

Supporting Information For

Mechanism and Origin of Stereoselectivity and Regioselectivity in Cobalt-Catalyzed C-H Functionalization of Arylphosphinamide

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Content

Part 1: Transformation of Co(OAc) ₂ to Co ^{II} -Saloxs	S2
Part 2: Pivolate-ligated cobalt species promoted C-H functionalization	S3
Part 3: Benchmark studies for different functionals	S4
Part 4: Testing for temperature	S5
Part 5: Energy information for all the stationary points	S6
Part 6: Cartesian coordinates of all the stationary points.....	S8

Part 1: Transformation of $\text{Co}(\text{OAc})_2$ to Co^{II} -Saloxs

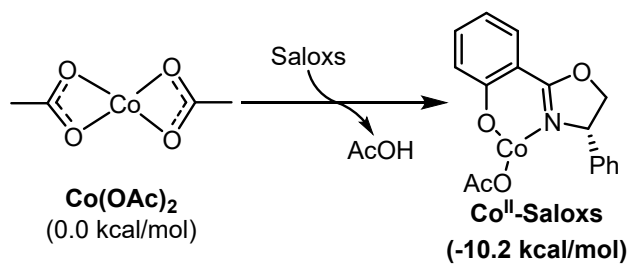


Fig. S1 Transformation of $\text{Co}(\text{OAc})_2$ to Co^{II} -Saloxs

Part 2: Pivolate-ligated cobalt species promoted C-H functionalization

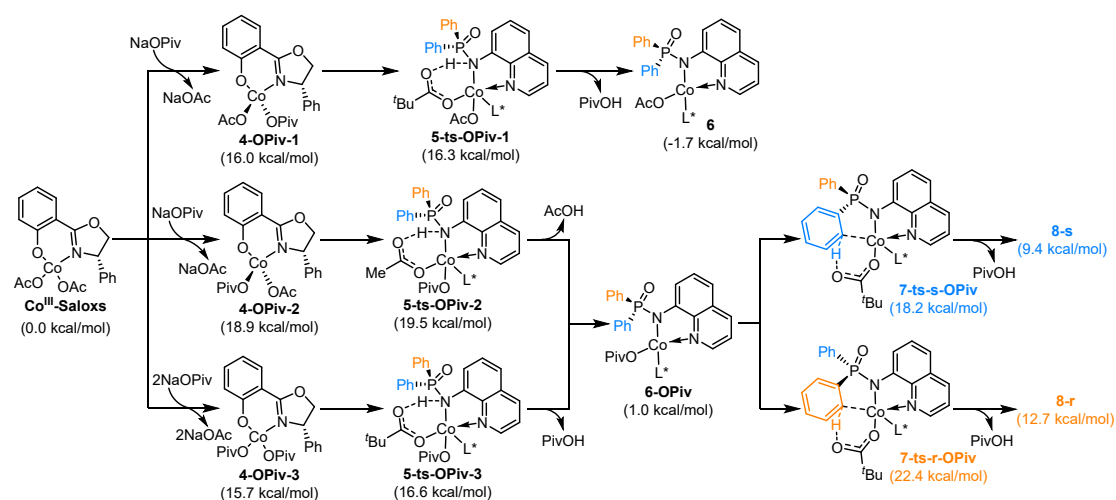


Fig. S2 Relative Gibbs free energy of pivolate-ligated cobalt species promoted C-H functionalization

Part 3: Benchmark studies for different functionals

Table S1. Method testing for the key stereoselectivity-determining states

	M06-L	M06-2X	B3LYP	B3PW91	Cam-B3LYP	ω B97X-D
7-ts-r	4.1	5.0	3.6	3.3	3.1	4.9
7-ts-s	0.0	0.0	0.0	0.0	0.0	0.0
9-ts-r	3.3	2.8	3.3	3.1	3.2	1.6
9-ts-s	0.0	0.0	0.0	0.0	0.0	0.0

Part 4: Testing for temperature

Table S2. Testing for temperature

	M06-L/6-31G(d, p)(sdd for Co)//IEF-PCM(^t BuOH)	
	T=298 K	T= 323 K
Co^{III}-Saloxs + 1a	0.0	0.0
4	14.7	16.7
5-ts	15.7	17.5

Part 5: Energy information for all the stationary points

Table S3. Energy information of all the stationary points

	Gibbs Free Energies (a.u.)	Thermal Correction to Free Energy (a.u.)	Imaginary frequency (cm ⁻¹)
Co(OAc)₃	-831.279739	0.11412	/
Co^{III}-Saloxs	-1386.608961	0.293526	/
AcOH	-229.037636	0.035119	/
Salox	-784.358228	0.206181	/
AcO	-228.553594	0.022639	/
R1	-1336.237462	0.280011	/
R2	-308.28335	0.078739	/
M1	-2722.821904	0.602274	/
TS1	-2722.820813	0.600728	1002.55 <i>i</i>
M2	-2493.807857	0.546544	/
TS2R	-2493.775006	0.540338	1426.56 <i>i</i>
TS2S	-2493.781018	0.539177	1331.78 <i>i</i>
M3R	-2264.744853	0.484194	/
M3S	-2264.749173	0.482001	/
TS3R	-2573.011849	0.590435	259.11 <i>i</i>
TS3S	-2573.016157	0.586436	251.76 <i>i</i>
M4R	-2573.058303	0.591627	/
M4S	-2573.062318	0.59049	/
TS3S-Regio	-2573.009351	0.586692	357.66 <i>i</i>
M4S-Regio	-2573.062594	0.589662	
TS4R	-2573.032052	0.592285	398.33 <i>i</i>
TS4S	-2573.037688	0.594919	261.33 <i>i</i>
PR	-1643.374893	0.367207	/
PS	-1643.378225	0.368658	/
Co^I-Saloxs	-929.620407	0.195907	/

Co(OAc)₂	-602.829864	0.066847	/
Co^{II}-Saloxs	-1158.166679	0.23927	/
NaOAc	-390.826284	0.020474	/
NaOPiv	-508.677292	0.101059	/
PivOH	-346.886243	0.116782	/
4-OPiv-1	-2840.672987	0.685387	/
4-OPiv-2	-2840.668418	0.686792	/
4-OPiv-3	-2,958.523159	0.763168	/
5-ts-OPiv-1	-2840.672763	0.682253	1013.14 <i>i</i>
5-ts-OPiv-2	-2840.669779	0.682759	1007.78 <i>i</i>
5-ts-OPiv-3	-2958.524594	0.762075	1069.95 <i>i</i>
6-OPiv	-2611.660325	0.627435	/
7-ts-s-OPiv	-2611.635751	0.617775	1429.24 <i>i</i>
7-ts-r-OPiv	-2611.626694	0.620108	1314.92 <i>i</i>

Part 6: Cartesian coordinates of all the stationary points

Co(OAc)₃

0 1

Co	0.00127500	-0.00127900	0.00930700
O	1.70309300	0.29077100	-0.87505900
C	2.24722500	-0.46311300	0.00341600
O	1.45359100	-0.93002300	0.89193700
O	0.08522900	1.72095900	0.88676200
C	-0.72106200	2.17411400	0.00269500
O	-1.10789800	1.32523800	-0.87287300
O	-1.53428500	-0.78584200	0.89213400
C	-1.52685800	-1.70971200	0.00675000
O	-0.59795800	-1.62258600	-0.86862400
C	3.68933100	-0.79872800	-0.02298300
H	4.06569400	-0.94647300	0.98936900
H	3.82505400	-1.73522700	-0.57122200
H	4.25576600	-0.01984800	-0.53262000
C	-1.15154900	3.59072100	-0.02047600
H	-2.15867600	3.67888100	-0.42762600
H	-1.10295500	4.02166400	0.97928400
H	-0.47589900	4.15615000	-0.66819800
C	-2.54211600	-2.78716400	-0.02333000
H	-3.37352500	-2.47254400	-0.66025600
H	-2.12044500	-3.69855300	-0.44705500
H	-2.93342400	-2.97437300	0.97640000

Co-Saloxs

0 1

Co	-0.45800600	1.15940800	0.11905900
O	1.29130000	1.94889500	-0.33568500
C	1.67865300	1.66702100	0.85017600
O	0.82381300	1.07620000	1.59349500
O	-1.17395300	2.97290100	0.42807400
C	-1.72678900	2.89453100	-0.71738100
O	-1.54092700	1.80267000	-1.36134800
C	3.04193300	1.98715800	1.33694000
H	2.98245800	2.59429900	2.24275100
H	3.55205800	1.05423500	1.59774300

H	3.61513200	2.51142800	0.57319000
C	-2.51487900	4.01215400	-1.29398300
H	-3.24034200	3.63959500	-2.01696000
H	-3.01671100	4.57192300	-0.50448700
H	-1.83797600	4.69708500	-1.81217600
C	-3.80317000	-0.90084100	1.41358700
C	-2.55692300	-0.66396100	0.78103200
C	-2.03974100	-1.70426200	-0.04666600
C	-2.76753100	-2.89824700	-0.22696400
C	-3.98083800	-3.09636300	0.39787000
C	-4.48998300	-2.08288700	1.22600900
H	-4.19956700	-0.11437000	2.04847200
H	-2.34588200	-3.66416200	-0.87038800
H	-4.53189300	-4.01928800	0.25153000
H	-5.44580300	-2.22316700	1.72485900
O	-1.96937400	0.48120600	1.00778900
C	-0.76706500	-1.55464400	-0.68927500
O	-0.32146300	-2.56924900	-1.44495300
C	1.25438000	-0.80155900	-1.39514400
C	0.87590800	-2.10980400	-2.11547000
H	1.63001100	-2.89217300	-2.02308900
N	0.03437300	-0.52825500	-0.61847300
H	0.62822200	-1.95933400	-3.16916400
H	1.40267700	0.00779100	-2.11735800
C	2.49610900	-0.93094900	-0.54587900
C	2.46723500	-1.59066000	0.68554200
C	3.71405200	-0.45220700	-1.03406100
C	3.64009300	-1.77160800	1.41328700
H	1.51962800	-1.94904300	1.08150000
C	4.88973900	-0.64139300	-0.31252800
H	3.73587700	0.07607500	-1.98546400
C	4.85489700	-1.30255400	0.91350300
H	3.60628600	-2.28085200	2.37229100
H	5.83037200	-0.26381500	-0.70280100
H	5.76936100	-1.44698300	1.48171200

AcOH

01

C	-0.09140900	0.12275400	0.00019700
O	-0.65052300	1.20027000	-0.00005400
O	-0.76508900	-1.04831200	-0.00003500
H	-1.70881200	-0.82600400	-0.00006500
C	1.38573100	-0.10175700	-0.00005300
H	1.67883500	-0.68259200	0.87737200

H	1.67841400	-0.68453900	-0.87630900
H	1.91053200	0.85148900	-0.00115800

Salox

0 1

C	3.87272100	-1.45572900	-0.28416700
C	2.56817800	-1.00556200	-0.52176600
C	2.16356100	0.24559800	0.00813100
C	3.07587900	1.00300800	0.75881600
C	4.36267200	0.54654400	0.98880400
C	4.75431000	-0.68841100	0.46130300
H	4.16810300	-2.41526800	-0.69690500
H	2.74949100	1.95863500	1.15682900
H	5.05833300	1.14142900	1.57124800
H	5.76176400	-1.05680200	0.63425400
O	1.75347900	-1.78590200	-1.24730800
C	0.81489700	0.72243300	-0.23252800
O	0.47237500	1.92020700	0.29012500
C	-1.30194100	0.88602800	-0.90231100
C	-0.89824800	2.15475400	-0.10797200
H	-1.49033000	2.30054200	0.79941500
N	-0.07818200	0.08091900	-0.90948100
H	-0.92304200	3.06830000	-0.70595200
H	-1.55860900	1.15106100	-1.93565400
C	-2.47255300	0.15195400	-0.29345700
C	-2.30149900	-0.63477200	0.84882800
C	-3.75180100	0.29511300	-0.83292300
C	-3.39155400	-1.26429100	1.44136400
H	-1.30369100	-0.75819500	1.26479500
C	-4.84553000	-0.33069300	-0.23906600
H	-3.88974900	0.90242100	-1.72555200
C	-4.66738600	-1.11199600	0.89983600
H	-3.24601100	-1.87717100	2.32671600
H	-5.83580200	-0.21165700	-0.66956900
H	-5.51795500	-1.60415100	1.36281300
H	0.87769900	-1.32387000	-1.31597800

AcO

-1 1

C	0.20111600	0.00045100	-0.00101700
O	0.81515400	-1.09804200	0.00025700
O	0.69406600	1.16011000	0.00025100
C	-1.34332400	-0.05825400	0.00009600
H	-1.74305200	0.46492400	0.87665600

H	-1.74476000	0.46695500	-0.87450700
H	-1.73269700	-1.08160700	-0.00068700
1a			
0 1			
O	-1.29648700	0.28642000	-2.37781300
P	-1.14650800	0.04168900	-0.90619700
C	-1.50701700	1.53099400	0.05702500
C	-0.99124200	1.72850600	1.34330400
C	-2.35537400	2.49335700	-0.50198000
C	-1.32034400	2.87506900	2.05897000
H	-0.31826500	0.99051000	1.77339600
C	-2.68744000	3.63673600	0.21885700
H	-2.74089300	2.34130500	-1.50680000
C	-2.17033700	3.82743700	1.49858300
H	-0.91028400	3.02846900	3.05282700
H	-3.34600500	4.38074300	-0.21966400
H	-2.42667100	4.72161900	2.05942200
C	-2.19883100	-1.29365200	-0.29354800
C	-3.15155600	-1.82762200	-1.16606500
C	-2.10891100	-1.77780500	1.01754100
C	-4.00136800	-2.84224000	-0.73424900
H	-3.21114900	-1.44539900	-2.18167400
C	-2.95797700	-2.79335600	1.44445300
H	-1.37408400	-1.36210600	1.70371600
C	-3.90405200	-3.32477900	0.56873900
H	-4.73729100	-3.25829700	-1.41578800
H	-2.88256800	-3.16998500	2.46023000
H	-4.56695800	-4.11688700	0.90499300
N	0.35724600	-0.46881800	-0.32318100
H	0.47924600	-1.44818200	-0.07841000
C	1.57286000	0.19515700	-0.44338200
C	2.73743300	-0.52699500	-0.02876700
C	1.71339300	1.48816500	-0.91946200
C	4.01575600	0.10175100	-0.09827200
C	2.98351800	2.09375500	-0.97908900
H	0.84142900	2.04116900	-1.25645000
C	3.62717200	-2.47562700	0.79400700
C	5.12547300	-0.66498100	0.32627400
C	4.11911400	1.42856000	-0.57801500
H	3.05556700	3.10946700	-1.35707900
C	4.93574000	-1.95041900	0.77304500
H	3.45761400	-3.49419300	1.14081800
H	6.11894900	-0.22410600	0.29048000

H	5.09574100	1.90181500	-0.62909100
H	5.76942600	-2.56144500	1.10288100
N	2.55841900	-1.80021900	0.41229700

2a

0 1

C	0.59300700	-0.00001400	0.00000300
C	-0.12000700	1.21153900	0.00000000
C	-0.12001900	-1.21154400	0.00000200
C	-1.50913600	1.20619800	-0.00000100
H	0.42804400	2.14907400	0.00000300
C	-1.50915800	-1.20618600	-0.00000300
H	0.42800100	-2.14909700	0.00000500
C	-2.20775000	0.00000600	-0.00000400
H	-2.04952800	2.14832600	-0.00000100
H	-2.04954300	-2.14831700	-0.00000300
H	-3.29372300	0.00002500	-0.00000600
C	2.01652200	-0.00000600	0.00001200
C	3.22999500	0.00000700	0.00000300
H	4.29601200	-0.00001700	-0.00007400

4

0 1

Co	-0.21732500	0.63117100	-0.80939200
P	-1.20807400	-2.56069200	0.23586600
O	-0.95228600	-3.98989800	-0.14664700
O	-0.12528700	2.50357900	-1.14920900
O	0.92317300	2.09886500	2.85545600
O	-3.31173200	1.87255800	-1.11877000
N	-0.12297500	-1.47732000	-0.64745800
N	1.48451900	0.31409000	-1.72762100
N	0.72860200	0.97913200	0.92182900
C	2.13175000	1.20651100	-2.45945400
H	1.61491700	2.14857800	-2.61677000
C	3.42052300	0.95973000	-2.95929500
H	3.91128400	1.72099400	-3.55481500
C	4.05391300	-0.21949700	-2.63966800
H	5.07129600	-0.41386300	-2.96894500
C	3.38314900	-1.19185900	-1.86547700
C	2.05436800	-0.89363200	-1.46023500
C	1.27575400	-1.83934900	-0.74673900
C	1.87021200	-3.01461500	-0.33539700
H	1.29462400	-3.76272100	0.19649200
C	3.21445100	-3.28383800	-0.67786200

