-3.53927800	-3.64097800	0.94133200
H	2.20131300	-1.75545600	1.75123700	H	-3.92625800	-1.89661300	2.18256000

H	-2.23996000	-2.08797600	1.68202300	H	-4.88001900	1.76276800	0.81392200
H	-4.28069700	-3.73578300	-2.07265400	H	-3.06954800	0.72255300	-2.60590500
H	-5.53469600	-2.58024100	-1.61758300	H	-2.05366100	2.14160400	-2.41462400
C	-4.78335500	-3.76095300	0.05642600	C	-4.13620500	2.59478600	-2.88294300
H	-2.66210100	-4.03541200	0.40223400	C	-4.55367700	3.78274400	-2.00939400
H	-3.64630900	-4.24627500	1.85648800	H	-6.31174900	3.26298700	-0.81451200
H	-5.03255400	-4.81925600	-0.12325700	H	-5.01692900	4.02822400	0.10771000
H	-5.64726100	-3.33164700	0.59729100	H	-3.76023800	2.93865800	-3.85983900
C	-3.55349600	-1.18849000	0.15230600	H	-5.02579200	1.97688900	-3.10002900
H	-4.56243700	-0.75932500	0.27824900	H	-5.23863400	4.45023500	-2.55664900
C	3.19813800	1.64679200	0.20467100	H	-3.65782100	4.38753300	-1.78023800
H	4.26964800	1.39514100	0.29435400	C	-3.23413000	1.71398400	-0.64359200
C	3.42575000	-1.21931400	-0.70702200	H	-2.67304400	2.57088300	-0.22911400
H	2.82583400	-2.14131900	-0.62151700	C	0.29355900	-2.78555700	0.11367900
C	-4.71546000	1.89979200	-0.26744300	O	1.36926200	-3.26134600	0.53869400
C	-3.05256800	1.73975900	-2.18643600	O	-0.25895100	-2.85638000	-1.00871700
C	-5.21557400	3.29953200	-0.69679600				
H	-5.31396600	1.12077900	-0.76842800				