

Supporting Information

Computational Insight into the Mechanism and Stereoselectivity of Cycloaddition between Donor-acceptor Spirocyclopropane and Aldehyde Catalyzed by Brønsted Acid TsOH

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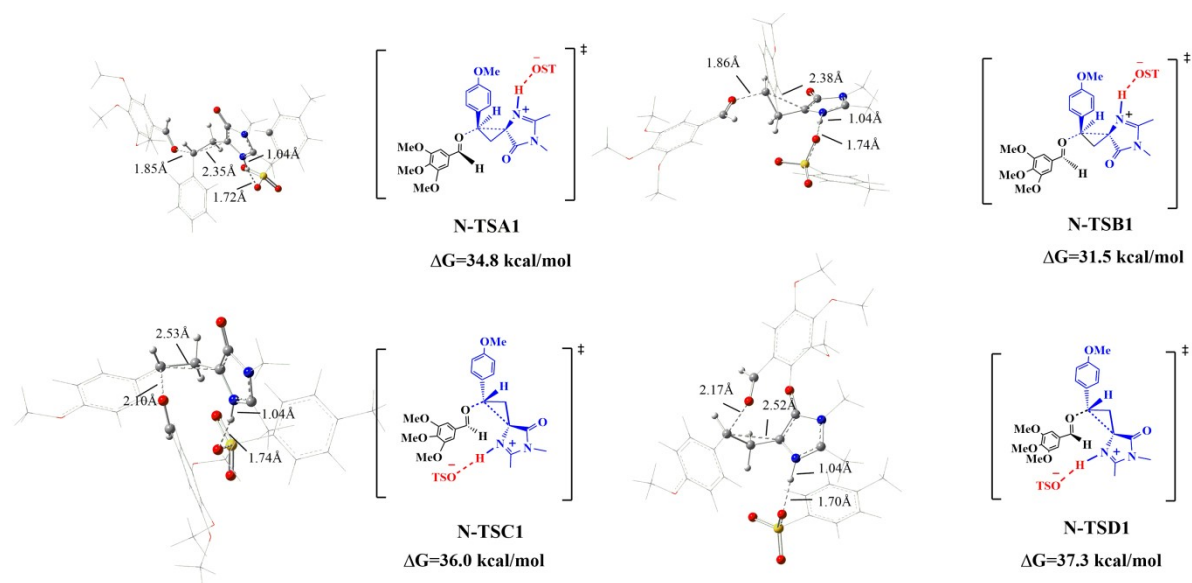


Figure S1. Optimized structures and Gibbs free energy barriers of the transition states of the rate-determining steps of paths A, B, C and D in reaction between aldehyde **2a** and ion-pair complex **1a-TsOH-N** (in dichloromethane, 273.15 K, energies are given in kcal/mol).

Table S1. List of absolute energies of optimized structures in this article.

Compounds	E (a.u.) ^a	G_{corr} (a.u.) ^b	G_{sol} (a.u.) ^c	Imag Freq(cm ⁻¹) ^d
1a	-802.976125987	0.239108	-802.737017987	
2a	-689.055362055	0.169349	-688.886013055	
TsOH	-895.310529745	0.108665	-895.201864745	
1a-TsOH-O	-1698.308615220	0.368802	-1697.939813220	
1a-TsOH-N	-1698.321215210	0.369754	-1697.951461210	
TSA1	-2387.344239310	0.559706	-2386.784533310	118.32 <i>i</i>
TSB1	-2387.340444320	0.563183	-2386.777261320	307.59 <i>i</i>
TSC1	-2387.322628990	0.559776	-2386.762852990	143.11 <i>i</i>
TSD1	-2387.343221750	0.562473	-2386.780748750	68.21 <i>i</i>
INTA1	-2387.364520460	0.568806	-2386.795714460	
INTB1	-2387.375803340	0.567986	-2386.807817340	
INTC1	-2387.345340060	0.564428	-2386.780912060	
INTD1	-2387.380236650	0.566414	-2386.813822650	
TSA2	-2387.363441520	0.570536	-2386.792905520	40.84 <i>i</i>
TSD2	-2387.381352800	0.566247	-2386.815105800	68.68 <i>i</i>
INTA2	-2387.378602450	0.567927	-2386.810675450	
INTD2	-2387.384050080	0.567688	-2386.816362080	
TSA3	-2387.380047200	0.566426	-2386.813621200	246.00 <i>i</i>
TSD3	-2387.385378380	0.566827	-2386.818551380	108.31 <i>i</i>
3aa	-2387.414561220	0.566610	-2386.847951220	
3'aa	-2387.412796320	0.568265	-2386.844531320	
3dd	-2387.413817510	0.565347	-2386.848470510	
3'dd	-2387.414496150	0.566884	-2386.847612150	
N-TSA1	-2387.341700810	0.559682	-2386.782018810	304.57 <i>i</i>
N-TSB1	-2387.348318250	0.560996	-2386.787322250	288.98 <i>i</i>
N-TSC1	-2387.338881100	0.560790	-2386.778091100	111.65 <i>i</i>
N-TSD1	-2387.335166660	0.560691	-2386.774475660	131.62 <i>i</i>
2b	-345.52950960	0.082747	-345.44676260	
2c	-437.76928708	0.078826	-437.69046108	
2d	-349.13341160	0.150286	-348.98312555	
2e	-666.29878192	0.049094	-666.24968792	
TSA1-2b	-2043.818430000	0.472249	-2043.346181000	142.16 <i>i</i>
TSA1-2c	-2136.058567740	0.469471	-2135.589096740	224.39 <i>i</i>
TSA1-2d	-2047.424436620	0.540678	-2046.883758620	150.22 <i>i</i>
TSA1-2e	-2364.594480310	0.441893	-2364.152587310	119.56 <i>i</i>

a. Electronic energies (E) calculated at the M06-2X/SMD/6-311+G(d,p)//B3LYP-D3/SMD/6-31G(d,p) level.

b. Frequency calculations were performed and the thermal free energy corrections (G_{corr}) were obtained

using the experimental temperature 273.15 K at the B3LYP-D3/SMD/6-31G(d,p) level on geometries optimized in the solution phase at the same level of theory.

c. Absolute free energies calculated with the equation: $G_{\text{sol}} = E + G_{\text{corr}}$.

d. Imaginary frequency (Imag Freq) was obtained from the optimized transition structure in the solution phase at the B3LYP-D3/SMD/6-31G(d,p) level of theory.

The optimized Cartesian coordinates (Å) for ground state and transition state geometries along the potential energy profiles in dichloromethane.