H	3.65447000	-4.21761800	-0.34189600
C	3.94986600	-2.41927500	-1.45287800
H	4.97142900	-2.65236900	-1.73890100
C	-0.95568300	-2.27928600	1.99891000
C	-0.52070500	-3.37905100	2.74976500
H	-0.30871400	-4.31594300	2.24125800
C	-0.38285300	-3.27170300	4.13079800
H	-0.04050800	-4.12571700	4.70734500
C	-0.70590700	-2.07815200	4.77208600
H	-0.61795500	-2.00096200	5.85187400
C	-1.14583300	-0.98315500	4.02895200
H	-1.39664400	-0.04958200	4.52711900
C	-1.25697800	-1.07128300	2.64430000
H	-1.57324900	-0.21198400	2.05572100
C	-2.85855700	-2.01644800	-0.24390700
C	-3.82937400	-1.67252800	0.70200500
H	-3.57304200	-1.62043900	1.75618100
C	-5.13153900	-1.39307100	0.29942300
H	-5.87466100	-1.11785400	1.04254000
C	-5.47889700	-1.46357500	-1.04699600
H	-6.49562400	-1.24287000	-1.35877700
C	-4.52162800	-1.82558100	-1.99264600
H	-4.78985500	-1.89281000	-3.04302600
C	-3.21960800	-2.11097400	-1.59512400
H	-2.48430300	-2.40585600	-2.33958000
C	-0.51634000	3.36643000	-0.24574700
C	-1.13178300	4.56814000	-0.66622600
H	-1.29355200	4.70495200	-1.73104900
C	-1.53304600	5.52340400	0.24902300
H	-2.01690700	6.42888200	-0.10910400
C	-1.34433600	5.33496800	1.62624000
H	-1.67545400	6.08582200	2.33599100
C	-0.72982200	4.17743000	2.06595400
H	-0.56135200	4.01026600	3.12583000
C	-0.31286200	3.19153800	1.15420600
C	0.42341800	2.04585900	1.60960600
C	1.71207500	0.20491800	1.69744300
H	1.40952700	-0.84875300	1.73930500
C	1.60352400	0.84569200	3.09190700
H	1.00503200	0.25784100	3.79106200
H	2.57315700	1.07282400	3.53705800
C	3.12476200	0.30422100	1.16895500
C	4.02346700	-0.72386600	1.46165300
H	3.66445000	-1.61659500	1.97167500

C	5.35955000	-0.62278600	1.08748500
H	6.04507200	-1.43664800	1.30804100
C	5.81191000	0.51275700	0.41853700
H	6.85341300	0.59144100	0.11972500
C	4.92121000	1.54461500	0.12967700
H	5.26523100	2.42897800	-0.40023000
C	3.58424100	1.44400200	0.50531100
H	2.88671300	2.24474800	0.26466200
C	-3.73117900	1.69225000	1.22558400
H	-3.40475200	2.64844300	1.65117600
H	-3.57372200	0.92193900	1.98508400
H	-4.79458300	1.76917000	0.99188300
C	-2.92439100	1.44481600	-0.03798600
O	-1.81549500	0.79908300	0.22490800
O	-1.11292600	0.58317800	-2.53349800
C	-1.05834500	-0.33495800	-3.42375800
O	-0.54381000	-1.47022900	-3.27909500
C	-1.73977700	0.00590500	-4.72391200
H	-1.24857000	-0.50242000	-5.55477000
H	-2.77234000	-0.35490800	-4.67815800
H	-1.76834800	1.08150400	-4.89828900
H	-0.42392700	-1.55433500	-1.66961700

5-ts

0 1

Co	-0.19249300	0.62421200	-0.81368600
P	-1.28770100	-2.47858400	0.25556500
O	-1.10254500	-3.91894300	-0.13279600
O	-0.05900300	2.48669400	-1.20831300
O	1.04034100	2.14839300	2.78762900
O	-3.23867600	1.89846900	-1.16901100
N	-0.16802600	-1.45415400	-0.60987700
N	1.49492400	0.23787800	-1.73719800
N	0.77279100	0.98658200	0.88978200
C	2.17376700	1.09016500	-2.48897100
H	1.69142300	2.04671700	-2.66746200
C	3.45183300	0.78233300	-2.98267200
H	3.97155500	1.51061600	-3.59491700
C	4.03814200	-0.41471000	-2.63921000
H	5.04600100	-0.65566800	-2.96736600
C	3.33362100	-1.34343800	-1.84193100
C	2.02014500	-0.98212700	-1.43713100
C	1.20008400	-1.87177000	-0.69185400
C	1.75994600	-3.05668600	-0.24811900

H	1.16377700	-3.76299700	0.31726100
C	3.08620500	-3.39189200	-0.59870100
H	3.49043700	-4.33347700	-0.23944800
C	3.85280500	-2.58263700	-1.40445400
H	4.86120600	-2.86619400	-1.69150600
C	-1.03942700	-2.23368600	2.02904800
C	-0.68887200	-3.36562100	2.77588500
H	-0.54778000	-4.31283800	2.26159200
C	-0.53976000	-3.27544600	4.15712600
H	-0.26050900	-4.15511000	4.72921900
C	-0.76752200	-2.06317100	4.80427600
H	-0.67044900	-1.99690800	5.88407400
C	-1.12342300	-0.93510200	4.06600400
H	-1.30189200	0.01266000	4.56855800
C	-1.24195700	-1.00905700	2.68083200
H	-1.49081000	-0.12533300	2.09600400
C	-2.93830900	-1.89717500	-0.20321700
C	-3.85691800	-1.41017700	0.73216600
H	-3.55686900	-1.25733400	1.76480000
C	-5.16241300	-1.11596900	0.34968000
H	-5.86326500	-0.73416500	1.08659400
C	-5.56637200	-1.30639000	-0.96905300
H	-6.58449700	-1.07200000	-1.26600700
C	-4.66429900	-1.81128400	-1.90261800
H	-4.97696500	-1.97932700	-2.92941700
C	-3.36236300	-2.11984500	-1.52091100
H	-2.67674100	-2.54174000	-2.24930000
C	-0.40131300	3.38848200	-0.32442200
C	-0.98490700	4.59819700	-0.76687500
H	-1.16345400	4.71054400	-1.83192600
C	-1.33393700	5.59248400	0.12789500
H	-1.79345600	6.50394700	-0.24678000
C	-1.12279700	5.43702600	1.50610500
H	-1.41142200	6.21975200	2.19993300
C	-0.54150200	4.27074700	1.96719200
H	-0.35884900	4.12754400	3.02819200
C	-0.17838400	3.24508500	1.07639300
C	0.51969000	2.08393900	1.55085000
C	1.73664700	0.19611200	1.67431700
H	1.40651400	-0.84831600	1.73149600
C	1.64371800	0.86183900	3.05621300
H	0.99789700	0.32006300	3.75099000
H	2.61639600	1.03923200	3.51633200
C	3.14986800	0.25602900	1.14067300

C	4.02729300	-0.78767900	1.44303900
H	3.65065400	-1.66680800	1.96350800
C	5.36349500	-0.72018600	1.06181000
H	6.03211400	-1.54597200	1.28972900
C	5.83752000	0.39691200	0.37692900
H	6.87915400	0.44933700	0.07304100
C	4.96846300	1.44442000	0.07877900
H	5.32933600	2.31466800	-0.46319700
C	3.63137000	1.37729300	0.46127300
H	2.95049600	2.18971500	0.21264200
C	-3.63946100	1.91774400	1.18376600
H	-3.38099600	2.95037800	1.44384400
H	-3.40169500	1.28765100	2.04467600
H	-4.71198000	1.88301500	0.98241400
C	-2.85442500	1.54225000	-0.06115100
O	-1.76840200	0.87386100	0.23642000
O	-1.09620900	0.55651600	-2.55504300
C	-1.12224800	-0.43207500	-3.34351400
O	-0.68877800	-1.59432900	-3.05607400
C	-1.75464800	-0.22828000	-4.68569800
H	-1.24855600	-0.82988800	-5.44179700
H	-2.79254800	-0.57167600	-4.63164000
H	-1.75747400	0.82274900	-4.97082500
H	-0.47169200	-1.56516000	-1.77720400

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Co	-0.02093100	-0.30738700	-0.98675400
P	1.29645800	1.78372600	1.18323700
O	0.92066900	2.93323100	2.08569600
O	-0.17266300	-1.81285600	-2.17701500
O	-0.57732600	-3.27957700	1.72021100
O	0.86923600	0.64072400	-2.47339600
N	0.06516700	1.33358300	0.12443900
N	-1.78009000	0.29969500	-1.42224800
N	-0.57916000	-1.41213600	0.49341000
C	-2.67157900	-0.35529600	-2.15065400
H	-2.41720900	-1.37956300	-2.40257300
C	-3.85868200	0.26311300	-2.57321300
H	-4.56778100	-0.30301200	-3.16675300
C	-4.09527000	1.57391100	-2.22827000
H	-5.00444600	2.07589600	-2.55017400
C	-3.15879000	2.28912300	-1.44716800
C	-1.98448700	1.59166600	-1.04669900

C	-0.97268200	2.18234300	-0.22497800
C	-1.16989000	3.52331900	0.12350100
H	-0.43436700	4.02257600	0.74085900
C	-2.32475600	4.21430200	-0.28165700
H	-2.42941300	5.25190400	0.02597100
C	-3.31721200	3.63118000	-1.04214500
H	-4.20372300	4.18187100	-1.34123000
C	1.75811200	0.36776600	2.24113100
C	1.34312700	0.47726800	3.57792700
H	0.79993100	1.36808000	3.88228200
C	1.62135600	-0.53073100	4.49590100
H	1.28940100	-0.43026900	5.52559600
C	2.32962300	-1.66293000	4.09445600
H	2.54662000	-2.45223500	4.80887100
C	2.76345900	-1.77288500	2.77582100
H	3.32489300	-2.64749700	2.45823900
C	2.48786700	-0.76378100	1.85449200
H	2.84155300	-0.85990900	0.83478300
C	2.73849400	2.20318400	0.16599000
C	4.04781700	1.88546000	0.54375700
H	4.22390700	1.26768800	1.42111300
C	5.12920000	2.35891600	-0.19699100
H	6.14141400	2.09924800	0.09986200
C	4.91367000	3.16931700	-1.30960800
H	5.75804000	3.54163100	-1.88283100
C	3.61278900	3.49854100	-1.68853100
H	3.44019900	4.12599000	-2.55855100
C	2.53178900	3.01353500	-0.95987000
H	1.51588000	3.25507700	-1.26706500
C	0.26762500	-2.99556300	-1.83165300
C	0.72430800	-3.87609400	-2.84144300
H	0.70788900	-3.51745600	-3.86656100
C	1.18795800	-5.14164600	-2.53466100
H	1.54530700	-5.78323300	-3.33664600
C	1.21603800	-5.60420000	-1.21046200
H	1.59188300	-6.59553500	-0.97989700
C	0.75231300	-4.77798100	-0.20489300
H	0.74847400	-5.11301700	0.82836100
C	0.27690400	-3.48538700	-0.49103800
C	-0.28603000	-2.68002300	0.55748900
C	-1.22623100	-0.99314100	1.74940000
H	-0.63973200	-0.18107200	2.18189100
C	-1.09120700	-2.25997700	2.61276000
H	-0.37166400	-2.13715800	3.42732100

H	-2.04211300	-2.62008700	3.01039100
C	-2.63645500	-0.49233800	1.57786200
C	-2.97020500	0.77659500	2.05360700
H	-2.19160700	1.39652200	2.49809100
C	-4.27277300	1.25619200	1.93926200
H	-4.51747100	2.25054000	2.30301100
C	-5.25284900	0.46615800	1.34443300
H	-6.26902200	0.83862900	1.24831000
C	-4.92754300	-0.80351400	0.86657700
H	-5.68927200	-1.41992600	0.39669500
C	-3.62635500	-1.28126900	0.98515100
H	-3.37064100	-2.26957500	0.60370800
C	3.23256400	0.28992700	-2.87019500
H	3.50519600	-0.66056500	-3.33761800
H	4.03932000	0.56515900	-2.18502900
H	3.12418700	1.05223200	-3.64099900
C	1.97048800	0.11503200	-2.10952900
O	1.93585800	-0.60001500	-1.04924600

7-ts-r

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Co	0.84738800	-0.23086400	0.73913700
P	-1.86071700	-1.64582100	0.75192500
O	-2.15167500	-2.12175800	2.15248000
O	2.72008200	-0.27867800	1.14656500
O	2.32427800	0.11078400	-3.06403500
O	0.56405100	-0.35313100	2.68010600
N	-1.10859100	-0.15792500	0.56822800
N	0.66406600	1.70130700	1.04573700
N	1.18484400	0.06355800	-1.14314900
C	1.63366900	2.59457300	1.15464500
H	2.64508200	2.23088100	0.99795600
C	1.36124600	3.93623300	1.47226900
H	2.18281500	4.63996600	1.54695700
C	0.06075300	4.32711300	1.69841400
H	-0.16934800	5.35684600	1.96018300
C	-0.99280200	3.38990600	1.59372100
C	-0.63500300	2.06247600	1.23416100
C	-1.60748400	1.03406600	1.05011200
C	-2.93518800	1.36073100	1.31954900
H	-3.71136900	0.60844200	1.21336700
C	-3.28843000	2.66925600	1.69642600
H	-4.33691300	2.88412100	1.88578100
C	-2.35704600	3.67968100	1.82178800

H	-2.65077800	4.68697000	2.10123700
C	-3.38463000	-1.66488400	-0.23803900
C	-4.60134000	-1.87319900	0.42095500
H	-4.59151200	-2.03637800	1.49572300
C	-5.79831800	-1.86719200	-0.29001000
H	-6.73830200	-2.02544800	0.23106600
C	-5.79003900	-1.66322400	-1.66827600
H	-6.72360800	-1.66074800	-2.22368600
C	-4.58252400	-1.46799900	-2.33693200
H	-4.57157500	-1.31813600	-3.41269500
C	-3.38762000	-1.46743400	-1.62392800
H	-2.44587500	-1.33070300	-2.15277800
C	-0.60876600	-2.59346200	-0.14556400
C	-0.88969600	-3.54796300	-1.12230800
H	-1.92031500	-3.78195100	-1.38027400
C	0.15575000	-4.19119300	-1.78469500
H	-0.06372900	-4.92951000	-2.55083300
C	1.48024900	-3.89111400	-1.46432900
H	2.29092800	-4.39949400	-1.97886700
C	1.75975800	-2.94807500	-0.48054700
H	2.79418400	-2.73284300	-0.21908700
C	0.72818300	-2.27919800	0.19983100
H	1.02135400	-2.24515500	1.47354800
C	3.73159800	-0.26906600	0.32405500
C	5.03486300	-0.40225900	0.86903200
H	5.11691400	-0.50190100	1.94714500
C	6.15531400	-0.41640900	0.06339700
H	7.13521500	-0.52664200	0.52148600
C	6.04789700	-0.29826600	-1.33205600
H	6.93354700	-0.31421500	-1.95806600
C	4.79507700	-0.16404600	-1.89384400
H	4.68100400	-0.07464500	-2.96972200
C	3.63310600	-0.13905500	-1.09504000
C	2.35064400	0.00931800	-1.72100500
C	0.15363100	0.30427300	-2.16695200
H	-0.65066400	-0.42429600	-2.02472300
C	0.93342300	0.02332300	-3.45640100
H	0.75963000	-0.98635300	-3.84228600
H	0.76249500	0.75505400	-4.24658200
C	-0.42183800	1.69774100	-2.08501000
C	-1.80186300	1.88595600	-2.01341000
H	-2.45509600	1.01589700	-1.97289900
C	-2.34151000	3.16816600	-1.95184700
H	-3.41798000	3.29709300	-1.87871300

C	-1.50137000	4.27781800	-1.95961400
H	-1.91907100	5.27897700	-1.89751300
C	-0.12007500	4.09972600	-2.03412500
H	0.54154100	4.96171300	-2.03291700
C	0.41608300	2.81747700	-2.09883300
H	1.49643800	2.68483900	-2.14395600
C	0.61126800	-1.43669900	4.78611400
H	-0.41744400	-1.75647100	4.97701600
H	0.74130000	-0.44130900	5.20974800
H	1.28032700	-2.14888500	5.26892800
C	0.82246600	-1.42480500	3.30477600
O	1.20991900	-2.49314400	2.74054500

7-ts-s

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Co	-0.33691300	-0.45491200	-0.62835900
P	2.08066600	-0.33178500	1.35616800
O	2.34930300	0.35205700	2.67329900
O	-1.67404700	-1.34261400	-1.66735400
O	-3.36444500	-0.44499400	2.12840000
O	0.78895300	-0.61984600	-2.24953300
N	1.15919100	0.45274300	0.21465800
N	-0.70028200	1.34233400	-1.36854900
N	-1.55014000	-0.16076600	0.85532000
C	-1.72960100	1.71808700	-2.10921900
H	-2.50493200	0.97523600	-2.27246300
C	-1.80172200	3.00813700	-2.66278200
H	-2.66365700	3.27948100	-3.26190000
C	-0.77516100	3.89862400	-2.44174300
H	-0.80980800	4.89844600	-2.86765000
C	0.33665300	3.52292000	-1.65262300
C	0.32220600	2.20642600	-1.11777100
C	1.36396200	1.71880800	-0.27214600
C	2.43471000	2.57334200	-0.01471500
H	3.24691900	2.24383300	0.62793600
C	2.45666400	3.86989500	-0.55892800
H	3.30635100	4.50824600	-0.33124600
C	1.43963100	4.35598600	-1.35604600
H	1.47211600	5.36377500	-1.75913300
C	1.02867600	-1.79564400	1.53727600
C	0.93279200	-2.42770200	2.77635200
H	1.54867400	-2.08210800	3.60435600
C	0.02243700	-3.46907000	2.95599000
H	-0.05862900	-3.95638800	3.92371200

C	-0.78965800	-3.87926100	1.89793200
H	-1.49672000	-4.69217200	2.04054400
C	-0.70156600	-3.23838700	0.66612500
H	-1.33901900	-3.55685300	-0.15700100
C	0.20359900	-2.18302800	0.45671900
H	0.73856900	-2.35628200	-0.74152500
C	3.63547200	-0.84060400	0.56985400
C	4.60054600	-1.49831800	1.34411200
H	4.41002000	-1.67892800	2.40002200
C	5.79720400	-1.91573400	0.77142800
H	6.53801000	-2.42990900	1.37731000
C	6.04662800	-1.66990500	-0.57841100
H	6.98268200	-1.99388400	-1.02458300
C	5.09789700	-1.00639300	-1.35309500
H	5.29506400	-0.80590700	-2.40287700
C	3.89485800	-0.59645500	-0.78341300
H	3.15109400	-0.07641200	-1.38366200
C	-2.87494000	-1.69784900	-1.30497400
C	-3.66457700	-2.41537600	-2.24053000
H	-3.22408400	-2.61827100	-3.21230600
C	-4.93678500	-2.84841200	-1.92833900
H	-5.50634000	-3.39930400	-2.67306500
C	-5.50035400	-2.59411000	-0.66721000
H	-6.49976600	-2.94198700	-0.42794400
C	-4.76198700	-1.89188100	0.26225000
H	-5.17352400	-1.67889500	1.24399100
C	-3.46197100	-1.42920800	-0.03144100
C	-2.74401600	-0.67476700	0.95620000
C	-1.26568800	0.62463000	2.07409300
H	-0.28415800	0.35135700	2.47304200
C	-2.37572900	0.13588400	3.00997600
H	-2.03170100	-0.65259200	3.68805500
H	-2.85985300	0.92935700	3.57981500
C	-1.27699600	2.11051900	1.81611900
C	-0.21980400	2.89697400	2.27579000
H	0.62285400	2.40978000	2.76519200
C	-0.22774800	4.27524000	2.07458800
H	0.60784800	4.87676700	2.42262700
C	-1.29215800	4.87686400	1.40809900
H	-1.29395300	5.95057500	1.24060400
C	-2.34960900	4.09563800	0.94248600
H	-3.17731000	4.55942500	0.41234900
C	-2.34239200	2.71964300	1.14624900
H	-3.16292100	2.11221500	0.76586600

C	2.06001600	-1.79727500	-3.86768200
H	1.35050000	-2.12282400	-4.63339400
H	2.86806700	-2.52737900	-3.82351700
H	2.44318300	-0.81932600	-4.16088500
C	1.34743800	-1.71338300	-2.55343300
O	1.33225000	-2.74447600	-1.81005200
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Co	0.86686600	0.13713100	-0.94814800
C	5.00078200	-0.45125000	-1.15124700
C	3.71116200	-0.29164900	-0.58549100
C	3.62758400	-0.22329800	0.83918300
C	4.79518300	-0.29271200	1.62514700
C	6.03789800	-0.43924900	1.04316900
C	6.12737500	-0.52174200	-0.35614000
H	5.07134300	-0.50760900	-2.23318300
H	4.69513200	-0.23098900	2.70446900
H	6.93059800	-0.49063300	1.65714800
H	7.10032400	-0.63822600	-0.82714300
O	2.67941400	-0.21687800	-1.37716900
C	2.34703800	-0.10439600	1.47334100
O	2.30846100	-0.09778400	2.81658100
C	0.11766900	-0.00842000	1.91820300
C	0.93731400	0.16323600	3.20649400
H	0.67461100	-0.54868100	3.99043500
N	1.17994300	-0.02560600	0.89589300
H	0.89199000	1.18068100	3.60522000
H	-0.51878300	0.86351200	1.74468900
C	-0.74334100	-1.24511300	1.88119800
C	-0.17186400	-2.51784500	1.97428900
C	-2.12976100	-1.12619000	1.78141600
C	-0.97545000	-3.65245300	1.95287500
H	0.91028700	-2.61985700	2.04839800
C	-2.93682200	-2.26166900	1.76507600
H	-2.57634400	-0.13593800	1.70478200
C	-2.36078400	-3.52614500	1.84708200
H	-0.52072300	-4.63776000	2.01147100
H	-4.01447000	-2.15512300	1.67215300
H	-2.98712500	-4.41363100	1.82027300
O	-2.50481000	2.24828900	-2.52981600
P	-1.64767700	1.92837700	-1.33408500
C	-0.10071600	2.81929700	-1.13541400
C	1.05557300	2.05005500	-0.90335300

C	-0.05081100	4.21742600	-1.18740600
C	2.25939600	2.73373500	-0.69457400
C	1.15954000	4.87378600	-0.99408200
H	-0.95996700	4.78695000	-1.37639800
C	2.31062700	4.12694400	-0.74102900
H	3.17725700	2.18285200	-0.50005900
H	1.20734100	5.95822700	-1.03400100
H	3.25949100	4.63454200	-0.58195100
C	-2.58579200	2.20854700	0.20211900
C	-3.94575500	1.87106100	0.24977700
C	-1.98201000	2.72144600	1.35893300
C	-4.66783100	1.99596700	1.43294900
H	-4.44556500	1.52604700	-0.65131000
C	-2.70532700	2.85201400	2.54170300
H	-0.93752800	3.02604600	1.33349700
C	-4.04643800	2.47701200	2.58430500
H	-5.71916300	1.72389700	1.45433700
H	-2.22096000	3.25061300	3.42909500
H	-4.61009100	2.57305100	3.50790000
N	-0.99282000	0.36857300	-1.29237900
C	-1.72779900	-0.78641700	-1.47801300
C	-0.97078500	-1.99505200	-1.39761500
C	-3.08720600	-0.90035900	-1.75971500
C	-1.57473300	-3.27070500	-1.54367200
C	-3.68486200	-2.16656800	-1.90849000
H	-3.68507700	-0.00558100	-1.89660700
C	1.13938800	-2.91635900	-1.11476100
C	-0.72342200	-4.39291500	-1.44319900
C	-2.96587300	-3.33731500	-1.79325200
H	-4.74959700	-2.21102600	-2.12136800
C	0.62745800	-4.21837400	-1.23396600
H	2.19892100	-2.73130700	-0.95401100
H	-1.14624000	-5.39024700	-1.53795600
H	-3.44354600	-4.30622500	-1.90501700
H	1.29958700	-5.06637700	-1.16124200
N	0.36486700	-1.84302400	-1.18982200
8-s			
O 1			
Co	-0.53547100	-0.53432700	-0.67825100
P	2.13257900	-0.98407500	0.82224800
O	2.42931200	-0.49722400	2.21986800
O	-2.02888900	-1.05257100	-1.71730000
O	-3.30712500	-0.22538000	2.22118600

N	-0.58592500	1.38508700	-1.44090400
N	1.22352400	0.01235100	-0.18107600
N	-1.55947200	-0.17751600	0.84282300
C	-1.57452700	2.01541000	-2.05872000
H	-2.48564600	1.44150900	-2.21172200
C	-1.45641900	3.34487000	-2.49659800
H	-2.29333000	3.81903400	-2.99742600
C	-0.27501700	4.02204800	-2.28465500
H	-0.15878600	5.05098200	-2.61706600
C	0.79953700	3.38279200	-1.62674600
C	0.58506500	2.04233600	-1.21134900
C	1.58460000	1.30144200	-0.51315300
C	2.79663400	1.93808600	-0.25422900
H	3.57809400	1.41545300	0.29050400
C	3.01512600	3.25990100	-0.68520100
H	3.97585600	3.71997900	-0.46928500
C	2.05063700	3.98481700	-1.35377300
H	2.23283100	5.00769700	-1.67004700
C	1.08247700	-2.43726800	0.68798200
C	-0.14289000	-2.28651500	0.01160200
C	-0.98079400	-3.40422000	-0.07852900
H	-1.93987100	-3.33123000	-0.58636400
C	-0.59983200	-4.62921800	0.47168300
H	-1.26513200	-5.48549500	0.38590800
C	0.62217100	-4.76536400	1.13100200
H	0.91180700	-5.72195500	1.55685800
C	1.46587400	-3.66570400	1.23825000
H	2.42569600	-3.75892500	1.74540800
C	3.67691500	-1.35823800	-0.05671100
C	3.66262700	-1.87969200	-1.35571500
H	2.71148200	-2.06731400	-1.85103800
C	4.85703100	-2.16169400	-2.01021900
H	4.84063300	-2.56725600	-3.01795800
C	6.07474500	-1.92344100	-1.37234600
H	7.00698200	-2.14428400	-1.88486700
C	6.09647200	-1.40479900	-0.08013200
H	7.04478600	-1.22053100	0.41706800
C	4.90062600	-1.12567300	0.57753900
H	4.90020400	-0.72278900	1.58762400
C	-3.25685800	-1.24717100	-1.32483400
C	-4.20605200	-1.73402400	-2.25772100
H	-3.86300700	-1.92496900	-3.27028500
C	-5.51769600	-1.96489600	-1.89234900
H	-6.21516500	-2.34336600	-2.63551600

C	-5.96020100	-1.72656400	-0.58124800
H	-6.99202700	-1.91500600	-0.30436800
C	-5.06097900	-1.24857700	0.34997300
H	-5.37606400	-1.05266400	1.37037800
C	-3.71772800	-0.99784400	0.00450700
C	-2.82023400	-0.47477100	0.99315900
C	-2.17625600	0.11459800	3.06363300
H	-1.96667200	-0.74938800	3.69961300
H	-2.46698400	0.96541800	3.68045500
C	-1.03424100	0.42178600	2.08384300
H	-0.11236200	-0.09595000	2.37329200
C	-0.74359400	1.89292200	1.91667200
C	-1.71066700	2.75446100	1.38800600
H	-2.66762800	2.35493500	1.05418100
C	-1.45021900	4.11516100	1.26866900
H	-2.20366600	4.77596000	0.84808500
C	-0.21990600	4.62856500	1.67982800
H	-0.01326500	5.69090200	1.58051200
C	0.74705700	3.77474100	2.20329000
H	1.71393100	4.16737800	2.50709000
C	0.48718000	2.41082200	2.31978400
H	1.24908300	1.72726800	2.69092100

9-ts-r

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Co	-0.91379800	0.17939200	-0.69990100
C	-5.10932400	0.63482700	-0.55158200
C	-3.81861300	0.16250300	-0.19321700
C	-3.76213500	-0.86510400	0.79849800
C	-4.94976400	-1.38378600	1.35307200
C	-6.18870500	-0.90798400	0.97479800
C	-6.25523700	0.11493000	0.01552200
H	-5.16176400	1.41901000	-1.30143700
H	-4.86672700	-2.17093600	2.09627000
H	-7.09382200	-1.31649600	1.41195900
H	-7.22281300	0.50256600	-0.29490800
O	-2.78914800	0.69060200	-0.79447900
C	-2.49478000	-1.36499900	1.25483900
O	-2.51218900	-2.32598700	2.20478100
C	-0.30802900	-1.68566600	1.67953400
C	-1.14793600	-2.78742800	2.33746600
H	-0.94370000	-2.93269200	3.39920200
N	-1.31361100	-0.98102700	0.87436400
H	-1.06666200	-3.74597100	1.81249500

H	0.44171600	-2.11069600	1.00740500
C	0.39577800	-0.77365700	2.65568300
C	-0.32315200	0.10945100	3.46722600
C	1.78578800	-0.82387800	2.77219300
C	0.33931500	0.92848400	4.37591700
H	-1.40637400	0.16996900	3.37242700
C	2.45059800	-0.00446600	3.68037200
H	2.34942000	-1.49395100	2.12287000
C	1.72848600	0.87420700	4.48364700
H	-0.22862600	1.61956300	4.99343600
H	3.53451400	-0.04148500	3.74846200
H	2.24627700	1.52324600	5.18473000
O	2.46130900	-0.56872900	-2.84113800
P	1.73228600	-1.16369700	-1.66101100
C	0.23704100	-2.11595100	-1.99253700
C	-0.99807900	-1.45650800	-1.82347600
C	0.26875000	-3.45046100	-2.41343700
C	-2.18431800	-2.16665600	-2.06335600
C	-0.91379100	-4.14465300	-2.64250500
H	1.22754700	-3.95001500	-2.54171800
C	-2.13929800	-3.49894300	-2.45540300
H	-3.14275200	-1.66432000	-1.95597000
H	-0.88506300	-5.18159500	-2.96297300
H	-3.06729200	-4.03833600	-2.62790300
C	2.86795500	-2.28195500	-0.77108400
C	4.24167700	-2.01633600	-0.84166100
C	2.43736500	-3.37592600	-0.00758700
C	5.15562400	-2.79094000	-0.13377000
H	4.58842200	-1.20266400	-1.47427900
C	3.35133300	-4.15930000	0.69201800
H	1.38230800	-3.63671000	0.02291500
C	4.71092600	-3.85972100	0.64134200
H	6.21645300	-2.56493300	-0.19418400
H	3.00080000	-5.00676000	1.27421900
H	5.42306700	-4.46677400	1.19307600
N	1.03274800	-0.09260600	-0.57946800
C	1.69078400	0.94795700	0.03376100
C	0.84284100	1.89333900	0.68661600
C	3.06528900	1.17264400	0.10054000
C	1.36381300	2.98596700	1.43130300
C	3.57966700	2.25797200	0.83088900
H	3.74874700	0.50124300	-0.40885700
C	-1.35491500	2.51207300	1.12934900
C	0.42208400	3.83586600	2.05617700

C	2.76577700	3.15060800	1.49841200
H	4.65825900	2.38908700	0.86611900
C	-0.92608600	3.59372300	1.91700000
H	-2.40637900	2.30221400	0.95353700
H	0.77568600	4.67934200	2.64440900
H	3.18116400	3.97921600	2.06444300
H	-1.66484000	4.23160600	2.39029300
N	-0.49562500	1.69801300	0.53561800
C	0.06573600	2.65744000	-2.30007000
C	-0.67399900	3.79085600	-1.92343900
C	1.42447900	2.79473900	-2.63573900
C	-0.06843600	5.04082800	-1.90564700
H	-1.71976600	3.67569900	-1.65012000
C	2.01914800	4.05074400	-2.60734300
H	1.99261800	1.90182200	-2.88954200
C	1.27840900	5.17506900	-2.24472500
H	-0.64857000	5.91389800	-1.62066900
H	3.07099100	4.15031100	-2.86139000
H	1.74928400	6.15380200	-2.22269000
C	-0.52605400	1.35591800	-2.30426500
C	-0.97765100	0.28152600	-2.79523600
H	-1.42840600	-0.15826500	-3.66662000