1a

C	-1.83571400	-1.14632900	-0.81689800
C	-1.00226400	-0.84069200	0.26524200
C	-1.49485500	0.04604000	1.24004400
C	-2.76440400	0.59724000	1.13169600
C	-3.58903500	0.27761100	0.04071600
C	-3.11771100	-0.60285600	-0.94003600
H	-1.48193000	-1.82891800	-1.58555600
H	-0.87454900	0.31998300	2.08611300
H	-3.14122500	1.28248900	1.88469600
H	-3.72888300	-0.87185500	-1.79305600
O	-4.81642400	0.87197800	0.03160500
C	-5.69606900	0.58632600	-1.05449100
H	-5.95102600	-0.47999800	-1.09823900
H	-6.60296100	1.16412600	-0.86692200
H	-5.26555000	0.89499300	-2.01532300
C	0.35073300	-1.45843600	0.33177800
C	1.14262300	-1.62017400	1.58843600
H	0.53112500	-2.22233100	-0.42111100
H	1.75117400	-2.51364400	1.69481200
H	0.74051300	-1.20996100	2.50945700
C	1.62336200	-0.60510800	0.57561500
C	2.81812400	-0.88495300	-0.27260700
C	2.56275300	1.31481600	0.18608600
N	1.55632600	0.80546700	0.81773900
N	3.35667800	0.37518500	-0.48646800
C	2.90951400	2.76360400	0.13824500
H	2.91261500	3.12937500	-0.89434500
H	2.17873900	3.33111100	0.71622200
H	3.90927900	2.93866200	0.55070800
C	4.54036400	0.63447000	-1.28611100
H	4.30260300	1.27229300	-2.14235500
H	5.32096000	1.11221000	-0.68738000
H	4.90559200	-0.32836200	-1.64780100
O	3.24367000	-1.94999000	-0.70349200

2a

C	-1.98752100	-0.38685900	0.07942100
C	-1.08780100	-1.46098300	0.08613100

C	0.28116800	-1.21239300	0.06184700
C	0.76468300	0.11246600	0.04484400
C	-0.14773800	1.19103100	0.00575900
C	-1.51729200	0.93034700	0.02438200
H	-1.43681300	-2.48882500	0.11145700
H	-2.21770500	1.75805600	0.00681400
O	0.22976000	2.50064400	0.02090900
O	2.11268400	0.36133400	0.05529500
O	1.14776500	-2.27524800	0.13141400
C	1.34162800	2.92517100	-0.78598000
H	2.29018500	2.80458700	-0.25786500
H	1.38225900	2.37196000	-1.72983000
H	1.16724000	3.98368400	-0.99498100
C	2.75721600	0.10793400	1.31887200
H	2.66207500	-0.94366500	1.60551200
H	3.81063100	0.35617900	1.17674700
H	2.33233500	0.74634500	2.10199700
C	1.97751500	-2.47282300	-1.02816200
H	2.57139400	-3.36669000	-0.82690900
H	1.36007400	-2.63918900	-1.91922200
H	2.64223000	-1.62092900	-1.19735000
C	-3.43788500	-0.65749800	0.10370500
O	-4.30517900	0.20251500	0.08175100
H	-3.70798800	-1.73382900	0.14377300

TsOH

C	1.95337000	1.20356900	0.00207900
C	0.56311800	1.22063300	-0.04525400
C	-0.12103500	0.00264000	-0.07291200
C	0.55411600	-1.21867100	-0.06006200
C	1.94632100	-1.21181000	-0.01290000
C	2.66491200	-0.00747400	0.01825000
H	2.49723500	2.14371200	0.02374500
H	0.01744400	2.15754400	-0.06518200
H	0.00299500	-2.15210500	-0.09194300
H	2.48308500	-2.15591900	-0.00339900
S	-1.89479400	0.00731800	-0.12260000
O	-2.39324900	-1.24576700	-0.69761900
O	-2.18088900	-0.02240700	1.49460400
H	-3.14219000	-0.14751000	1.63168400
O	-2.37982200	1.28156600	-0.65927500
C	4.17128000	-0.00311700	0.04371400
H	4.57161300	0.28219600	-0.93682700
H	4.55313300	0.72177200	0.76999700

H 4.57257700 -0.98853900 0.29436500

1a-TSOH-N

C -2.48800200 1.25153400 -0.89455700
C -3.05613100 0.92610200 0.34162200
C -3.02420600 1.88566800 1.36395200
C -2.43181600 3.12581100 1.15822900
C -1.84169200 3.42938000 -0.07793900
C -1.88631000 2.48766000 -1.11520700
H -2.48169600 0.51435600 -1.69213200
H -3.45913400 1.65661700 2.33262800
H -2.39282100 3.86723000 1.95005000
H -1.41747000 2.68701100 -2.06974600
O -1.26256500 4.65503700 -0.17354700
C -0.46810700 4.93425000 -1.32926600
H -1.08007400 4.97428800 -2.23965900
H -0.02953700 5.91942600 -1.15720700
H 0.32748500 4.19098700 -1.44223000
C -3.64679100 -0.42840800 0.56519400
C -3.43571800 -1.15941700 1.84779500
H -4.56202000 -0.66693100 0.02463600
H -4.21259700 -1.82617000 2.20943000
H -2.81519300 -0.69204700 2.60590800
C -2.69472100 -1.63817400 0.61355000
C -3.04733700 -2.91648200 -0.05020700
C -0.81833200 -2.53934300 -0.23081200
N -1.27999300 -1.51220900 0.44149900
N -1.81897700 -3.40771900 -0.54381100
C 0.59833200 -2.71145100 -0.63116800
H 0.75916100 -2.20438500 -1.58771800
H 1.24949700 -2.23636500 0.10296600
H 0.85286200 -3.76765900 -0.72833300
C -1.68726700 -4.65611900 -1.28645100
H -1.23990800 -4.46973600 -2.26463500
H -1.07927700 -5.37072900 -0.72738800
H -2.69253900 -5.05781100 -1.41493000
O -4.12831200 -3.45829900 -0.16951300
C 4.92053500 -0.66571300 -0.85758400
C 3.63133000 -0.16772500 -1.04785300
C 2.87001200 0.21825900 0.05657400
C 3.39522400 0.10490900 1.34639100
C 4.68451500 -0.39408600 1.52375100
C 5.46936500 -0.78376300 0.42736500
H 5.50770200 -0.97217300 -1.71966200

H	3.20607500	-0.09268000	-2.04313000
H	2.78990000	0.38697900	2.20154100
H	5.08742900	-0.48842800	2.52907200
S	1.22118200	0.90732200	-0.19122600
O	0.73464900	0.33315100	-1.47399700
O	0.43754500	0.39616500	1.00263000
H	-0.66275000	-0.67940000	0.69201600
O	1.37494600	2.38297900	-0.17675300
C	6.87457200	-1.29553900	0.62714500
H	7.17905300	-1.96102900	-0.18637800
H	7.59201000	-0.46548200	0.65538500
H	6.97288100	-1.83990500	1.57160900