9-ts-s

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Co	-0.51078000	-0.26399000	-0.64793600
C	-4.29698300	-0.06439500	-2.49933400
C	-3.33669500	-0.31354600	-1.48331200
C	-3.81515300	-0.89586600	-0.27102000
C	-5.18067900	-1.21643200	-0.12921200
C	-6.08801800	-0.96580500	-1.13872700
C	-5.62959500	-0.38085200	-2.32982800
H	-3.93843200	0.38017300	-3.42383300
H	-5.50830400	-1.66422500	0.80396000
H	-7.13632200	-1.21588300	-1.01236300
H	-6.33050200	-0.17704700	-3.13607000
O	-2.09656700	-0.00078300	-1.73222000
C	-2.91657600	-1.14248200	0.82385400
O	-3.44614900	-1.69695600	1.93632500
C	-1.16910000	-1.18845000	2.24466900
C	-2.33000200	-2.02409300	2.79454500
H	-2.61067500	-1.78139000	3.82024700
N	-1.64703200	-0.87146300	0.88729000
H	-2.14655600	-3.10043000	2.70634100

H	-0.25830700	-1.79347300	2.18548000
C	-0.87267300	0.05969200	3.04042900
C	-1.79528300	1.10873600	3.10737500
C	0.33106300	0.16432400	3.73892300
C	-1.51730300	2.24370600	3.86241300
H	-2.72892300	1.04474800	2.54966700
C	0.60774900	1.29900500	4.49818600
H	1.06194300	-0.63757300	3.64521700
C	-0.31460100	2.33992900	4.56239300
H	-2.23552800	3.05900000	3.89742500
H	1.55521600	1.37766300	5.02548400
H	-0.09299200	3.23020700	5.14490500
O	2.15972400	-2.19721500	2.07917300
P	1.93201100	-1.74419200	0.65636100
C	3.52988800	-1.74529100	-0.20981400
C	4.52527800	-2.62594600	0.23289100
C	3.80215000	-0.89704400	-1.28882000
C	5.76435600	-2.66393100	-0.39924700
H	4.32182700	-3.26841200	1.08585500
C	5.04473300	-0.92898200	-1.91544200
H	3.03210300	-0.21107400	-1.63230900
C	6.02556200	-1.81503800	-1.47345600
H	6.52971600	-3.35114400	-0.04949300
H	5.24853000	-0.25969000	-2.74685400
H	6.99514600	-1.84082000	-1.96324600
C	0.76233000	-2.79282600	-0.23237200
C	-0.23778600	-2.19882800	-1.02428100
C	0.75766100	-4.17596500	-0.01995900
C	-1.21543600	-3.01042900	-1.61371800
C	-0.22049300	-4.97379000	-0.60229500
H	1.51614900	-4.61840800	0.62394000
C	-1.20794500	-4.38418300	-1.39625200
H	-1.97906700	-2.56045800	-2.24353800
H	-0.22043500	-6.04713800	-0.43713900
H	-1.97949500	-5.00225200	-1.84856200
N	1.15789300	-0.29911900	0.37637000
C	1.55538900	0.92965900	0.83987300
C	0.59270900	1.97019800	0.66916800
C	2.76447900	1.26422500	1.44979000
C	0.82702500	3.29442000	1.12772200
C	3.00110100	2.57986000	1.88582500
H	3.52435300	0.50232100	1.60177100
C	-1.49961500	2.52685600	-0.18038000
C	-0.20820100	4.23323700	0.91399100

C	2.06499200	3.58514500	1.74422100
H	3.95558300	2.80214800	2.35636200
C	-1.36424700	3.85138600	0.27158300
H	-2.37463000	2.18957600	-0.72951800
H	-0.07564600	5.25737400	1.25478100
H	2.26346000	4.59347900	2.09554700
H	-2.16773100	4.55758700	0.09240000
N	-0.55411800	1.62234100	0.01980700
C	0.67389200	1.72684000	-2.68905100
C	1.82152400	2.44267400	-2.30880000
C	-0.33075500	2.37973200	-3.42528500
C	1.96468800	3.77598000	-2.67434800
H	2.58767700	1.95206100	-1.71236400
C	-0.17399700	3.71130100	-3.78876500
H	-1.22792500	1.82805400	-3.69061100
C	0.97046700	4.41452700	-3.41397600
H	2.85501100	4.32007300	-2.37201800
H	-0.95366500	4.20533500	-4.36150500
H	1.08610800	5.45710800	-3.69561700
C	0.48415400	0.36233300	-2.29751200
C	0.48875700	-0.89487200	-2.40532800
H	0.77707800	-1.72789400	-3.01989700

10-r

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Co	-0.47718000	-0.69895500	0.29931400
C	-3.94854100	-2.98986700	-0.04310100
C	-3.01599100	-1.96893700	-0.36533100
C	-3.50294200	-0.88160300	-1.15607200
C	-4.85413200	-0.84064500	-1.55229000
C	-5.73969100	-1.83967800	-1.20013800
C	-5.26850600	-2.92263600	-0.44183100
H	-3.58504100	-3.82178300	0.55397400
H	-5.18980400	0.00642100	-2.14298100
H	-6.77922500	-1.78926700	-1.50703600
H	-5.95088500	-3.71982100	-0.15543200
O	-1.79538300	-2.09998100	0.07699800
C	-2.62016800	0.18017200	-1.55781900
O	-3.10645700	1.10060500	-2.41592700
C	-0.84147500	1.51957700	-1.87420600
C	-2.07501400	2.09697000	-2.59630800
H	-1.92916500	2.23847300	-3.66931400
N	-1.38698000	0.34829000	-1.18541200
H	-2.43086400	3.03194700	-2.15309600

H	-0.47069400	2.22811800	-1.12074400
C	0.30908700	1.15983600	-2.78671000
C	0.35886000	-0.07377200	-3.44093600
C	1.33201600	2.08373600	-3.01423300
C	1.42840800	-0.38967700	-4.27477200
H	-0.43182400	-0.80126800	-3.26921500
C	2.40793000	1.76730300	-3.83959100
H	1.28187900	3.06180300	-2.54053500
C	2.46235500	0.52466000	-4.46637800
H	1.46088100	-1.35970000	-4.76427900
H	3.20370600	2.49129900	-3.99081500
H	3.30418200	0.27130500	-5.10464500
O	1.22525000	1.37633600	3.21993900
P	0.52503200	1.59572900	1.90572700
C	-1.27580600	1.24783300	1.90198300
C	-1.75730100	0.01794300	2.42730600
C	-2.19235800	2.18607700	1.39545500
C	-3.14620300	-0.20421900	2.45635400
C	-3.55478600	1.92806000	1.40581800
H	-1.82664900	3.12488900	0.98595400
C	-4.03290100	0.73085400	1.94770800
H	-3.51240300	-1.14764000	2.85400400
H	-4.24846600	2.65909600	1.00022000
H	-5.09982500	0.52424300	1.95427600
C	0.71771700	3.33080300	1.40516100
C	1.35780200	3.67545100	0.21141500
C	0.29330400	4.34971100	2.26916100
C	1.56509300	5.01239800	-0.12113500
H	1.70538500	2.88697400	-0.45207000
C	0.48780000	5.68466400	1.93086500
H	-0.19417000	4.09476600	3.20810300
C	1.12458600	6.01776500	0.73530700
H	2.07220400	5.26741000	-1.04815300
H	0.14661200	6.46753200	2.60209900
H	1.28091300	7.06092400	0.47566500
N	0.89588000	0.64569100	0.58801200
C	2.12758800	0.22352100	0.15243000
C	2.08341300	-0.98026800	-0.60552800
C	3.36982900	0.82761600	0.33275600
C	3.23817400	-1.54409300	-1.20804800
C	4.51797200	0.26693900	-0.25470500
H	3.44962800	1.73439600	0.92659700
C	0.71275600	-2.70286700	-1.38990000
C	3.05466700	-2.73567800	-1.94768700

C	4.47345600	-0.88397000	-1.01751400
H	5.47161600	0.76453100	-0.09986600
C	1.80228300	-3.30003500	-2.04458100
H	-0.28616800	-3.12577000	-1.40038800
H	3.90986500	-3.19867600	-2.43317500
H	5.37223200	-1.29370900	-1.46820100
H	1.63814700	-4.21329700	-2.60598800
N	0.86037200	-1.58117400	-0.69676700
C	1.16463600	-2.41904300	2.17044300
C	2.34821500	-1.93433800	2.75406300
C	1.14067400	-3.73862900	1.69017000
C	3.47379300	-2.74795500	2.84676700
H	2.36374700	-0.90630200	3.11227100
C	2.26474000	-4.55029400	1.79580100
H	0.22975200	-4.11204300	1.22696100
C	3.43796600	-4.05587000	2.36606400
H	4.38413500	-2.35883300	3.29615600
H	2.22882400	-5.57130800	1.42417300
H	4.31846500	-4.68855900	2.43653700
C	0.04020000	-1.51457600	1.98710400
C	-0.80479000	-1.01923300	2.89544200
H	-0.83906700	-1.33967900	3.94010300

10-s

0 1

Co	0.48841900	-0.27934000	0.36625600
C	3.93885100	-1.26210500	2.54496900
C	3.15887400	-0.86433500	1.42720600
C	3.85507700	-0.64080000	0.19911200
C	5.24936700	-0.83919800	0.13002600
C	5.97529600	-1.23839900	1.23368400
C	5.30270600	-1.44648100	2.44885200
H	3.41327300	-1.42608200	3.48191700
H	5.74593800	-0.66682100	-0.81991100
H	7.04799200	-1.38575600	1.16319900
H	5.86075300	-1.75765500	3.32874400
O	1.87301000	-0.74271000	1.60587100
C	3.14604300	-0.19746400	-0.96886900
O	3.86890300	0.02021400	-2.08721900
C	1.60363400	0.60248900	-2.39954100
C	2.92306800	0.32973900	-3.13681700
H	3.30877200	1.18507500	-3.69421500
N	1.86987300	0.04154800	-1.06476900
H	2.86250700	-0.54103600	-3.79751900

H	0.77701000	0.05670600	-2.86950200
C	1.22330900	2.06001900	-2.30491400
C	1.96485400	2.94543500	-1.51625000
C	0.12146700	2.54031200	-3.01339200
C	1.60966100	4.28853700	-1.43976800
H	2.81437400	2.57648000	-0.94290700
C	-0.23436800	3.88478300	-2.93942100
H	-0.47509600	1.83965400	-3.59593900
C	0.50874200	4.76159500	-2.15331300
H	2.18681600	4.96519400	-0.81497900
H	-1.10502700	4.24329500	-3.48234100
H	0.22466000	5.80836200	-2.08658300
O	-1.50794200	-0.85361500	-3.28276300
P	-1.51816200	-1.11727300	-1.79755900
C	-3.16215900	-1.69627200	-1.29334500
C	-3.89531000	-2.47707700	-2.19660700
C	-3.73341100	-1.36174900	-0.06119200
C	-5.16854000	-2.92888800	-1.86313300
H	-3.46421900	-2.71522200	-3.16596700
C	-5.01152800	-1.80397200	0.26674300
H	-3.17045500	-0.75272700	0.63894500
C	-5.72783900	-2.59218400	-0.63129900
H	-5.72867800	-3.53724300	-2.56771400
H	-5.44747200	-1.53071200	1.22390500
H	-6.72480400	-2.93961600	-0.37443600
C	-0.25987600	-2.35900100	-1.34197500
C	-0.03788300	-2.87028300	-0.03643700
C	0.54121200	-2.80225700	-2.40590900
C	0.97677400	-3.83191700	0.13061200
C	1.55569900	-3.72675200	-2.20675700
H	0.34586200	-2.39579000	-3.39561500
C	1.76749400	-4.24946100	-0.92912700
H	1.15002900	-4.22828600	1.12857100
H	2.17188600	-4.04902000	-3.04111700
H	2.55309600	-4.98072000	-0.76146400
N	-1.01828000	0.09955900	-0.78996800
C	-1.59038800	1.31752500	-0.55159700
C	-0.89652700	2.07861900	0.43192100
C	-2.73118800	1.87962800	-1.12208200
C	-1.31596300	3.37674800	0.82057100
C	-3.14836800	3.16589100	-0.73687200
H	-3.28814700	1.32787500	-1.87469100
C	0.85359800	2.06858000	1.98200000
C	-0.55370800	4.01770400	1.82360600

C	-2.46714500	3.91640500	0.20230800
H	-4.03891500	3.57959000	-1.20308300
C	0.51850400	3.36878200	2.39491700
H	1.66259200	1.50060400	2.42891600
H	-0.83160100	5.01746500	2.14734900
H	-2.80491900	4.90999100	0.48083700
H	1.10875900	3.83685300	3.17474700
N	0.16711400	1.45690200	1.02259700
C	-1.22498300	-0.62093000	2.84186000
C	-2.18873600	0.40269400	2.88504700
C	-0.69577600	-1.07907900	4.06104100
C	-2.60782200	0.94059700	4.09622300
H	-2.61413900	0.77991500	1.95739000
C	-1.11463900	-0.53714500	5.27256700
H	0.05884900	-1.86183000	4.03976100
C	-2.07002000	0.47685400	5.29632200
H	-3.35570800	1.72954900	4.10161900
H	-0.69089800	-0.90764500	6.20227100
H	-2.39398700	0.90261900	6.24176700
C	-0.72071400	-1.16657300	1.58683600
C	-0.78663100	-2.43742300	1.17223800
H	-1.28096500	-3.21811300	1.76011200

9'-ts-s

01

Co	0.18437000	0.49251100	-0.56198400
C	0.70494700	4.51176500	-1.72667800
C	0.82944600	3.33953700	-0.93413500
C	1.47628300	3.48393800	0.33210600
C	1.93337900	4.74837800	0.75465000
C	1.78864500	5.86958300	-0.03705700
C	1.17007900	5.73607300	-1.29027700
H	0.21774100	4.40783600	-2.69238800
H	2.41227600	4.82095500	1.72636600
H	2.14815800	6.83505100	0.30321000
H	1.04839500	6.60808800	-1.92888300
O	0.34106600	2.22970700	-1.41178700
C	1.69385900	2.34102200	1.17730700
O	2.34107500	2.55454300	2.34479100
C	1.88212900	0.26381600	2.02852700
C	2.27635900	1.31102800	3.07806600
H	3.25202600	1.13913300	3.53524700
N	1.36261300	1.10831500	0.93977500
H	1.51835400	1.42421000	3.86016200

H	1.08279400	-0.38142700	2.41048900
C	3.02150700	-0.60836400	1.55971000
C	4.09614200	-0.06327900	0.84966900
C	3.01912900	-1.97279700	1.85035600
C	5.15158900	-0.87119100	0.43928100
H	4.09972800	0.99777600	0.60376000
C	4.07796600	-2.78204600	1.44429600
H	2.16047700	-2.39729800	2.36928300
C	5.14514400	-2.23367600	0.73792500
H	5.97695700	-0.43912800	-0.12082400
H	4.05866700	-3.84640800	1.66366600
H	5.96562700	-2.86674900	0.41051400
O	-0.49749100	-2.40202200	2.55337700
P	-1.00042000	-1.73255000	1.29715000
C	-2.35453900	-2.70822500	0.57790400
C	-3.34872200	-3.21020200	1.42965200
C	-2.45792900	-2.93899400	-0.79833800
C	-4.43441000	-3.90891100	0.91127700
H	-3.26531400	-3.05453700	2.50303400
C	-3.53720800	-3.65079100	-1.31479600
H	-1.68658500	-2.55726400	-1.46138800
C	-4.53060200	-4.12788400	-0.46243400
H	-5.20308100	-4.28803700	1.57891100
H	-3.60406400	-3.83172900	-2.38401200
H	-5.37709700	-4.67583800	-0.86701000
C	-1.62258000	-0.06200600	1.59209100
C	-1.35599200	0.94926800	0.65064900
C	-2.25419400	0.25179400	2.80062000
C	-1.73333500	2.26804000	0.94093800
C	-2.63459500	1.56223900	3.07127800
H	-2.42286900	-0.53255400	3.53653800
C	-2.36350800	2.57073900	2.14155400
H	-1.54572700	3.05243700	0.21112200
H	-3.13215800	1.80273400	4.00647300
H	-2.64864500	3.59721300	2.35758600
N	0.07973200	-1.34669200	0.09706000
C	0.91549800	-2.22019600	-0.54898300
C	1.83270600	-1.60383700	-1.45230500
C	0.98222000	-3.60684800	-0.40887600
C	2.80831800	-2.35370300	-2.16355700
C	1.93642500	-4.34828800	-1.12684700
H	0.30832600	-4.11295100	0.27778000
C	2.56073900	0.40685900	-2.36927400
C	3.68673300	-1.62285600	-2.99725600

C	2.84149400	-3.75545800	-1.98533100
H	1.96160000	-5.42622200	-0.98794700
C	3.57027800	-0.25427200	-3.09082900
H	2.41220200	1.48123500	-2.42959800
H	4.45371700	-2.15347600	-3.55619900
H	3.57943500	-4.34514200	-2.52120400
H	4.23726800	0.32537600	-3.71965900
N	1.72205100	-0.25118200	-1.58367500
C	-1.03474900	-0.00804200	-1.98871000
C	-1.97942300	0.46148500	-1.28500000
C	-3.34162800	0.94619300	-1.19934300
C	-3.70093800	2.06843200	-1.96127100
C	-4.31175400	0.30200600	-0.41653500
C	-5.01134000	2.53376300	-1.94223700
H	-2.94023900	2.56750900	-2.55613600
C	-5.61865600	0.77083300	-0.40774800
H	-4.03116800	-0.56191700	0.18100700
C	-5.97116300	1.88785000	-1.16602400
H	-5.28202300	3.40309200	-2.53407300
H	-6.36718100	0.26330600	0.19385000
H	-6.99366900	2.25385500	-1.15014600
H	-0.81607100	-0.48625300	-2.93048400

10'-s

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Co	0.43541000	0.41104800	-0.55136800
C	1.62507300	4.13690400	-2.07586700
C	1.61871600	3.00696900	-1.21604700
C	2.42672900	3.09084100	-0.03927300
C	3.16011400	4.26244300	0.23620700
C	3.13166300	5.34817600	-0.61485700
C	2.35488400	5.27105000	-1.78189100
H	1.01620100	4.07998200	-2.97362800
H	3.75560300	4.29097000	1.14353700
H	3.70096100	6.24314600	-0.38649400
H	2.32010400	6.11650700	-2.46509900
O	0.87739300	1.99012000	-1.56191800
C	2.51030900	1.98325300	0.87126900
O	3.33705200	2.11106500	1.93051900
C	2.33506800	-0.02719100	1.86962500
C	3.15036500	0.93476200	2.74911900
H	4.13689600	0.55834000	3.02601800
N	1.88065700	0.84918000	0.78037300
H	2.60884200	1.23947600	3.65044200

H	1.46486300	-0.40517400	2.41909300
C	3.10611300	-1.20764200	1.33184100
C	4.08893700	-1.03803500	0.35147800
C	2.84781100	-2.48905900	1.81975600
C	4.79895800	-2.13248800	-0.13214000
H	4.28607100	-0.04395500	-0.04771100
C	3.56172100	-3.58511500	1.34194200
H	2.05957200	-2.62283500	2.55886600
C	4.53799900	-3.40926700	0.36433900
H	5.55065800	-1.99052600	-0.90412600
H	3.34222900	-4.57985800	1.72092700
H	5.08651600	-4.26563000	-0.01884800
O	-0.76812900	-1.49113900	3.00986800
P	-1.17191300	-0.98233600	1.64926000
C	-2.81707700	-1.60055700	1.20231300
C	-3.80659900	-1.60150200	2.19539200
C	-3.13914500	-2.04721000	-0.08354500
C	-5.10078700	-2.01651600	1.89867200
H	-3.55631200	-1.27400600	3.20202300
C	-4.43091900	-2.47482100	-0.37516300
H	-2.37792400	-2.03860100	-0.86007100
C	-5.41470600	-2.44981500	0.61150300
H	-5.86445700	-2.00240400	2.67129900
H	-4.67289300	-2.81547100	-1.37824400
H	-6.42665600	-2.76857600	0.37739800
C	-1.18818200	0.84567900	1.60852600
C	-1.58045000	1.62023500	0.48744500
C	-0.68801600	1.48222700	2.75422400
C	-1.43337700	3.01795900	0.56146700
C	-0.54171500	2.86106500	2.79694500
H	-0.40268200	0.86261000	3.60125900
C	-0.91056600	3.63049300	1.69043200
H	-1.72291700	3.61433300	-0.30071800
H	-0.13846300	3.33900200	3.68548300
H	-0.78889300	4.70988200	1.71169500
N	-0.11412700	-1.19727600	0.39036200
C	0.28722000	-2.34715900	-0.22974700
C	1.11197300	-2.11509900	-1.36655500
C	0.01893000	-3.66983600	0.11909300
C	1.69831300	-3.17534900	-2.10646100
C	0.58204800	-4.72060500	-0.62524300
H	-0.60367200	-3.88649300	0.98306900
C	2.09262900	-0.48580100	-2.72730100
C	2.53115000	-2.80962800	-3.18944700

C	1.41224400	-4.50101200	-1.70814100
H	0.36152600	-5.74130300	-0.32384700
C	2.72802900	-1.48029300	-3.48992400
H	2.19624300	0.57290000	-2.93803700
H	3.01049400	-3.58686400	-3.77893100
H	1.84942700	-5.32841800	-2.25863500
H	3.36102700	-1.17847500	-4.31689700
N	1.31516800	-0.80434000	-1.69862500
C	-1.21750500	0.32196600	-1.47737500
C	-2.13152700	1.00274400	-0.76808300
C	-3.56300200	1.15817000	-1.07495500
C	-4.07622000	0.82142400	-2.33895400
C	-4.46563900	1.59549900	-0.09300000
C	-5.43617200	0.90581900	-2.60365600
H	-3.39381200	0.49137800	-3.11896900
C	-5.82930500	1.67909800	-0.35872900
H	-4.09478800	1.85436400	0.89686500
C	-6.32298000	1.33322300	-1.61376200
H	-5.80924500	0.63969300	-3.58939200
H	-6.50860300	2.01057300	0.42232600
H	-7.38719400	1.39769000	-1.82223500
H	-1.41712800	-0.22484300	-2.40175700

11-ts-r

0 1

Co	0.47446700	0.49959900	0.55997400
C	1.79273800	4.30045400	1.16241600
C	0.83651900	3.26947200	0.99240000
C	-0.39263400	3.63017800	0.35946000
C	-0.62093800	4.94718800	-0.07394400
C	0.34568500	5.92307800	0.08072800
C	1.55351100	5.58518400	0.71077200
H	2.72716200	4.04540300	1.65550100
H	-1.57503600	5.17552300	-0.54276000
H	0.17237700	6.93356100	-0.27475600
H	2.32010900	6.34467300	0.84448400
O	1.09642700	2.07245500	1.45459800
C	-1.43801400	2.64834300	0.30915900
O	-2.71443000	3.07590800	0.32672500
C	-2.57235600	0.74250400	0.58737700
C	-3.54005400	1.88675900	0.25613500
H	-4.35697600	2.00413900	0.96961300
N	-1.26798000	1.35850900	0.32223100
H	-3.93808500	1.81147600	-0.76129800

H	-2.73498900	-0.09112000	-0.10663500
C	-2.67725700	0.20456200	1.99957800
C	-1.68630800	0.41401800	2.96219700
C	-3.80067800	-0.55653800	2.33978700
C	-1.81029800	-0.14564500	4.23450200
H	-0.81274200	1.01764600	2.71869700
C	-3.93119800	-1.10202400	3.61223100
H	-4.57141700	-0.73510300	1.59122600
C	-2.92981100	-0.90447500	4.56282000
H	-1.02753300	0.01872500	4.97017100
H	-4.80843500	-1.69384500	3.85861700
H	-3.02519900	-1.33870900	5.55383100
O	-0.05659500	-2.12447000	-3.18068100
P	-0.65605200	-1.46215100	-1.96815800
C	-1.44509100	0.09104300	-2.38231200
C	-0.62162900	1.23062600	-2.58673900
C	-2.79120800	0.10814100	-2.75892200
C	-1.20912800	2.35450500	-3.20321800
C	-3.35482000	1.24233000	-3.33543500
H	-3.40328200	-0.77905800	-2.59883500
C	-2.54819200	2.36320800	-3.56208700
H	-0.59313300	3.23570500	-3.37146200
H	-4.40343300	1.25047900	-3.61583800
H	-2.97445000	3.25190700	-4.02045300
C	-1.82478900	-2.56255400	-1.13121000
C	-1.95432400	-2.61405300	0.26231100
C	-2.59536900	-3.42436500	-1.92440800
C	-2.84463300	-3.50800000	0.85026900
H	-1.35458700	-1.95574500	0.89006000
C	-3.49263000	-4.30855000	-1.33374000
H	-2.47454800	-3.40519900	-3.00484800
C	-3.61670000	-4.35150300	0.05398100
H	-2.93474900	-3.54102000	1.93245600
H	-4.08822500	-4.97029500	-1.95568600
H	-4.31163700	-5.04740700	0.51506000
N	0.47762600	-1.03761500	-0.73584100
C	1.33694800	-2.06433000	-0.27284000
C	2.06714100	-1.75115000	0.90044900
C	1.55364300	-3.30097700	-0.86802100
C	3.01444500	-2.65292800	1.45180800
C	2.47889100	-4.20524600	-0.31261400
H	1.02941300	-3.56444100	-1.77952800
C	2.47699700	-0.16927700	2.55531800
C	3.69063400	-2.24351600	2.62376100

C	3.20770500	-3.89966200	0.81555100
H	2.61941800	-5.16513500	-0.80085100
C	3.41106900	-1.01314600	3.17489700
H	2.26442000	0.82970000	2.92325200
H	4.42132600	-2.90754100	3.07738400
H	3.92089200	-4.60425300	1.23276200
H	3.91121700	-0.67338300	4.07518600
N	1.82644200	-0.52349400	1.44931100
C	2.82034100	0.28806400	-1.21337300
C	3.35802200	-0.61250200	-2.14299500
C	3.68044000	0.94330700	-0.32539100
C	4.72436700	-0.87527100	-2.16381100
H	2.68057600	-1.12302700	-2.82554600
C	5.04952200	0.69879600	-0.36322000
H	3.25231100	1.62192700	0.40931500
C	5.57274600	-0.21963900	-1.27353100
H	5.12773300	-1.58946500	-2.87640500
H	5.70947100	1.21555400	0.32882800
H	6.63998400	-0.42365800	-1.28783200
C	1.35285900	0.50153100	-1.18826300
C	0.76324700	1.21805500	-2.21183900
H	1.42991800	1.88616400	-2.75565000

11-ts-s

0 1

Co	0.63869200	-0.12429800	0.86536500
C	3.10119900	-2.41652300	3.13029300
C	2.74207000	-1.56884800	2.05348700
C	3.43787100	-1.77095100	0.81801600
C	4.41122800	-2.77850400	0.70631200
C	4.72368800	-3.60067300	1.77395700
C	4.06097700	-3.40362500	2.99288600
H	2.58525200	-2.26733200	4.07493600
H	4.91142600	-2.90451700	-0.24991200
H	5.46983200	-4.38144700	1.66844200
H	4.29464400	-4.03896600	3.84413100
O	1.83936900	-0.64117800	2.26282100
C	3.16266300	-0.92413100	-0.31683100
O	3.98336100	-1.00638300	-1.38720500
C	2.22742700	0.55048600	-1.73505000
C	3.55356000	0.01929300	-2.31291600
H	4.33291800	0.78849800	-2.34517800
N	2.18610000	-0.08036400	-0.41071900
H	3.45576800	-0.43483800	-3.30044500

H	1.37301600	0.17879300	-2.31885100
C	2.12439100	2.05202000	-1.66174600
C	2.96998300	2.78013000	-0.81959300
C	1.17607100	2.73006200	-2.42882800
C	2.86843200	4.16496800	-0.74532600
H	3.69610400	2.25111700	-0.20335100
C	1.08143200	4.11919900	-2.36378500
H	0.49104300	2.15574500	-3.05084400
C	1.92500900	4.83835800	-1.52128900
H	3.52097600	4.72100500	-0.07706500
H	0.33333000	4.63745900	-2.95823300
H	1.84045500	5.91997600	-1.45789300
O	-1.30741300	0.39657100	-3.05828800
P	-1.38058300	-0.40826300	-1.78770800
C	-3.05445300	-1.04283600	-1.45613200
C	-4.04635400	-0.27322000	-0.83152600
C	-3.38030300	-2.33692300	-1.88519000
C	-5.32704100	-0.78242400	-0.64790800
H	-3.81348600	0.71675000	-0.45035600
C	-4.66313600	-2.84537300	-1.69940700
H	-2.62268600	-2.95544600	-2.36107800
C	-5.63995600	-2.06864400	-1.08244000
H	-6.07781900	-0.17667700	-0.14763800
H	-4.89638700	-3.85218400	-2.03410500
H	-6.63961100	-2.46686600	-0.93323000
C	-0.30730100	-1.84067300	-1.80349400
C	0.11017100	-2.45716400	-0.60228600
C	0.14220100	-2.30947600	-3.04095500
C	0.97191100	-3.56698700	-0.70798200
C	1.00462900	-3.39818700	-3.12047600
H	-0.18110900	-1.79125800	-3.94126600
C	1.41326700	-4.02457300	-1.94099300
H	1.31746500	-4.04469400	0.20735800
H	1.35561400	-3.75174800	-4.08487900
H	2.08705100	-4.87669000	-1.98340000
N	-0.85038000	0.42494100	-0.38267700
C	-1.15068400	1.78120100	-0.20564600
C	-0.36497400	2.49048500	0.75234300
C	-2.10648300	2.50592500	-0.91402300
C	-0.58298800	3.87143500	1.01223900
C	-2.30766200	3.87588500	-0.66991500
H	-2.68146000	2.02423100	-1.69652400
C	1.34360800	2.38345300	2.32440000
C	0.23127900	4.48322200	1.99383600

C	-1.57812400	4.55647000	0.27939100
H	-3.06304400	4.39862000	-1.24955300
C	1.18666100	3.74122100	2.64916000
H	2.09046700	1.75451600	2.80303200
H	0.09163100	5.53816200	2.21564600
H	-1.74771900	5.61255400	0.46935200
H	1.82626100	4.18577900	3.40406300
N	0.59597700	1.78007900	1.41119400
C	-2.26017500	-0.74211000	1.83287700
C	-3.08042400	-1.88507600	1.90888400
C	-2.69264300	0.44801300	2.45179100
C	-4.29178500	-1.83946200	2.58406000
H	-2.75258500	-2.79779200	1.41636600
C	-3.91856000	0.49551000	3.09881000
H	-2.04886300	1.32285300	2.42529600
C	-4.71847200	-0.64755200	3.16965700
H	-4.91642200	-2.72658000	2.63574100
H	-4.24839900	1.41853600	3.56669400
H	-5.67272300	-0.60853700	3.68754600
C	-0.98693100	-0.83090500	1.17720600
C	-0.17776000	-1.92311900	0.71670700
H	0.10758200	-2.58995800	1.53729300

3a-r

01

O	-1.37343100	-0.66940900	-2.32650000
P	-1.50448200	-0.20392100	-0.91047500
C	-2.20835500	1.42891800	-0.70535200
C	-1.68197800	2.34962800	0.22967000
C	-3.31572000	1.76742300	-1.49119200
C	-2.32565900	3.59532200	0.35858000
C	-3.93033300	3.00498900	-1.34946500
H	-3.69577200	1.04953600	-2.21494200
C	-3.43023700	3.91586000	-0.41448300
H	-1.93226200	4.31339100	1.07399400
H	-4.79384700	3.25827400	-1.95623300
H	-3.90710000	4.88453700	-0.29408700
C	-2.47206000	-1.37321000	0.07478700
C	-3.36593000	-2.22675000	-0.58022100
C	-2.36530400	-1.42136700	1.47104000
C	-4.14380000	-3.11898600	0.15198000
H	-3.43432100	-2.19149400	-1.66435800
C	-3.14295000	-2.31599600	2.19949700
H	-1.66820600	-0.76258600	1.98591000

C	-4.03211800	-3.16349000	1.54013900
H	-4.83337200	-3.78374000	-0.36014800
H	-3.05366200	-2.35455100	3.28114300
H	-4.63676100	-3.86248800	2.11095800
N	-0.00214900	-0.06407600	-0.06618300
C	1.04432800	-0.90148900	-0.56296300
C	2.16135300	-0.31549200	-1.22835900
C	0.94436500	-2.27265300	-0.45318600
C	3.18704900	-1.18207300	-1.72209300
C	1.94858700	-3.11612900	-0.96581500
H	0.08068400	-2.69839800	0.05283000
C	3.25591200	1.54684700	-1.98964500
C	4.29296900	-0.57724700	-2.36295100
C	3.05796200	-2.58330000	-1.57818500
H	1.84384600	-4.19118800	-0.85942300
C	4.33291100	0.78823000	-2.49652600
H	3.26459500	2.63096400	-2.10147200
H	5.09382400	-1.20593800	-2.74493000
H	3.84407200	-3.22657700	-1.96530300
H	5.16401700	1.28537400	-2.98549300
N	2.20569100	1.03507800	-1.37657300
C	1.45167000	0.76603700	1.73537100
C	1.69317000	-0.46819300	2.35574700
C	2.30727200	1.83971100	2.01359000
C	2.75493700	-0.61818300	3.24028000
H	1.02874400	-1.30524400	2.15681500
C	3.37021700	1.68700600	2.89695100
H	2.13826900	2.78984400	1.51304100
C	3.59777400	0.45791900	3.51307800
H	2.92137900	-1.57704000	3.72268900
H	4.02833100	2.52762100	3.09789600
H	4.43000300	0.33825100	4.20079500
C	0.28234900	0.95659000	0.85390300
C	-0.51890900	2.04353500	1.01771000
H	-0.24941900	2.73777300	1.80741900