1a-TsOH-O

C	-0.88842500	-1.91495700	-0.96184500	
C		-1.25427400	-1.31586000	0.25009700
C		-1.95459300	-2.09688700	1.18636300
C		-2.26977700	-3.42149800	0.91611000
C		-1.89117600	-4.01060100	-0.30201900
C		-1.19397800	-3.24825900	-1.24690300
H		-0.34929000	-1.32911100	-1.70215600
H		-2.26784700	-1.66437500	2.13034200
H		-2.81253500	-4.02427800	1.63761000
H		-0.88778200	-3.67212300	-2.19559300
O		-2.24616600	-5.31627600	-0.46349300
C		-1.90877200	-5.95999700	-1.69162400
H		-0.82341700	-5.98891400	-1.84879000
H		-2.28573700	-6.98096800	-1.60939900
H		-2.38615100	-5.46893500	-2.54871000
C		-0.86677000	0.10106700	0.47655100
C		-0.73912800	0.75900500	1.80422700
H		-0.21337700	0.49183600	-0.29522300
H		0.06036600	1.48091500	1.93880600
H		-1.02376300	0.20156500	2.69062600
C		-1.89907000	1.18291800	0.92407700
C		-1.91589200	2.46989300	0.19155800
C		-3.98213000	1.76809300	0.73535900
N		-3.24887400	0.83282300	1.23731900
N		-3.24173900	2.78143400	0.09181500
C		-5.46793700	1.84247700	0.78752700
H		-5.88968100	1.87264200	-0.22301400
H		-5.85498700	0.96766800	1.31161200
H		-5.79597100	2.74894100	1.30804700
C		-3.77333000	3.95891100	-0.57780600

H	-4.42230800	3.66601300	-1.40686900
H	-4.33708300	4.57637100	0.12588300
H	-2.92989800	4.53104600	-0.96547200
O	-0.98610600	3.15643300	-0.27308400
C	3.53298300	-1.47210200	0.60519700
C	2.73845300	-0.56272000	-0.09106900
C	3.22399100	0.72657900	-0.31188400
C	4.48651600	1.11469600	0.14360900
C	5.26434100	0.19201200	0.83693900
C	4.80187100	-1.11173400	1.07987900
H	3.16007400	-2.47730100	0.77980200
H	1.76215600	-0.85578600	-0.45907600
H	4.85250700	2.11784200	-0.04682000
H	6.24726700	0.48560800	1.19503700
S	2.20115800	1.91137500	-1.16594900
O	1.20244200	1.19367900	-1.97664400
O	1.45926500	2.61139000	0.06816300
H	0.46049800	2.80255500	-0.12730400
O	3.06724300	2.89229800	-1.82857800
C	5.66853000	-2.10027100	1.81745900
H	5.10788900	-2.99509500	2.10065600
H	6.51340100	-2.41706500	1.19393900
H	6.08940900	-1.65563100	2.72560000

1a-TsOH-O+2a Complex

C	-1.87054200	-3.27244700	-0.29841300
C	-1.14447400	-2.07861800	-0.15040000
C	-1.61841800	-1.12853300	0.76163600
C	-2.79386000	-1.33297400	1.48607200
C	-3.51979100	-2.51570200	1.30593700
C	-3.03904300	-3.49168100	0.41888300
H	-1.52597300	-4.03882900	-0.98391000
H	-1.07422700	-0.19723800	0.88818400
H	-3.14419000	-0.55997100	2.15772200
H	-3.60892600	-4.40696200	0.29263700
O	-4.69141900	-2.81074700	1.93844600
C	-5.34791400	-1.75797600	2.64618200
H	-5.53429700	-0.90325800	1.98598700
H	-6.29906100	-2.17226900	2.98654800
H	-4.77118900	-1.43104400	3.52083300
C	0.07226900	-1.75549500	-0.94203400
C	0.48521400	-2.45798300	-2.18219500
H	-0.09849900	-3.30347100	-2.52950900
H	0.96772300	-1.87333200	-2.95979500

C	1.31405900	-2.70575500	-0.93466800
C	2.66415000	-2.12595000	-0.78410300
C	2.45193800	-4.08600200	0.29576000
N	1.28231200	-3.94950500	-0.23140000
N	3.33056800	-3.02164800	0.00326700
C	2.90137800	-5.21839700	1.15121100
H	3.18585100	-4.86155700	2.14736400
H	2.08959800	-5.94036800	1.24899900
H	3.77614700	-5.71527000	0.71801100
C	4.70415700	-2.87027700	0.45884400
H	5.32816700	-3.67983700	0.07162300
H	5.07560500	-1.91576100	0.08504400
H	4.74381400	-2.87223100	1.55112200
O	3.15269200	-1.07707700	-1.24506000
C	-2.21868700	0.91371100	-2.10304300
C	-1.63853500	2.06450000	-1.55554200
C	-2.25986100	2.72972300	-0.50026100
C	-3.46895700	2.23345900	0.02832800
C	-4.06251600	1.08921500	-0.55207400
C	-3.43784800	0.43349500	-1.60341400
H	-0.68962300	2.44634400	-1.91688300
H	-3.88743900	-0.46063700	-2.02052900
O	-5.24264000	0.58077100	-0.05846200
O	-4.05690600	2.92049900	1.05411400
O	-1.69590100	3.88282300	-0.02591100
C	-6.39840200	1.40663400	-0.28598300
H	-6.30728200	2.37479700	0.21666100
H	-6.55208200	1.56719700	-1.35975700
H	-7.24967800	0.85993200	0.12439100
C	-4.22914100	2.19923800	2.28934800
H	-3.26697300	1.81414800	2.64539800
H	-4.61426200	2.92598800	3.00720000
H	-4.93886200	1.37600600	2.18154500
C	-1.14953300	3.81009200	1.30061300
H	-0.52379000	4.69683700	1.42182600
H	-1.94081200	3.82071600	2.05689200
H	-0.52823300	2.91680100	1.41622900
C	-1.51664200	0.19554300	-3.18091200
O	-1.93409200	-0.81243200	-3.73285900
H	-0.54106300	0.63845300	-3.47053800
H	0.36186500	-0.71282800	-0.87825000
H	2.37998300	0.19698300	-1.58932000
C	5.36340900	0.87258700	1.52453700
C	4.02843100	0.87623000	1.12315700

C	3.58421800	1.88786100	0.27138800
C	4.44707500	2.88940200	-0.18129300
C	5.77590400	2.86811300	0.23056800
C	6.25582500	1.85984300	1.08318700
H	5.71611400	0.09065200	2.19087000
H	3.34212300	0.11152600	1.46739200
H	4.07981100	3.67317300	-0.83510600
H	6.45318900	3.64537300	-0.11253300
C	7.70422100	1.84320000	1.49981100
H	7.88883700	1.10860500	2.28813900
H	8.34908600	1.59320300	0.64866200
H	8.02171800	2.82614300	1.86383300
S	1.89305400	1.87505500	-0.29691700
O	1.46618500	3.24227500	-0.59905500
O	1.10586900	1.06325400	0.64530300
O	1.96237100	1.12423800	-1.71478500