3a-s

0 1

O	1.93274700	0.37248900	-2.55888700
P	1.65604800	0.28457600	-1.08632900
C	2.17560500	-1.29530100	-0.38730600
C	1.86892400	-1.63543800	0.93645200
C	2.92105600	-2.17231000	-1.17855200
C	2.29935000	-2.85036300	1.45670100

H	1.27648700	-0.95256400	1.54453800
C	3.35762500	-3.38493600	-0.65064500
H	3.14824800	-1.89651200	-2.20502500
C	3.04537400	-3.72351600	0.66383600
H	2.05417500	-3.11847300	2.48016100
H	3.93838000	-4.06593600	-1.26580800
H	3.38356800	-4.67089100	1.07376900
C	2.37553500	1.56994300	-0.07141800
C	1.58442000	2.64653600	0.39245900
C	3.75229700	1.53942600	0.18629400
C	2.23217500	3.69449100	1.07706800
C	4.36416000	2.57331400	0.88091400
H	4.34459500	0.69706100	-0.16663600
C	3.59511400	3.65783300	1.31703300
H	1.63716800	4.53508200	1.42623800
H	5.43147600	2.54314600	1.07635600
H	4.06909500	4.47565900	1.85240800
N	-0.00614500	0.40541900	-0.63442000
C	-0.78665000	-0.78726500	-0.65319200
C	-1.48952500	-1.18543600	0.52346800
C	-0.80480800	-1.59162100	-1.77540700
C	-2.25182900	-2.39349900	0.48267300
C	-1.53135900	-2.79773800	-1.78892200
H	-0.25254700	-1.27302700	-2.65624600
C	-2.05869000	-0.80582400	2.71170800
C	-2.95925200	-2.75301800	1.65310500
C	-2.25815700	-3.18666700	-0.68855600
H	-1.52764100	-3.40763700	-2.68666300
C	-2.87112600	-1.95838100	2.76866600
H	-1.95630500	-0.17629600	3.59541400
H	-3.55964200	-3.65938700	1.65199800
H	-2.83879800	-4.10532300	-0.69852500
H	-3.40062100	-2.20528400	3.68293400
N	-1.38906700	-0.41893500	1.64224300
C	-2.04202900	1.78543600	-0.44665000
C	-2.67679900	1.35765100	-1.62121300
C	-2.80826300	2.41165800	0.54453600
C	-4.04103600	1.55932600	-1.79931300
H	-2.09099600	0.88548500	-2.40515900
C	-4.17247300	2.61179500	0.36491300
H	-2.32391400	2.71639100	1.46906100
C	-4.79398200	2.18465600	-0.80719600
H	-4.51648400	1.23208800	-2.71963800
H	-4.75358600	3.09309000	1.14638300

H	-5.86057000	2.33617400	-0.94590800
C	-0.58523700	1.63143100	-0.26622400
C	0.16321800	2.67485900	0.18476900
H	-0.36011300	3.60095900	0.40161900

Co(I)-Saloxs

0 1

Co	0.22994100	-1.93914700	-0.61426000
C	3.83698100	-0.74472600	0.82846000
C	2.53872600	-0.67339700	0.27236100
C	2.01738300	0.62493800	-0.03946200
C	2.80724800	1.76886400	0.21493700
C	4.06967100	1.66567700	0.76061400
C	4.58210800	0.39296000	1.06773500
H	4.22774000	-1.73103500	1.06362400
H	2.39084100	2.74152800	-0.03052200
H	4.65989000	2.55667200	0.95023600
H	5.57583400	0.29813800	1.49828700
O	1.88296300	-1.79500200	0.07334200
C	0.71087500	0.77638800	-0.59216800
O	0.23094500	2.02723100	-0.81291800
C	-1.41377200	0.40918100	-1.28831200
C	-0.99635000	1.86451200	-1.54986200
H	-1.71173200	2.60352900	-1.18674600
N	-0.12362000	-0.19366900	-0.90452100
H	-0.78697700	2.04480200	-2.60953900
H	-1.77715000	-0.05054400	-2.21310300
C	-2.46405900	0.25499700	-0.21253900
C	-2.12288400	0.22489600	1.14316900
C	-3.81255600	0.20074600	-0.57381500
C	-3.11542700	0.14274100	2.11678900
H	-1.07565200	0.25519100	1.43556700
C	-4.80551200	0.11905200	0.39939400
H	-4.08423200	0.21874900	-1.62765200
C	-4.45822100	0.09041800	1.74834200
H	-2.83788400	0.11833700	3.16680000
H	-5.84971000	0.07332300	0.10325200
H	-5.23058000	0.02264800	2.50919100

Co(OAc)₂

0 2

Co	-0.00003000	-0.00047200	0.00501100
O	1.64042900	-1.09487500	0.02678400

C	2.31100700	-0.00911900	0.01568800
O	1.62955300	1.07570500	0.02462300
O	-1.63917600	1.09548200	-0.01368600
C	-2.31077800	0.01059400	-0.01273800
O	-1.63036700	-1.07523800	-0.01739500
C	3.79520600	0.00839700	-0.03030200
H	4.18640300	0.77344700	0.64196700
H	4.20638500	-0.96689400	0.22716800
H	4.11999800	0.26955100	-1.04143100
C	-3.79560200	-0.00696600	0.00163800
H	-4.16729700	-0.60707700	-0.83200800
H	-4.14617200	-0.48434700	0.91991900
H	-4.20102200	1.00203000	-0.05923700

Co^{II}-Saloxs

O 2

Co	0.06797000	1.38393900	-0.18176600
O	1.90781500	1.72917200	-0.79257600
C	1.83215200	2.89663400	-0.27058300
O	0.72768000	3.20905600	0.28260900
C	2.99491300	3.82411600	-0.29097400
H	2.67836700	4.84952700	-0.10256200
H	3.70170100	3.53183200	0.49095200
H	3.52042500	3.75859800	-1.24475900
C	-3.90615600	1.06581000	0.96406200
C	-2.64471000	0.68293200	0.44266500
C	-2.54934700	-0.62248400	-0.13368500
C	-3.67805500	-1.46798200	-0.16721800
C	-4.89127700	-1.06233400	0.34800700
C	-4.99396700	0.21837600	0.91687500
H	-3.98515300	2.05654200	1.40187200
H	-3.56992200	-2.45155500	-0.61451500
H	-5.75256800	-1.72111200	0.31296600
H	-5.94466100	0.55225600	1.32538300
O	-1.66055800	1.54031300	0.52150400
C	-1.30547800	-1.07873600	-0.67697800
O	-1.22161500	-2.34678600	-1.11851000
C	0.87346200	-1.26044500	-1.25728200
C	0.08512700	-2.49681000	-1.72206800
H	0.50412000	-3.44412900	-1.38048200
N	-0.20514000	-0.38165700	-0.78256900
H	-0.04957400	-2.52534300	-2.80674000
H	1.38146800	-0.78752900	-2.10393200

C	1.88889600	-1.53751600	-0.17358200
C	1.50800100	-1.65547000	1.16567200
C	3.23066200	-1.71719700	-0.51604700
C	2.45437800	-1.95258300	2.14365200
H	0.46778100	-1.50440000	1.44788200
C	4.17680700	-2.01708000	0.45978400
H	3.53451400	-1.61323600	-1.55592900
C	3.79034300	-2.13571500	1.79306800
H	2.14675600	-2.03798900	3.18213100
H	5.21821700	-2.14986800	0.18001500
H	4.52824500	-2.36346500	2.55698100

NaOAc

0 1

C	0.55035600	0.01167500	0.00006800
O	-0.04050500	1.13036300	-0.00031500
O	-0.03006700	-1.11402400	-0.00031200
Na	-2.05082900	-0.00994100	0.00022900
C	2.07322300	-0.00149900	0.00032700
H	2.44235700	-0.54866200	0.87296500
H	2.44233500	-0.53805100	-0.87894000
H	2.49752300	1.00430400	0.00611400

NaOPiv

0 1

C	-0.42211900	0.03027100	0.00021200
O	-1.01893100	1.14521200	0.00027600
O	-1.00141200	-1.09683400	0.00023100
Na	-3.02975700	-0.00005300	-0.00021900
C	1.12658300	0.01143100	-0.00006500
C	1.70507400	1.42071700	-0.00136100
H	1.38235500	1.98323200	0.87946900
H	2.80151200	1.38679600	-0.00142500
H	1.38225800	1.98164400	-0.88318300
C	1.59690700	-0.74139900	1.24655700
H	1.17334400	-1.74909300	1.26837300
H	2.69034000	-0.82352800	1.26332300
H	1.28956500	-0.22471700	2.16336700
C	1.59663300	-0.74356500	-1.24545800
H	1.28917200	-0.22845200	-2.16311700
H	2.69006300	-0.82578700	-1.26227200
H	1.17299100	-1.75126300	-1.26549000

PivOH

O 1			
C	-0.94922900	-0.13034200	-0.00018800
O	-1.62051500	1.03806900	-0.00014300
O	-1.51628300	-1.20630900	-0.00014000
C	0.56496200	0.02979900	-0.00004000
C	1.00941100	1.48862200	-0.00184300
H	0.64823700	2.02250800	0.88113500
H	2.10291800	1.53772600	-0.00171600
H	0.64854600	2.02020200	-0.88634300
C	1.09232900	-0.68201500	1.25139000
H	0.77261500	-1.72684900	1.26917500
H	2.18619200	-0.65438800	1.25934400
H	0.73733600	-0.19821400	2.16698000
C	1.09314800	-0.68540300	-1.24916900
H	0.73883100	-0.20406200	-2.16631400
H	2.18701800	-0.65787900	-1.25644100
H	0.77337200	-1.73025400	-1.26437600
H	-2.56440800	0.81315600	-0.00007500

4-OPiv-1

O 1			
Co	-0.31170400	0.50953000	0.53301200
P	-0.75180700	-1.18153800	-2.49357900
O	-0.53901700	-0.92356700	-3.95771700
O	-0.46093300	1.09524400	2.34182900
O	1.71099200	-2.44677000	2.54215500
O	-3.43741000	0.14105800	1.57476000
N	-0.04788200	0.12403800	-1.52629800
N	1.07725300	1.83679300	0.14278300
N	1.05363800	-0.81295900	1.15357000
C	1.41795400	2.84862800	0.92613200
H	0.82063600	2.96459300	1.82609700
C	2.50689000	3.68368500	0.62552100
H	2.74603700	4.50339700	1.29325600
C	3.27611600	3.41325900	-0.48295000
H	4.15522700	4.01015500	-0.71108500
C	2.92953600	2.34433900	-1.33708800
C	1.76840900	1.59822300	-1.00625600
C	1.28702300	0.57739700	-1.86414100
C	2.04483800	0.21849400	-2.96034000
H	1.69213000	-0.54453600	-3.64353100
C	3.24470600	0.90749400	-3.24718400
H	3.81821400	0.60492200	-4.11766100
C	3.66538100	1.97016400	-2.48391600

H	4.56664500	2.52099100	-2.73709700
C	0.02341400	-2.71824500	-1.95886300
C	0.84207000	-3.36326300	-2.89408400
H	0.99461200	-2.90712200	-3.86861600
C	1.43369000	-4.58314100	-2.58099300
H	2.07421900	-5.07570300	-3.30637800
C	1.18524900	-5.17937200	-1.34665300
H	1.63158800	-6.14082600	-1.10887400
C	0.36132300	-4.54554700	-0.41636700
H	0.16995200	-5.00943400	0.54808400
C	-0.20770200	-3.30937600	-0.70783400
H	-0.82397200	-2.79005000	0.02423200
C	-2.49528600	-1.19182700	-2.04560000
C	-3.15592100	-2.38717700	-1.74110300
H	-2.59888500	-3.31649600	-1.66056200
C	-4.53215000	-2.39324800	-1.53526900
H	-5.03345800	-3.32485100	-1.28832200
C	-5.26033400	-1.21182200	-1.63996900
H	-6.33383500	-1.21747500	-1.47499900
C	-4.61139800	-0.02372300	-1.96886600
H	-5.17848000	0.89772700	-2.06617400
C	-3.23721200	-0.01036700	-2.17815200
H	-2.74402800	0.92115700	-2.44759900
C	-0.64235600	0.23167500	3.30856800
C	-1.43970700	0.60017700	4.41681500
H	-1.90556600	1.58124600	4.39680300
C	-1.63674200	-0.26770900	5.47506500
H	-2.26861100	0.04266500	6.30364400
C	-1.05353500	-1.54337500	5.48703100
H	-1.22565200	-2.22061000	6.31706100
C	-0.25450200	-1.92474200	4.42514100
H	0.21893200	-2.90212600	4.41346900
C	-0.03940400	-1.06004000	3.33807600
C	0.88020600	-1.42045400	2.29477300
C	2.26340800	-1.36224400	0.52157200
H	2.04577900	-1.64140000	-0.51653000
C	2.53448600	-2.62078000	1.36762100
H	2.23489100	-3.54694300	0.87292000
H	3.57142100	-2.69839800	1.69803300
C	3.45486300	-0.43339900	0.54720800
C	4.45049800	-0.60432900	-0.41732500
H	4.29774800	-1.32550400	-1.21917700
C	5.62010000	0.14734700	-0.36755300
H	6.38061200	0.01410600	-1.13208300

C	5.80692900	1.07787000	0.65223500
H	6.71589700	1.67150500	0.68994000
C	4.82028000	1.24717000	1.62217600
H	4.95618700	1.97763100	2.41529900
C	3.65027800	0.49349100	1.57333200
H	2.87290400	0.63841400	2.32209200
C	-3.23354300	-2.23517100	1.74021500
H	-2.85430000	-2.43526700	2.74951600
H	-2.85113100	-3.02091400	1.08367700
H	-4.32377700	-2.27677600	1.76977400
C	-2.75984400	-0.85031300	1.33188500
O	-1.57117800	-0.90110600	0.78301000
O	-1.61889900	1.90198800	0.21692000
C	-1.69658400	2.70397500	-0.77419800
O	-1.15784600	2.53710900	-1.89571500
C	-2.59776200	3.92624900	-0.53965900
H	-0.62221100	0.99133300	-1.75943000
C	-2.08142900	5.10025000	-1.36766200
H	-2.03515500	4.84267100	-2.42796700
H	-2.74088900	5.96610400	-1.24604900
H	-1.07544600	5.39683600	-1.05006100
C	-4.00056200	3.52816700	-1.01560600
H	-4.37652500	2.66638200	-0.45307200
H	-4.69926800	4.35942800	-0.87285200
H	-3.99665000	3.27112500	-2.08085000
C	-2.63720900	4.29798600	0.94018200
H	-1.63357300	4.52471700	1.31673900
H	-3.26193600	5.18565100	1.08787900
H	-3.04068700	3.48240800	1.54498600

4-OPiv-2

O 1

Co	-0.06407700	0.52355400	-0.87130700
P	-0.70288300	-2.86602500	0.05188900
O	-0.25349800	-4.21900800	-0.41740900
O	-0.14073800	2.36777500	-1.31300600
O	0.91238100	2.22237700	2.74758100
O	-3.20715400	1.33396900	-1.47559700
N	0.26486500	-1.58821800	-0.68950300
N	1.72308500	0.36667100	-1.69840800
N	0.76268400	0.99205200	0.88030500
C	2.30867000	1.31306900	-2.41582200
H	1.69639100	2.18296500	-2.63398200
C	3.64570600	1.20743700	-2.83276900

H	4.08057000	2.00692300	-3.42165400
C	4.38903700	0.11649000	-2.44459500
H	5.44028300	0.03482100	-2.70845300
C	3.78697700	-0.91109200	-1.68602600
C	2.40969900	-0.76208600	-1.36974600
C	1.69995200	-1.78297100	-0.69084600
C	2.40002200	-2.87276600	-0.21416400
H	1.88587700	-3.67713300	0.29808600
C	3.78497100	-2.98979800	-0.46540300
H	4.30706300	-3.86034300	-0.08050800
C	4.46406800	-2.05773000	-1.21265400
H	5.52192900	-2.17435300	-1.42969200
C	-0.55044200	-2.65994900	1.83120100
C	-0.07687500	-3.74598100	2.57564000
H	0.24348000	-4.64598600	2.05686300
C	-0.03439300	-3.66972800	3.96482900
H	0.34047100	-4.50973100	4.54180300
C	-0.49607800	-2.52613600	4.61283800
H	-0.48622500	-2.47654200	5.69775700
C	-0.97669500	-1.44636800	3.87229200
H	-1.34522000	-0.55822300	4.38042600
C	-0.98747400	-1.49911100	2.48135000
H	-1.33713600	-0.65074000	1.89255400
C	-2.40412000	-2.52325700	-0.43250600
C	-3.42585500	-2.47597900	0.52291700
H	-3.18780900	-2.48229800	1.58266300
C	-4.75764800	-2.44699100	0.12178800
H	-5.54305300	-2.42122600	0.87195400
C	-5.08202400	-2.44653100	-1.23229400
H	-6.12246900	-2.41524000	-1.54203600
C	-4.06999900	-2.49857100	-2.18853600
H	-4.31819300	-2.50926800	-3.24573400
C	-2.73772500	-2.55490900	-1.79448600
H	-1.95640300	-2.63326700	-2.54620500
C	-0.43282400	3.32140900	-0.47107400
C	-0.97024000	4.52582000	-0.98738600
H	-1.15961100	4.57373000	-2.05529700
C	-1.24118400	5.59870200	-0.16068400
H	-1.65616900	6.50686200	-0.59104700
C	-1.00581300	5.52897900	1.22155200
H	-1.23255100	6.37428200	1.86252500
C	-0.48694000	4.36512200	1.75371600
H	-0.29288800	4.28393500	2.81892300
C	-0.19506400	3.25875100	0.93179000

C	0.46404900	2.11245000	1.48381700
C	1.72443000	0.27890400	1.74185200
H	1.49346500	-0.79190800	1.77017000
C	1.44483000	0.92534300	3.09957400
H	0.68265700	0.39095400	3.67396400
H	2.33442300	1.07989500	3.70990800
C	3.16749200	0.48938100	1.33329700
C	4.12542600	-0.43856400	1.74940800
H	3.80391800	-1.34275700	2.26441900
C	5.47675500	-0.22188600	1.49939000
H	6.20920700	-0.95791900	1.81975600
C	5.88667800	0.92947700	0.82962000
H	6.94096600	1.09918000	0.62999500
C	4.93656800	1.85879000	0.41194700
H	5.24660100	2.75345200	-0.12150300
C	3.58434600	1.64245700	0.66348600
H	2.84689000	2.36458300	0.31778500
C	-3.82461900	1.57335900	0.82607400
C	-2.86311700	1.13550500	-0.31474700
O	-1.73021800	0.63107100	0.10297500
O	-0.83618200	0.34693400	-2.65420200
C	-0.60614000	-0.55435900	-3.53154000
O	0.00252900	-1.63505000	-3.33418400
C	-1.19067200	-0.26945300	-4.89069400
H	-0.68264200	-0.85338000	-5.65874900
H	-2.24669300	-0.55799500	-4.88526800
H	-1.14529400	0.79391800	-5.12857500
H	0.05026300	-1.67396800	-1.73559900
C	-5.23492000	1.08315900	0.50183900
H	-5.95274100	1.49771900	1.21870100
H	-5.52618200	1.39621800	-0.50380100
H	-5.30347300	-0.00652200	0.54924700
C	-3.40310100	1.08087700	2.20404900
H	-3.42219200	-0.01328600	2.26126000
H	-2.39064200	1.41643100	2.45860800
H	-4.09004900	1.46438300	2.96781300
C	-3.83670000	3.10615000	0.81170700
H	-2.86004400	3.52156600	1.07224300
H	-4.11255500	3.48197600	-0.17795600
H	-4.56637600	3.48011100	1.53957500
5-ts-OPiv-1			
O 1			
Co	-0.26724200	0.43950700	0.62351100

P	-0.89429500	-0.87900100	-2.52043200
O	-0.78617100	-0.44070600	-3.95467200
O	-0.31820400	0.87712100	2.48043800
O	1.96565800	-2.59275400	2.24444600
O	-3.29101600	-0.15051100	1.83267600
N	-0.11967600	0.26677000	-1.45670200
N	1.05998900	1.84718400	0.27389700
N	1.16530400	-0.87761200	1.04396600
C	1.44364800	2.77882100	1.13339400
H	0.89736700	2.80509700	2.07212200
C	2.51414800	3.64441400	0.85477700
H	2.79070800	4.39574100	1.58581300
C	3.21949900	3.48978800	-0.31675800
H	4.08258400	4.11386000	-0.53368100
C	2.83152500	2.50335400	-1.25040800
C	1.69468400	1.71757800	-0.92463400
C	1.17361000	0.75430100	-1.82952100
C	1.88596000	0.49505000	-2.98749700
H	1.51737000	-0.22967800	-3.70340200
C	3.05255700	1.23201600	-3.28467600
H	3.58321700	1.00695200	-4.20511300
C	3.50561000	2.23813100	-2.46376300
H	4.38776500	2.81818500	-2.71824600
C	-0.13185600	-2.49678300	-2.25920600
C	0.48932000	-3.08791500	-3.36651700
H	0.51242900	-2.54631400	-4.30865600
C	1.05515700	-4.35559600	-3.25929700
H	1.54258800	-4.80460500	-4.11974000
C	0.97761100	-5.05274400	-2.05611800
H	1.40052000	-6.05022800	-1.97775400
C	0.35612700	-4.47035100	-0.95209800
H	0.29550400	-5.01284900	-0.01163200
C	-0.18049600	-3.18868000	-1.04063200
H	-0.63519800	-2.71398300	-0.17186200
C	-2.62181900	-0.93166600	-1.98977000
C	-3.23668000	-2.09381300	-1.51360900
H	-2.65376100	-2.99791800	-1.36370200
C	-4.59844400	-2.10335900	-1.22697900
H	-5.05947100	-3.01216700	-0.85020600
C	-5.36370900	-0.95620800	-1.41878100
H	-6.42517400	-0.96452500	-1.18912800
C	-4.76573300	0.19748800	-1.92123900
H	-5.36044500	1.09032000	-2.09533700
C	-3.40729700	0.20739500	-2.22007700

H	-2.95791600	1.10291800	-2.63916700
C	-0.39486700	-0.05707100	3.39250500
C	-1.12596000	0.19748400	4.57499300
H	-1.63134700	1.15512000	4.65665000
C	-1.21217200	-0.74870100	5.57925600
H	-1.79706200	-0.52559500	6.46814500
C	-0.57613000	-1.99375800	5.46038200
H	-0.66103700	-2.73374600	6.24924600
C	0.15906300	-2.26501100	4.32136000
H	0.66778600	-3.21769800	4.20569600
C	0.26019500	-1.31834700	3.28629600
C	1.09947600	-1.57087700	2.14908100
C	2.32222100	-1.35876400	0.27211900
H	2.02748800	-1.53227200	-0.77042600
C	2.63433300	-2.69372400	0.96631700
H	2.22357800	-3.55680300	0.43608800
H	3.69740800	-2.84576300	1.15642900
C	3.51578600	-0.43151300	0.31116100
C	4.44944800	-0.50722000	-0.72472900
H	4.24698500	-1.15239800	-1.57819200
C	5.61762300	0.24671100	-0.68108000
H	6.32883600	0.18842700	-1.50071800
C	5.86488800	1.08623500	0.40309400
H	6.77250600	1.68218800	0.43652400
C	4.93860900	1.16358700	1.44123600
H	5.12046900	1.82372100	2.28535000
C	3.77083700	0.40576000	1.39947000
H	3.04375700	0.47757300	2.20672400
C	-2.96894800	-2.52096600	1.81681000
H	-2.50493900	-2.77280100	2.77774800
H	-2.60298800	-3.23985500	1.07874900
H	-4.05052900	-2.61762900	1.92533100
C	-2.59033900	-1.08982100	1.47572800
O	-1.44833100	-1.04302300	0.83441900
O	-1.67713100	1.78574200	0.50745000
C	-1.87209200	2.57818100	-0.45691100
O	-1.32781800	2.45694500	-1.60251600
C	-2.78162300	3.77340400	-0.18958400
H	-0.75467700	1.30273100	-1.57415200
C	-3.94885000	3.35171100	0.70226400
H	-4.58491800	4.21767800	0.91227700
H	-4.56473300	2.58810600	0.21529700
H	-3.59665700	2.93495500	1.64775600
C	-3.29565400	4.35759100	-1.50156300

H	-3.92823100	5.22724400	-1.29709000
H	-2.47562900	4.67364900	-2.15049300
H	-3.89704600	3.62799400	-2.05401800
C	-1.91538800	4.80719400	0.54593100
H	-2.50587500	5.70400600	0.75904900
H	-1.54895500	4.40492000	1.49556600
H	-1.05082300	5.10700700	-0.05658500

5-ts-OPiv-2

O 1

Co	-0.05409500	0.51900700	-0.87539000
P	-0.72369000	-2.81288000	0.04427100
O	-0.30602800	-4.17768000	-0.42772000
O	-0.12852100	2.36213600	-1.33748800
O	0.92784300	2.23522700	2.72203300
O	-3.18225500	1.33666800	-1.49427300
N	0.25354000	-1.56722000	-0.68951400
N	1.73383200	0.35436800	-1.69891800
N	0.77287000	0.99611000	0.86234400
C	2.33290200	1.29562900	-2.41287000
H	1.73059200	2.17128100	-2.63559600
C	3.67088600	1.17432700	-2.82124500
H	4.11902000	1.96851900	-3.40741200
C	4.39830000	0.07299100	-2.43100600
H	5.44927700	-0.02180500	-2.69207000
C	3.78240000	-0.94742100	-1.67399100
C	2.40653300	-0.78000600	-1.36008700
C	1.67175000	-1.78430300	-0.67654600
C	2.36443400	-2.88226800	-0.19626900
H	1.84251100	-3.67595700	0.32450700
C	3.74527900	-3.02239100	-0.45269600
H	4.25327100	-3.90069400	-0.06551400
C	4.44254500	-2.10356300	-1.20068400
H	5.49858600	-2.23731000	-1.41636000
C	-0.58098600	-2.63663000	1.83265100
C	-0.13015900	-3.73837000	2.56761700
H	0.17206100	-4.63911300	2.03910900
C	-0.08631100	-3.67784400	3.95790800
H	0.27142200	-4.53138900	4.52605800
C	-0.52483000	-2.53245300	4.61859400
H	-0.51421900	-2.49431200	5.70404500
C	-0.98289200	-1.43589200	3.88846800
H	-1.33386600	-0.54529100	4.40491600
C	-0.99282500	-1.47441800	2.49699700

H	-1.32468400	-0.61225700	1.91782200
C	-2.43796200	-2.47448500	-0.41521700
C	-3.44623500	-2.39547700	0.55271200
H	-3.19276700	-2.37339200	1.60840800
C	-4.78495700	-2.37352100	0.17309500
H	-5.55693400	-2.32383200	0.93600900
C	-5.13354100	-2.40896000	-1.17418400
H	-6.17889800	-2.38025800	-1.46728100
C	-4.13714700	-2.49782300	-2.14369000
H	-4.40141600	-2.54241200	-3.19627500
C	-2.79942600	-2.55179300	-1.76811400
H	-2.03506300	-2.67556100	-2.52882700
C	-0.39911900	3.32984400	-0.50579600
C	-0.91836600	4.53874900	-1.03073100
H	-1.10813700	4.58165800	-2.09883600
C	-1.17580600	5.62027700	-0.21124500
H	-1.57881300	6.53092500	-0.64775300
C	-0.94218200	5.55685700	1.17182000
H	-1.15836500	6.40936100	1.80686400
C	-0.43793400	4.39042000	1.71188200
H	-0.24487100	4.31359600	2.77760200
C	-0.16012400	3.27483000	0.89723400
C	0.48353800	2.12412300	1.45728600
C	1.72178400	0.27603800	1.73253900
H	1.47859800	-0.79159400	1.76340100
C	1.44076100	0.93289400	3.08448300
H	0.66758900	0.41150800	3.65623000
H	2.32799000	1.07928000	3.70019400
C	3.16960100	0.46910600	1.33292700
C	4.11237900	-0.47109800	1.75616800
H	3.77478600	-1.37126400	2.26790000
C	5.46796900	-0.27288100	1.51459700
H	6.18849200	-1.01855100	1.83972100
C	5.89734600	0.87227900	0.84640700
H	6.95503000	1.02751700	0.65288000
C	4.96237300	1.81383000	0.42192900
H	5.28779000	2.70361600	-0.11058200
C	3.60576100	1.61612900	0.66528800
H	2.88002300	2.34723200	0.31366800
C	-3.80443200	1.62282800	0.80155400
C	-2.84474100	1.15499500	-0.32835100
O	-1.71932400	0.64418900	0.09992900
O	-0.82234500	0.33883900	-2.67965600
C	-0.62023200	-0.61452300	-3.48407700

O	-0.04848400	-1.71066700	-3.17444200
C	-1.13431200	-0.46232500	-4.88245700
H	-2.06922400	-1.02434100	-4.97349300
H	-1.33368700	0.58063100	-5.12333900
H	-0.42788600	-0.89123200	-5.59465200
H	0.05784400	-1.68090400	-1.88159400
C	-5.21977400	1.14544900	0.47904400
H	-5.30273400	0.05717900	0.53849600
H	-5.93449800	1.57800800	1.18831100
H	-5.50319300	1.45038700	-0.53136900
C	-3.39208200	1.14740700	2.18841600
H	-3.41508800	0.05441300	2.26076200
H	-2.37977400	1.48293500	2.44406900
H	-4.08142100	1.54433600	2.94310300
C	-3.79768400	3.15531100	0.76431000
H	-2.81794800	3.56174700	1.02671000
H	-4.06140700	3.52121400	-0.23236700
H	-4.52775500	3.54842800	1.48153200

5-ts-OPiv-3

O 1

Co	0.03871700	0.62885500	0.50511600
P	0.56253400	-2.80999900	-0.01586100
O	0.20134700	-4.09999800	0.66752300
O	0.17401400	2.52176400	0.64571800
O	-1.20947000	1.76130800	-3.22785600
O	3.16518100	1.52620100	0.71571000
N	-0.28179600	-1.45581400	0.68307300
N	-1.64347900	0.64389400	1.52267700
N	-0.93049600	0.84462900	-1.20356100
C	-2.14929200	1.69822700	2.14464200
H	-1.52359000	2.58559800	2.14361300
C	-3.42675000	1.66978100	2.72642800
H	-3.79910100	2.55517500	3.22913600
C	-4.19660200	0.53578100	2.60403300
H	-5.20875100	0.50373400	2.99903400
C	-3.67642700	-0.60429200	1.95387600
C	-2.34635400	-0.51895700	1.45917100
C	-1.69613400	-1.63765100	0.87477300
C	-2.44555000	-2.78294500	0.66571300
H	-1.99050800	-3.66531000	0.23369900
C	-3.78852500	-2.84912300	1.09554500
H	-4.33931500	-3.76808400	0.91866000
C	-4.39179900	-1.80600400	1.75674900

H	-5.41491300	-1.87940200	2.11385300
C	0.17257900	-2.86169400	-1.77611300
C	-0.54561500	-3.94751900	-2.28672900
H	-0.89539100	-4.72161200	-1.60775200
C	-0.77967800	-4.04256000	-3.65631200
H	-1.34155200	-4.88311400	-4.05282200
C	-0.26957100	-3.07457700	-4.51887800
H	-0.43324300	-3.16251800	-5.58916400
C	0.45684600	-1.99650500	-4.01170500
H	0.85775000	-1.24241500	-4.68541500
C	0.66311500	-1.87750600	-2.64089600
H	1.19286800	-1.02192000	-2.22471600
C	2.33884600	-2.50160200	0.09538300
C	3.12106200	-3.38430600	-0.66729200
H	2.64569900	-4.05257500	-1.38273400
C	4.50142500	-3.42462700	-0.50783700
H	5.09326100	-4.11147800	-1.10555700
C	5.11819200	-2.58864100	0.42039000
H	6.19635800	-2.61999800	0.54970100
C	4.35144100	-1.69569200	1.16418000
H	4.83025000	-1.01197100	1.85977400
C	2.96904300	-1.64954300	1.00527600
H	2.40144200	-0.91101000	1.55707100
C	0.43566400	3.31091600	-0.36039700
C	1.02998000	4.56795800	-0.09265900
H	1.28311100	4.79399400	0.93882100
C	1.27823600	5.47083900	-1.10869200
H	1.74018700	6.42519700	-0.86744200
C	0.96355000	5.16824000	-2.44305800
H	1.17414300	5.87976500	-3.23446000
C	0.38220100	3.94927100	-2.73331400
H	0.11985700	3.69103800	-3.75485700
C	0.10905000	3.01593400	-1.71486700
C	-0.64460300	1.83182000	-2.01060100
C	-1.98806500	0.04021400	-1.84004100
H	-1.76805700	-1.02834200	-1.73275500
C	-1.85751100	0.47109200	-3.30571800
H	-1.21589000	-0.19430900	-3.88888100
H	-2.81452900	0.60669900	-3.80974700
C	-3.37277600	0.33354200	-1.30648600
C	-4.36207700	-0.64247900	-1.44741200
H	-4.09160100	-1.62004700	-1.84482500
C	-5.67527400	-0.37829400	-1.07168200
H	-6.43218100	-1.15102100	-1.17456700