TSA1

C	1.41280200	-4.00797600	-0.19278600	
C		1.21487600	-2.69641300	0.29750500
C		1.25076500	-2.48242600	1.69097500
C		1.47900500	-3.52542900	2.57744000
C		1.67544900	-4.82293100	2.07100300
C		1.63927400	-5.05364200	0.67934300
H		1.40287400	-4.19648700	-1.25975100
H		1.10589700	-1.47383200	2.06899400
H		1.50703000	-3.33070300	3.64205400
H		1.79885400	-6.06467300	0.31966800
O		1.90864800	-5.91228500	2.83106100
C		1.99615000	-5.75945800	4.25329800
H		1.05324200	-5.39211800	4.67332300
H		2.20220700	-6.75627200	4.64482300
H		2.81300700	-5.08374300	4.52982100
C		0.95593200	-1.56143400	-0.55060600
C		1.29814900	-1.48583700	-2.00428600
H		0.99909000	-2.38053600	-2.55436600
H		0.80904200	-0.61491600	-2.44751100
C		2.79448900	-1.33022300	-2.01937900
C		3.54429700	-0.17067000	-1.90071400
C		4.87175300	-1.94770400	-1.97160600
N		3.64667700	-2.42531800	-2.04116000
N		4.86444400	-0.57055200	-1.88186800
C		6.13194700	-2.74518900	-1.98632300
H		6.71145100	-2.60675800	-1.06552000

H	5.87967700	-3.80359100	-2.07765800
H	6.78177800	-2.46815200	-2.82515800
C	6.01719300	0.31272500	-1.80994800
H	6.48841900	0.42499600	-2.79158700
H	5.68644200	1.29160400	-1.46227600
H	6.74892700	-0.08795200	-1.10500000
O	3.25936200	1.13435300	-1.86290800
C	-3.00200800	-0.29009600	-0.65707400
C	-3.49748600	1.02327000	-0.68024800
C	-4.86774200	1.25682100	-0.58961500
C	-5.75722800	0.16296400	-0.48722400
C	-5.24414900	-1.15929000	-0.47572300
C	-3.87939800	-1.38404000	-0.54755100
H	-2.81846200	1.86867000	-0.71805900
H	-3.50339900	-2.40080800	-0.54229800
O	-6.09129200	-2.23610500	-0.38498200
O	-7.09415700	0.41606600	-0.47736300
O	-5.28645000	2.55282500	-0.64838500
C	-6.87058700	-2.48732400	-1.57066900
H	-7.52828200	-1.64442800	-1.80572600
H	-6.21414700	-2.68814400	-2.42556100
H	-7.47292400	-3.37222200	-1.35691500
C	-7.84748900	-0.04899500	0.66459800
H	-7.44132300	0.38211400	1.58578400
H	-8.86591200	0.31031300	0.51078000
H	-7.84037800	-1.13829400	0.73456100
C	-6.20236200	3.01834000	0.35917100
H	-6.08283100	4.10369900	0.39127200
H	-7.23569100	2.76982700	0.10757800
H	-5.95068800	2.60181300	1.34108900
C	-1.56908700	-0.47385200	-0.73966800
O	-1.01798500	-1.58724100	-0.62554800
H	-0.96087100	0.42078600	-0.91151900
H	0.99682400	-0.60550600	-0.03844300
H	2.33279900	1.30934700	-1.50875500
C	3.58348900	4.90255700	0.65033700
C	2.89531700	3.71844900	0.40638200
C	1.54994800	3.61876500	0.77837700
C	0.90224700	4.68995700	1.38967100
C	1.60692000	5.87215500	1.62932200
C	2.95307400	5.99765800	1.26603500
H	4.62769000	4.98382400	0.35857400
H	3.39516700	2.88520900	-0.07672700
H	-0.14163600	4.59691400	1.66894400

H	1. 10059900	6. 70807000	2. 10468000
C	3. 72011500	7. 27156700	1. 51977300
H	4. 60964300	7. 08084300	2. 13118400
H	4. 06834800	7. 71588200	0. 57991800
H	3. 10722200	8. 01495000	2. 03674100
S	0. 67231800	2. 07336000	0. 51194800
O	-0. 76723100	2. 33714700	0. 76004800
O	1. 29323600	1. 06844500	1. 41947400
O	0. 91604900	1. 72227000	-0. 94712000

INTA1

O	0. 99255200	-0. 73064900	-2. 80622400
O	-2. 09824600	1. 03127800	-0. 30393400
O	6. 41327600	-2. 04425900	0. 32582800
O	2. 50068600	2. 50457800	1. 19985400
O	0. 61786900	4. 50447300	1. 02225500
O	-0. 99018000	4. 72610000	-0. 99349300
N	-3. 29643300	-0. 29473100	-1. 79678100
N	-1. 93529400	-2. 01776800	-2. 16679400
C	-1. 31870100	-1. 14891300	-1. 27632100
C	-2. 16903500	-0. 07150600	-1. 03431600
C	-3. 10475900	-1. 48784600	-2. 46297400
C	0. 39520500	0. 43384100	-2. 72227000
H	-0. 22047700	0. 64574000	-3. 59688700
C	-0. 00499900	-1. 45460000	-0. 64873700
H	-0. 07051000	-2. 37555100	-0. 05900900
H	0. 27178400	-0. 66286300	0. 04578900
C	1. 10239200	-1. 70549100	-1. 68075500
H	0. 87199600	-2. 62772400	-2. 22131800
C	2. 51505500	-1. 76798700	-1. 14584900
C	2. 78690900	-1. 93155500	0. 22209600
H	1. 98462600	-1. 95390900	0. 95164200
C	4. 09788600	-2. 02688200	0. 67667300
H	4. 31042700	-2. 14491400	1. 73452200
C	5. 17159200	-1. 95019000	-0. 22263500
C	4. 91340500	-1. 78064300	-1. 59115400
H	5. 72139000	-1. 71267300	-2. 30951300
C	3. 59365300	-1. 70171100	-2. 03570200
H	3. 40324700	-1. 56902000	-3. 09653900
C	0. 60597600	1. 47737900	-1. 79769600
C	1. 55594100	1. 42217900	-0. 74952200
H	2. 24156300	0. 59120300	-0. 68807500
C	1. 61012900	2. 44127800	0. 18351100
C	0. 69066300	3. 52583600	0. 11052900

C	-0.19436700	3.62776300	-0.99514100
C	-0.24043200	2.61077900	-1.93311000
H	-0.96202700	2.63278000	-2.73950500
C	-4.12501200	-2.05727700	-3.38830700
H	-3.74053000	-2.98677400	-3.81248900
H	-4.35859500	-1.36739900	-4.20795000
H	-5.06607300	-2.27495300	-2.86907000
C	7.54542700	-1.98167000	-0.54170300
H	8.42090900	-2.09358800	0.09990700
H	7.60209200	-1.01785600	-1.06269500
H	7.53435100	-2.79259000	-1.28022000
C	3.20280100	1.30266200	1.54919400
H	2.49598700	0.50039000	1.78047000
H	3.78403900	1.55103100	2.43870800
H	3.88620700	0.99412800	0.75071800
C	0.72103700	4.18564100	2.43442500
H	1.75863300	4.23253600	2.76691200
H	0.30444200	3.19588300	2.63412600
H	0.12966600	4.95314400	2.93800000
C	-2.00307000	4.81634200	-1.99569900
H	-2.70450400	3.97532000	-1.93124800
H	-1.57282600	4.85803200	-3.00396500
H	-2.53730000	5.74648600	-1.79618500
C	-4.45870000	0.57690200	-1.85312800
H	-4.45845400	1.17460600	-2.77019000
H	-4.43211600	1.24521200	-0.99211700
H	-5.37297400	-0.01876800	-1.81388100
H	-1.43954400	0.95878100	0.46199000
C	-4.19749100	-1.38044800	1.72484700
C	-3.14188600	-0.56949700	2.13420200
C	-1.88612100	-1.13713400	2.36727400
C	-1.69908500	-2.51182400	2.22708400
C	-2.76570000	-3.31500800	1.82185800
C	-4.02490700	-2.76270200	1.55066100
H	-5.16856100	-0.93364000	1.52746800
H	-3.28538600	0.50030700	2.24112000
H	-0.72010700	-2.93840500	2.41522400
H	-2.61347800	-4.38452900	1.70233300
S	-0.50098400	-0.06969000	2.80204800
O	0.72102300	-0.91302800	2.69490300
O	-0.53763200	1.00969700	1.73330200
O	-0.76110000	0.48832800	4.14965400
C	-5.15413100	-3.62257400	1.04059500
H	-5.14978200	-3.65206400	-0.05664200

H	-5.06571200	-4.65450500	1.39341900
H	-6.12862900	-3.23434500	1.35266200

TSA2

01.01489000	-0.73265500	-2.77767100	
O	-2.15202400	0.96497400	-0.27237600
O	6.44393700	-1.96552200	0.35803300
O	2.52314300	2.62132900	1.04072500
O	0.59075900	4.57205400	0.90681100
O	-1.16632100	4.66498300	-1.00673000
N	-3.29653700	-0.37279900	-1.78328900
N	-1.86581000	-2.02931300	-2.20203200
C	-1.27767500	-1.15516600	-1.29445600
C	-2.18209800	-0.12129500	-1.01718400
C	-3.05581700	-1.54275100	-2.48032100
C	0.28377500	0.36184300	-2.68837700
H	-0.38959500	0.49910500	-3.53439200
C	0.02129500	-1.46114700	-0.63646400
H	-0.05811500	-2.37612800	-0.03988400
H	0.29135600	-0.66047800	0.05107700
C	1.13288600	-1.71413900	-1.65992000
H	0.91497900	-2.64289000	-2.19494700
C	2.54357400	-1.75520400	-1.11972500
C	2.81691900	-1.86865200	0.25273500
H	2.01517200	-1.87093000	0.98303200
C	4.12847800	-1.94164500	0.71023000
H	4.34178100	-2.02205500	1.77148300
C	5.20128000	-1.89292400	-0.19196000
C	4.94189700	-1.77152600	-1.56552900
H	5.74971200	-1.72450700	-2.28571700
C	3.62174300	-1.71417200	-2.01178000
H	3.42989300	-1.61905900	-3.07648300
C	0.50074800	1.45759000	-1.81985400
C	1.51498300	1.46644200	-0.83485800
H	2.22790300	0.65685000	-0.79252300
C	1.58557300	2.51189900	0.06932200
C	0.63326200	3.56622900	0.01687100
C	-0.32513600	3.60001800	-1.02778700
C	-0.39524500	2.55122200	-1.93119700
H	-1.16831600	2.52041000	-2.68782400
C	-4.05623200	-2.13288900	-3.41332900
H	-3.63070400	-3.02750500	-3.87152500
H	-4.33362800	-1.42803800	-4.20573500
H	-4.97718600	-2.41479500	-2.88910500

C	7.57478100	-1.92635500	-0.51248400
H	8.45164300	-2.01134700	0.13145500
H	7.62544000	-0.98043700	-1.06604300
H	7.56791800	-2.76208400	-1.22301800
C	3.23302700	1.43124900	1.41501100
H	2.53167800	0.64136800	1.70060100
H	3.84392600	1.71153300	2.27480300
H	3.88971200	1.08630200	0.60913800
C	0.70879000	4.26757400	2.31980000
H	1.75112200	4.30381300	2.63948500
H	0.28388700	3.28439700	2.53643500
H	0.13353600	5.04538200	2.82676100
C	-2.29764000	4.63116900	-1.87731300
H	-2.91867900	3.74773300	-1.68557700
H	-1.99913300	4.64715300	-2.93276600
H	-2.87168500	5.53222400	-1.65577800
C	-4.49163900	0.45585500	-1.81803500
H	-4.47597200	1.13470800	-2.67644100
H	-4.53486500	1.04190800	-0.89972500
H	-5.37720200	-0.17882000	-1.87834800
H	-1.46126400	0.93081500	0.47771100
C	-4.14396100	-1.45271900	1.80518700
C	-3.10825500	-0.60420900	2.18816800
C	-1.82990600	-1.12829900	2.40050200
C	-1.60039200	-2.49728300	2.26806400
C	-2.64734400	-3.33836000	1.88871300
C	-3.92868500	-2.82974800	1.63658900
H	-5.13342200	-1.04019200	1.62546100
H	-3.28614600	0.46068000	2.29231300
H	-0.60499600	-2.89010500	2.44300200
H	-2.46246100	-4.40339700	1.77589500
S	-0.47210600	-0.01125000	2.79580300
O	0.77314800	-0.82057400	2.70623700
O	-0.54262800	1.03451200	1.69319100
O	-0.74355300	0.58160800	4.12551000
C	-5.03956700	-3.73042300	1.15735300
H	-5.06216200	-3.76359000	0.06032500
H	-4.90647600	-4.75722200	1.51099000
H	-6.01883100	-3.37479200	1.49260700