C	-6.01336500	0.86885000	-0.54990700
H	-7.03680600	1.07618300	-0.25012400
C	-5.03153800	1.84756800	-0.40960600
H	-5.28604400	2.81952400	0.00507500
C	-3.71764800	1.58392000	-0.78819800
H	-2.95119900	2.34650400	-0.66131200
C	3.64849600	1.32961700	-1.62560800
C	2.75417300	1.12706600	-0.37176900
O	1.60704200	0.55114300	-0.61817700
O	0.93227400	0.72120700	2.24745800
C	0.84197400	-0.09902900	3.20664000
O	0.38034300	-1.27926500	3.09838100
C	1.41630500	0.34375200	4.54976600
H	0.08942600	-1.42391700	1.83232400
C	1.34703400	1.86196900	4.68746400
H	1.78930300	2.16905600	5.64067700
H	1.88479300	2.36008000	3.87715600
H	0.31033000	2.21494300	4.66914700
C	2.88250500	-0.11401200	4.55161300
H	3.35105600	0.14140600	5.50748000
H	2.96063700	-1.19733700	4.41221400
H	3.44779700	0.37900700	3.75377700
C	0.65635100	-0.33359000	5.68745400
H	1.08876900	-0.04017200	6.64932600
H	-0.39882000	-0.04066500	5.68985400
H	0.70380800	-1.42143600	5.60389200
C	4.99235300	0.64803200	-1.36881900
H	4.88246600	-0.44011700	-1.31787200
H	5.69474600	0.87894300	-2.17799000
H	5.42396500	0.98978400	-0.42397300
C	3.04422500	0.78480400	-2.91401900
H	2.98843500	-0.30818800	-2.89781100
H	2.03632200	1.17757000	-3.09209400
H	3.67230300	1.06446000	-3.76831100
C	3.86790200	2.83908300	-1.76549400
H	2.93670800	3.35659700	-2.01731300
H	4.25108900	3.26220500	-0.83309000
H	4.59143100	3.03980100	-2.56422500

6-OPiv

O 1

Co	0.15567000	0.34466000	-0.78322600
P	-0.97043900	-1.75871200	1.50228100
O	-0.45321000	-2.89737400	2.34788700

O	0.29950100	1.90945000	-1.89895300
O	1.44657500	3.04286100	1.96189000
O	-1.04824000	-0.37049200	-2.18074200
N	0.05742100	-1.35097400	0.23138800
N	1.74537700	-0.41510600	-1.53543700
N	1.03840400	1.27779700	0.65436600
C	2.57966800	0.18660400	-2.36955700
H	2.42187200	1.25027600	-2.51481700
C	3.58853300	-0.53048500	-3.03207200
H	4.25438700	-0.00443000	-3.70704200
C	3.70886400	-1.88363700	-2.81422900
H	4.47882700	-2.45979000	-3.32130000
C	2.83248100	-2.54481000	-1.92333400
C	1.84100700	-1.74938900	-1.28381500
C	0.90841000	-2.28233300	-0.34021300
C	0.97802400	-3.66151200	-0.11644800
H	0.29047900	-4.12411100	0.57986800
C	1.95543100	-4.44775700	-0.75028400
H	1.97249700	-5.51225400	-0.53032600
C	2.87969600	-3.92441600	-1.63134600
H	3.62724700	-4.54958000	-2.11001400
C	-1.23760400	-0.32606300	2.60156300
C	-0.57461100	-0.39084600	3.83659100
H	0.06354700	-1.24710300	4.04132800
C	-0.73882500	0.61249800	4.78682400
H	-0.21680300	0.54727000	5.73761200
C	-1.57880800	1.69271200	4.51938300
H	-1.70936700	2.47771500	5.25898300
C	-2.26590900	1.75065000	3.30944900
H	-2.93832300	2.57910000	3.10418900
C	-2.10673300	0.74388000	2.35892100
H	-2.65870300	0.79432900	1.42743000
C	-2.58780300	-2.16692200	0.78631200
C	-3.74866400	-2.08691200	1.56738400
H	-3.70342300	-1.63868200	2.55774200
C	-4.95830500	-2.58191700	1.08881000
H	-5.85285200	-2.50799400	1.70063100
C	-5.01834100	-3.18034400	-0.16873000
H	-5.95984000	-3.57535700	-0.53917200
C	-3.86883500	-3.26737600	-0.95165000
H	-3.91322500	-3.73206100	-1.93315600
C	-2.66107700	-2.75517500	-0.48254000
H	-1.76868900	-2.80741500	-1.10265300
C	0.07816200	3.11096000	-1.43187100

C	-0.37807300	4.11460300	-2.32048200
H	-0.54843300	3.83029400	-3.35478000
C	-0.61415700	5.40535800	-1.88725800
H	-0.97990900	6.14325400	-2.59711900
C	-0.40073700	5.77333200	-0.55002400
H	-0.59624800	6.78765100	-0.21829000
C	0.07053600	4.82395300	0.33595500
H	0.26424700	5.08314300	1.37282300
C	0.31511500	3.50175100	-0.07953000
C	0.91182600	2.56299300	0.82958600
C	1.84883000	0.71274200	1.75007200
H	1.28377400	-0.09621000	2.21832900
C	1.95732400	1.91029500	2.70718300
H	1.33617700	1.79211700	3.59972200
H	2.98264900	2.14439700	2.99953700
C	3.16820500	0.14864100	1.28971500
C	3.48054800	-1.18354200	1.56575200
H	2.74748800	-1.80332500	2.08153400
C	4.70001300	-1.72316900	1.16272300
H	4.92522500	-2.76553100	1.37135000
C	5.61851900	-0.92947500	0.48092100
H	6.56826400	-1.34799100	0.15953900
C	5.31543000	0.40449700	0.20532000
H	6.02848700	1.02491100	-0.33093500
C	4.09712400	0.94045600	0.60848800
H	3.85830700	1.97947200	0.38368400
C	-3.33391600	0.49692600	-2.31244200
C	-1.99783200	0.28635500	-1.64164600
O	-1.73089400	0.85684700	-0.52770200
C	-3.56253000	-0.54628200	-3.40032300
H	-4.52299700	-0.36128800	-3.89098000
H	-2.77818300	-0.50777400	-4.16031300
H	-3.58414100	-1.55743000	-2.98465300
C	-4.44612500	0.45757600	-1.26479800
H	-4.28027800	1.20700000	-0.48594700
H	-5.40904000	0.66817900	-1.74075300
H	-4.51270700	-0.52468300	-0.78641000
C	-3.26430700	1.89784100	-2.94309000
H	-2.44580600	1.96491400	-3.66709800
H	-4.20237900	2.10915300	-3.46598300
H	-3.11019400	2.66876300	-2.18255500

7-ts-s-OPiv

0 1

Co	0.30427400	-0.49450900	0.31583200
P	-1.54688300	0.65602300	-1.92431000
O	-1.40246200	1.66481200	-3.03605600
O	1.17605800	-1.89485000	1.28952400
O	3.78759800	-0.65401800	-1.82841500
O	-1.15336500	-0.73201400	1.62334500
N	-0.75048800	0.92420200	-0.48899300
N	0.84146100	0.94278600	1.56178700
N	1.85106300	-0.18876000	-0.81452800
C	1.73441900	0.87405300	2.53451400
H	2.28953400	-0.05614500	2.61606600
C	1.93898100	1.94892700	3.41753400
H	2.68441500	1.85635500	4.19952100
C	1.18615000	3.09338800	3.27863900
H	1.32644200	3.93220700	3.95616600
C	0.22246600	3.19204100	2.24791500
C	0.09187300	2.06676100	1.39013900
C	-0.80862300	2.05637100	0.28219900
C	-1.59980700	3.18702300	0.08668600
H	-2.28840100	3.22462100	-0.75316600
C	-1.48511300	4.29208600	0.94859000
H	-2.11524800	5.15771000	0.76106100
C	-0.59790800	4.31834200	2.00648400
H	-0.51814500	5.18686400	2.65317200
C	-0.78507700	-0.93743700	-2.32182800
C	-0.55002300	-1.28027800	-3.65241500
H	-0.88271000	-0.61377000	-4.44583000
C	0.13769900	-2.45542500	-3.95429200
H	0.32816700	-2.72115500	-4.99042000
C	0.58463400	-3.28726300	-2.92702700
H	1.11432700	-4.20593800	-3.16535400
C	0.36114500	-2.93475100	-1.59943700
H	0.71250500	-3.58698800	-0.80135100
C	-0.32146800	-1.75183500	-1.26404100
H	-1.13619500	-2.04467300	-0.25547700
C	-3.29933600	0.36133900	-1.54967400
C	-4.18132200	0.10653300	-2.60862100
H	-3.80706800	0.09902700	-3.63046100
C	-5.52937200	-0.13103600	-2.36179000
H	-6.20417400	-0.33432700	-3.18844600
C	-6.01377100	-0.10258800	-1.05469700
H	-7.06737200	-0.28331700	-0.86147900
C	-5.14705600	0.16414200	0.00283600
H	-5.52816300	0.20105900	1.02088900

C	-3.79360300	0.38775800	-0.24070200
H	-3.11501900	0.59760200	0.58405700
C	2.31037000	-2.47835900	1.01672200
C	2.69850300	-3.58726800	1.81204900
H	2.02880900	-3.88391200	2.61455800
C	3.87077400	-4.27418700	1.56810600
H	4.12692000	-5.12418000	2.19597600
C	4.72826400	-3.89780200	0.52144000
H	5.64497700	-4.44680300	0.33346600
C	4.38458500	-2.81730000	-0.26416800
H	5.02778800	-2.50244000	-1.08003800
C	3.19678400	-2.09307200	-0.03447000
C	2.89395500	-0.96674700	-0.87053400
C	2.00514200	0.89030400	-1.81035600
H	1.09797100	0.95806400	-2.41929700
C	3.17351300	0.36373500	-2.65258100
H	2.84037900	-0.11486600	-3.57934700
H	3.93159700	1.11477200	-2.87720000
C	2.25639600	2.23204400	-1.16865400
C	1.48440900	3.33261400	-1.54217600
H	0.67732700	3.18961000	-2.25965900
C	1.71726900	4.58242700	-0.97295400
H	1.09987500	5.42966400	-1.25925500
C	2.72225500	4.73983700	-0.02233200
H	2.89529200	5.71158200	0.43201200
C	3.49755200	3.64367600	0.35577900
H	4.27779800	3.75959200	1.10327600
C	3.26741600	2.39680700	-0.21681800
H	3.86738100	1.54079300	0.08975100
C	-2.84658600	-1.98163400	2.75914200
C	-1.94615800	-1.71390500	1.55719600
O	-1.98842500	-2.51483700	0.57057500
C	-3.24222500	-0.66692300	3.42825100
H	-3.84120000	-0.87269600	4.32075400
H	-2.36432000	-0.08858600	3.72540300
H	-3.84667000	-0.04363000	2.76055300
C	-4.08805400	-2.76146400	2.33697900
H	-3.82407300	-3.71894300	1.88249100
H	-4.71634700	-2.95685600	3.21150500
H	-4.68370500	-2.19716800	1.61147700
C	-1.99896200	-2.82047000	3.72843100
H	-2.58697300	-3.05938900	4.62012600
H	-1.68300500	-3.76184500	3.26783900
H	-1.10488800	-2.27362800	4.04379700

7-ts-r-OPiv

O 1

Co	-0.85227000	0.29976800	0.07956000
P	1.76497600	1.53373900	-0.95057200
O	1.88239500	2.96857100	-0.50452600
O	-2.76638800	0.33903000	0.19604700
O	-1.68757800	-3.11672800	-2.02345500
O	-0.90327500	1.90982300	1.19583000
N	1.10429400	0.43390600	0.12761800
N	-0.60223900	-0.59358000	1.81828200
N	-0.87315200	-1.39811000	-0.85140200
C	-1.52740400	-1.16899700	2.56788200
H	-2.52222100	-1.23970700	2.13791400
C	-1.23376800	-1.64713500	3.85638300
H	-2.01830300	-2.11903500	4.43743600
C	0.03786400	-1.49382900	4.36149400
H	0.28155900	-1.84366100	5.36175800
C	1.04305100	-0.87366700	3.58378200
C	0.66934700	-0.44499700	2.28043500
C	1.59570900	0.17434300	1.38787200
C	2.88467400	0.40014600	1.86644100
H	3.62240900	0.88307700	1.23228900
C	3.25233100	-0.01445500	3.15934300
H	4.27115300	0.17303900	3.48854000
C	2.37131300	-0.64895500	4.01087500
H	2.67545200	-0.96728500	5.00347600
C	3.39146500	0.93268800	-1.50315500
C	4.51200100	1.71259000	-1.19305500
H	4.36338700	2.65007000	-0.66273300
C	5.78867400	1.29418500	-1.55727800
H	6.65042300	1.90623800	-1.30740600
C	5.95917100	0.09548900	-2.24623300
H	6.95458100	-0.23042500	-2.53438100
C	4.85003900	-0.68241600	-2.57411300
H	4.97735900	-1.61231700	-3.12106100
C	3.57473900	-0.26653000	-2.20236900
H	2.71503600	-0.87233300	-2.48084800
C	0.57516400	1.23111900	-2.27676800
C	0.91769700	1.07359800	-3.61894000
H	1.95851200	1.13418800	-3.92995800
C	-0.07646700	0.81885600	-4.56349700
H	0.19215000	0.68850900	-5.60817200
C	-1.41255900	0.73567000	-4.17120500

H	-2.18428400	0.54606400	-4.91223200
C	-1.75508800	0.90320300	-2.83292800
H	-2.80106300	0.85770500	-2.53485500
C	-0.77546100	1.15366700	-1.85671500
H	-1.21280900	2.10445700	-1.06181700
C	-3.63307100	-0.47125700	-0.34297000
C	-5.01169400	-0.18340000	-0.16814500
H	-5.26732600	0.69937000	0.41038400
C	-5.99059400	-0.98702000	-0.71529400
H	-7.03553400	-0.72913100	-0.55972600
C	-5.65867300	-2.12443900	-1.46995500
H	-6.43514300	-2.74906800	-1.89892400
C	-4.32752100	-2.43352700	-1.65763200
H	-4.04098300	-3.30571700	-2.23699800
C	-3.30550700	-1.63435600	-1.10440100
C	-1.93368300	-2.00523200	-1.30241000
C	0.31572000	-2.19257300	-1.19983700
H	1.06221900	-1.52520200	-1.63923200
C	-0.25824300	-3.15161000	-2.24866500
H	-0.07427600	-2.81202300	-3.27308900
H	0.07329300	-4.18447200	-2.13717400
C	0.91484100	-2.88050300	0.00319500
C	2.27938100	-2.77300500	0.27228600
H	2.90083800	-2.15288100	-0.37212400
C	2.83799700	-3.42023800	1.37199500
H	3.89965400	-3.31459800	1.57859300
C	2.03290400	-4.18195700	2.21434800
H	2.46452200	-4.67683400	3.08013500
C	0.66863500	-4.29926900	1.94969100
H	0.03436800	-4.88851300	2.60644500
C	0.11405300	-3.65386500	0.84944400
H	-0.95472300	-3.73663000	0.65592500
C	-1.46388600	4.17870000	1.71567200
C	-1.32832500	3.01100200	0.74077800
O	-1.60415000	3.20268800	-0.48346100
C	-0.15477300	4.97550900	1.62972400
H	0.01705200	5.34946000	0.61630000
H	-0.20408800	5.83194000	2.30999800
H	0.70333500	4.35871500	1.91124600
C	-1.66114500	3.65816900	3.13690300
H	-1.74406400	4.50024600	3.83129400
H	-2.57401500	3.05981500	3.21945200
H	-0.82215700	3.03197800	3.45013200
C	-2.63758300	5.06451100	1.30234800

H	-3.58422500	4.51581200	1.33403500
H	-2.71850600	5.91312000	1.98900200
H	-2.50525000	5.45237700	0.28991600