INTA2

C	4.78498500	1.13003800	-0.66646300
C		4.25651700	-0.03408200
C		5.00538600	-1.21057700

C	6.26218000	-1.24398300	-0.74805800
C	6.77537600	-0.07777800	-1.33012100
C	6.02359500	1.11014100	-1.28978200
H	4.21339100	2.05324200	-0.64026000
H	4.60771000	-2.12105700	0.30320700
H	6.81956800	-2.17245900	-0.76933300
H	6.43653300	2.00250100	-1.74932700
O	7.97931100	0.01062500	-1.95678800
C	8.80548000	-1.15313100	-2.00358200
H	8.32364500	-1.96787100	-2.55766800
H	9.71515600	-0.85327900	-2.52664600
H	9.06648000	-1.50227200	-0.99712800
C	2.92688900	-0.01140900	0.60875100
C	2.86853500	0.89848500	1.87511700
H	3.41838500	1.82137200	1.67670700
H	3.39149700	0.35470600	2.66869900
C	1.47585600	1.25804800	2.26457900
C	0.47996100	0.43382800	2.79643400
C	-0.29342400	2.48849200	2.47995300
N	0.96826400	2.53252100	2.09265200
N	-0.64091000	1.22714000	2.92446700
C	-1.27148700	3.60697000	2.41239600
H	-2.10834600	3.35888600	1.74856200
H	-1.69319300	3.84302400	3.39604100
H	-0.77130900	4.49373400	2.01957100
C	-1.94114700	0.81715300	3.43621700
H	-2.71777900	1.02154800	2.69592300
H	-1.92058600	-0.25252600	3.63915000
H	-2.17093100	1.35468100	4.35987600
O	0.55199800	-0.83159800	3.18524600
C	-0.40932800	1.03255000	-0.35993100
C	-0.25367800	2.30630800	-0.93852200
C	-1.37352900	3.08218000	-1.20325800
C	-2.66837800	2.60951300	-0.86353100
C	-2.81573700	1.32377400	-0.27745400
C	-1.69503400	0.54543100	-0.03475200
H	0.72882300	2.69349700	-1.17802500
H	-1.78576200	-0.41200000	0.46072900
O	-4.07685000	0.96456200	0.08257200
O	-3.70146400	3.46234600	-1.04390200
O	-1.16443200	4.32272900	-1.72729600
C	-4.30278000	-0.41300500	0.42103800
H	-5.37622800	-0.49984300	0.59387700
H	-4.00639000	-1.06772600	-0.40375100

H	-3.76479800	-0.70344600	1.32945000
C	-4.91441300	2.99496300	-1.67357200
H	-4.68852600	2.28647400	-2.47616100
H	-5.58045000	2.52921600	-0.94648300
H	-5.38401300	3.88552700	-2.09552000
C	-1.96275300	4.73750000	-2.85135600
H	-1.34854500	5.45144700	-3.40565300
H	-2.20281900	3.89008100	-3.50296200
H	-2.88651400	5.22046600	-2.52619700
C	0.69270800	0.23207800	0.03422400
O	1.92057900	0.53146800	-0.31576400
H	2.60869300	-1.02473600	0.87460800
H	0.52718000	-0.74884300	0.47574600
H	-0.18438400	-1.38681400	2.75225300
C	-4.08467500	-3.83158900	-1.23254600
C	-3.17704800	-3.88876700	-0.17746100
C	-1.94340300	-3.24395800	-0.29767800
C	-1.61709200	-2.55107300	-1.46317900
C	-2.53610400	-2.49958500	-2.51194900
C	-3.78066700	-3.13719700	-2.41514400
H	-5.04361500	-4.33510700	-1.14080200
H	-3.41532300	-4.43558700	0.72891900
H	-0.65418900	-2.05926500	-1.54595200
H	-2.28079000	-1.95829100	-3.41909100
S	-0.80514200	-3.24471000	1.09268800
O	0.54242800	-2.93593600	0.53903600
O	-1.30670100	-2.09350400	1.96379800
O	-0.94225400	-4.55614700	1.76109800
C	-4.75945200	-3.11292300	-3.56252800
H	-4.71085700	-4.04922400	-4.13240600
H	-5.78939500	-3.00537800	-3.20722800
H	-4.54649100	-2.29365900	-4.25517700

TSA3

C	4.99515600	0.72172100	-0.40837100
C		4.40231400	-0.52980400
C		5.12503300	-1.68242600
C		6.41743900	-1.61074000
C		6.99575000	-0.35707200
C		6.27161300	0.81112100
H		4.44304300	1.62883600
H		4.67850400	-2.65819400
H		6.95265600	-2.52494500
H		6.73490000	1.77335700

O	8.24200100	-0.16113700	-1.75191600
C	9.02310800	-1.30696400	-2.09164900
H	8.53483200	-1.91232900	-2.86502000
H	9.96681400	-0.92073100	-2.48070700
H	9.22491400	-1.93269900	-1.21358900
C	3.02964100	-0.62281500	0.42933200
C	2.90215800	-0.06252900	1.88303100
H	3.60803000	0.75936200	2.01882600
H	3.15957400	-0.85791200	2.58706400
C	1.52201500	0.47250900	2.12080000
C	0.40801000	-0.21261200	2.70390300
C	0.10341100	1.98995900	2.74265600
N	1.30696200	1.85175800	2.26321500
N	-0.49527600	0.75073400	3.02361800
C	-0.63278900	3.26623000	2.92948300
H	-1.49184000	3.31125700	2.24877800
H	-1.01047600	3.37307100	3.95168500
H	0.03472500	4.09821000	2.70118500
C	-1.83867400	0.55090900	3.55407300
H	-2.57567100	0.94777500	2.85345800
H	-2.01265700	-0.51512000	3.69172900
H	-1.93595000	1.05989600	4.51535400
O	0.23722700	-1.49021900	2.83582100
C	-0.13117700	1.04935800	-0.21371400
C	0.22786000	2.32103700	-0.67319800
C	-0.75141800	3.29423000	-0.87323200
C	-2.10283700	3.00984400	-0.57813000
C	-2.45722600	1.71939100	-0.11492500
C	-1.47907800	0.74198700	0.05069400
H	1.26423200	2.57102900	-0.86399800
H	-1.73829100	-0.23787400	0.43164600
O	-3.76935400	1.54462300	0.20622700
O	-3.02914700	4.01269700	-0.65584500
O	-0.31255500	4.52109400	-1.27769000
C	-4.24288300	0.20003700	0.37216300
H	-5.31862900	0.28435200	0.53349700
H	-4.05027900	-0.38765100	-0.52810000
H	-3.78608100	-0.29421900	1.23569500
C	-4.07967100	3.84734000	-1.62819800
H	-3.66102100	3.71310200	-2.63218600
H	-4.72166100	2.99910400	-1.38029200
H	-4.66060100	4.77131700	-1.59973200
C	-1.04551100	5.22425800	-2.29332900
H	-0.33665100	5.92587500	-2.73984100

H	-1.40403600	4.53800600	-3.06894000
H	-1.88975900	5.77395500	-1.87232600
C	0.86630700	0.06034500	0.14943600
O	2.10405300	0.17029400	-0.36165500
H	2.67662400	-1.66060600	0.41819800
H	0.52425900	-0.96323400	0.32140900
H	-0.69507900	-1.84125300	2.43811800
C	-5.00478800	-2.96548100	-1.42642000
C	-4.09148900	-3.29545600	-0.42904100
C	-2.75004000	-2.93368100	-0.58252700
C	-2.32183100	-2.25588500	-1.72283600
C	-3.24861000	-1.93403800	-2.71627300
C	-4.59972300	-2.28206400	-2.58563500
H	-6.04857000	-3.24499300	-1.30923400
H	-4.41150300	-3.83457700	0.45659000
H	-1.27737600	-1.98536200	-1.82885500
H	-2.91540300	-1.40543300	-3.60530700
S	-1.57902200	-3.31517200	0.72097900
O	-0.22050600	-3.14755800	0.14825300
O	-1.85656400	-2.22729200	1.77895100
O	-1.91657400	-4.66025200	1.22889600
C	-5.59818600	-1.95842500	-3.66862100
H	-5.86538500	-2.86010400	-4.23342200
H	-6.52592600	-1.55727000	-3.24697500
H	-5.19964600	-1.22840700	-4.37866500

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O	0.41180400	-1.40504000	-1.60673800
O	-2.27463900	-0.49882400	1.72186400
O	6.31420300	-0.37725500	0.58513000
O	1.15497500	3.19627800	0.50387400
O	-1.15934800	4.52775600	0.15332900
O	-3.35484300	3.29306800	-0.74743400
N	-3.36505400	-2.34431700	0.82847300
N	-1.81316800	-3.20097800	-0.58274200
C	-1.26485200	-1.95356200	-0.02930000
C	-2.32020400	-1.44737500	0.95655500
C	-2.98569100	-3.34969900	-0.07309800
C	-0.89790700	-0.98992100	-1.21146200
H	-1.58246200	-1.19174600	-2.04204500
C	0.10700600	-2.16281500	0.61930400
H	0.14058600	-3.07142200	1.22278100
H	0.33199300	-1.30187200	1.25498000
C	1.04813500	-2.21165200	-0.59423800

H	1.08913900	-3.24183300	-0.97530700
C	2.45605200	-1.71612500	-0.32046100
C	3.14302300	-2.12589000	0.83409200
H	2.66789200	-2.80552300	1.53615700
C	4.42671700	-1.66778600	1.10579200
H	4.95373800	-1.97648300	2.00324500
C	5.06319200	-0.78146700	0.22202000
C	4.39843300	-0.37663400	-0.94164500
H	4.86508200	0.30173400	-1.64562500
C	3.10811300	-0.85047400	-1.20149600
H	2.59200200	-0.52081500	-2.09598600
C	-0.94687500	0.48808400	-0.86983100
C	0.18362600	1.13274200	-0.36819900
H	1.10769200	0.58375600	-0.26981800
C	0.11144600	2.48196600	-0.00528700
C	-1.09340000	3.18923900	-0.15633800
C	-2.22973500	2.52861100	-0.65778500
C	-2.14964700	1.18110900	-1.03179100
H	-3.01709500	0.66153500	-1.42205800
C	-3.92105300	-4.47300300	-0.36717000
H	-3.45249800	-5.16347600	-1.06966300
H	-4.85267400	-4.09390700	-0.80158900
H	-4.18214100	-5.01157200	0.55022900
C	6.99535200	0.54563100	-0.26302200
H	7.95855900	0.73748600	0.21315200
H	6.44489400	1.49043300	-0.35621200
H	7.16597900	0.12706700	-1.26267100
C	2.40920600	2.52820100	0.64919800
H	2.34001400	1.67464000	1.33471800
H	3.09442900	3.26827500	1.06681100
H	2.79570500	2.18218500	-0.31641600
C	-1.38651600	4.78162400	1.54559900
H	-0.58410500	4.35841600	2.16148100
H	-2.34995100	4.36954200	1.87143800
H	-1.39983500	5.86769200	1.66857800
C	-4.54852200	2.67230900	-1.21813400
H	-4.85299200	1.83838700	-0.57275900
H	-4.43984700	2.31113100	-2.24861900
H	-5.31856800	3.44567800	-1.19144800
C	-4.59105500	-2.28176400	1.60445800
H	-5.46448600	-2.28277500	0.94729900
H	-4.56962000	-1.35097600	2.17361000
H	-4.66015300	-3.12445900	2.29885600

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C	3.32849800	0.19371500	0.47133400	
C		3.39677600	-0.27020600	-0.85441900
C		4.59115700	-0.10524400	-1.55495700
C		5.70975000	0.49583100	-0.96564100
C		5.62741400	0.95046200	0.35534700
C		4.42609800	0.79531600	1.06976100
H		2.40484100	0.06799500	1.02874900
H		4.66173100	-0.44956600	-2.58399700
H		6.62104900	0.60623200	-1.54096700
H		4.38151400	1.15545700	2.09304600
O		6.64445600	1.55086200	1.03670400
C		7.88720800	1.74349100	0.36329400
H		7.77461000	2.39309800	-0.51364700
H		8.54846900	2.22679500	1.08472300
H		8.33103900	0.78945800	0.05225400
C		2.20200200	-0.92938600	-1.49856500
C		1.67669500	-2.21493100	-0.78597400
H		2.32916900	-2.54244100	0.02440500
H		1.57088800	-3.03203200	-1.50447100
C		0.28579300	-1.82603500	-0.26116700
C		-0.74063100	-2.95355800	-0.25577300
C		-0.55378700	-1.98746800	1.77827400
N		0.31334900	-1.31266100	1.10970600
N		-1.22546000	-2.97350800	1.03429600
C		-0.88063900	-1.79167100	3.21876900
H		-1.93425800	-1.51668800	3.33845300
H		-0.71390800	-2.71389600	3.78575000
H		-0.25487600	-0.99691400	3.62687600
C		-2.28105000	-3.85536500	1.49935800
H		-3.14861000	-3.27900600	1.83316100
H		-2.57078600	-4.48771100	0.65840200
H		-1.93032600	-4.48711100	2.31992600
O		-1.10032400	-3.66306200	-1.18513900
C		-1.23092500	0.17939500	-0.85210400
C		-0.98401100	1.41366400	-0.26485400
C		-2.04853700	2.20659400	0.18619100
C		-3.37035500	1.74274100	0.08195700
C		-3.60877800	0.47715500	-0.50449000
C		-2.54608500	-0.28841800	-0.98675800
H		0.02737400	1.78566900	-0.15976200
H		-2.72437900	-1.25086500	-1.45066000
O		-4.91382800	0.08190100	-0.53214200
O		-4.40162600	2.47582700	0.62178500
O		-1.70464500	3.38955400	0.78190300

C	-5.21836400	-1.19645800	-1.08889800
H	-6.29846200	-1.31549400	-0.98827900
H	-4.94663200	-1.24962100	-2.15011900
H	-4.71400600	-2.00439100	-0.54427300
C	-5.34369800	3.01663500	-0.31937400
H	-4.83928200	3.64228600	-1.06564300
H	-5.90108000	2.22410500	-0.82632900
H	-6.03325000	3.63431800	0.26065800
C	-2.45126000	4.57093900	0.46142200
H	-1.80177800	5.41291200	0.71513100
H	-2.68427100	4.61349600	-0.60897400
H	-3.37621100	4.63632400	1.03870000
C	-0.10615000	-0.72013800	-1.29464700
O	1.09559300	0.00088000	-1.49376300
H	2.44599300	-1.17515000	-2.54046400
H	-0.39953900	-1.25413100	-2.21396700

TSB1

C	3.04002800	-3.17970200	-0.24481200
C	1.90957600	-2.34113600	-0.13815400
C	1.37507300	-2.08521500	1.13733600
C	1.94319600	-2.63436700	2.28093600
C	3.06392800	-3.47197400	2.15713300
C	3.60797000	-3.73827400	0.88393800
H	3.47630600	-3.38468400	-1.21534000
H	0.52382800	-1.41933200	1.24055900
H	1.52215300	-2.40059900	3.25066200
H	4.47859400	-4.38230000	0.81766800
O	3.69492100	-4.06683400	3.19333800
C	3.19549800	-3.85349800	4.51848900
H	2.16390600	-4.21048300	4.61777100
H	3.84388600	-4.43486600	5.17546000
H	3.24745500	-2.79547200	4.79872700
C	1.26393400	-1.74240800	-1.29819400
C	2.02207100	-1.41155200	-2.55778800
H	2.58175100	-2.27587600	-2.92247800
H	1.30833100	-1.11200400	-3.33056200
C	2.95541600	-0.28440900	-2.22116300
C	2.64509400	1.05519100	-2.13370900
C	4.73914400	0.70935600	-1.50240700
N	4.26408100	-0.48492000	-1.81291900
N	3.79218800	1.68699500	-1.69412600
C	6.11692900	1.00089400	-1.00858000
H	6.09948200	1.47961000	-0.02236100

H	6.66853700	0.06212600	-0.92541500
H	6.66584200	1.66599600	-1.68627300
C	3.86977000	3.08745400	-1.31503400
H	4.89465500	3.44440700	-1.42754900
H	3.21741900	3.66806000	-1.96890500
H	3.54008000	3.21296700	-0.27983900
O	1.52246900	1.74481500	-2.40609300
C	-2.02560800	-2.64107400	-1.18411400
C	-3.12167200	-3.35405600	-0.65505000
C	-4.25763300	-2.69140600	-0.20550600
C	-4.32658300	-1.28224600	-0.31830800
C	-3.23110800	-0.56945700	-0.86893700
C	-2.09288700	-1.23698000	-1.29552900
H	-3.09792500	-4.43686600	-0.58699200
H	-1.29221500	-0.64181700	-1.70963700
O	-3.28151300	0.78995200	-1.00108900
O	-5.42593100	-0.64750300	0.16129200
O	-5.23976100	-3.45410200	0.34785600
C	-3.23494500	1.52586900	0.24212900
H	-4.19486400	1.47483200	0.76663600
H	-2.43972900	1.14088900	0.88349200
H	-3.01776400	2.55895900	-0.03024500
C	-6.19341300	0.14873500	-0.77136100
H	-6.60343400	-0.49246800	-1.55889400
H	-7.00765000	0.57981600	-0.18802900
H	-5.58825300	0.94026000	-1.21650500
C	-6.60525500	-3.22395200	-0.04688100
H	-7.13299000	-4.15795700	0.15923600
H	-7.05625500	-2.41166200	0.52596800
H	-6.67343200	-3.00370100	-1.11810900
C	-0.91450900	-3.44612300	-1.62176200
O	0.26515100	-3.12199800	-1.90429100
H	-1.12469700	-4.51806600	-1.73767600
H	0.51191500	-1.00602600	-1.03745800
H	0.85162800	1.52351500	-1.68814500
C	-0.45299500	5.42742100	0.05040100
C	0.03322100	4.12666700	-0.03601600
C	-0.21176700	3.23007500	1.01002400
C	-0.93381800	3.63252300	2.13075500
C	-1.41858200	4.94101300	2.20352100
C	-1.18731900	5.85647000	1.16977700
H	-0.26732800	6.12357700	-0.76376800
H	0.58725100	3.80434800	-0.91230100
H	-1.12246800	2.92224500	2.92830900

H	-1.98721600	5.25152500	3.07622100
C	-1.70604400	7.27130000	1.24186600
H	-2.34294600	7.50361800	0.38056400
H	-2.29052300	7.44008700	2.15051200
H	-0.88148400	7.99408500	1.23280600
S	0.42952700	1.55328400	0.89295400
O	-0.20666400	0.77780800	1.98969200
O	1.90830100	1.65704100	0.95841000
O	-0.05302700	1.08023900	-0.46837400

INTB1

O	0.33701700	-2.06059100	-1.79988200
O	-1.14194800	0.21032800	1.21182900
O	-4.52215300	-4.81918400	1.20968300
O	5.31181400	-0.66151800	-1.80947600
O	5.93458000	-0.43719000	0.79791400
O	4.16705200	-0.89057000	2.72144200
N	0.79685700	1.35850500	0.62929100
N	0.90479400	1.10232900	-1.58248700
C	-0.22452500	0.43812200	-1.11730200
C	-0.31895700	0.64249600	0.28150100
C	1.50696300	1.61284900	-0.53192500
C	0.68404000	-1.69011900	-0.58062600
H	-0.03387200	-1.85642600	0.22146100
C	-1.16602400	-0.19810000	-2.09129800
H	-0.87484400	0.16812000	-3.07786000
H	-2.19848900	0.11553200	-1.92314500
C	-1.06534700	-1.75431800	-2.12052700
H	-1.15850400	-2.10905000	-3.14859500
C	-1.99930400	-2.54644100	-1.22362800
C	-3.08201100	-1.98221300	-0.53667500
H	-3.31124700	-0.92837000	-0.61568700
C	-3.90354000	-2.76712300	0.26514500
H	-4.73654300	-2.32259400	0.80019800
C	-3.66430900	-4.14154800	0.39956700
C	-2.58791300	-4.72390000	-0.28789300
H	-2.38019600	-5.78423000	-0.20889600
C	-1.77507600	-3.92387600	-1.08925000
H	-0.93997800	-4.38277100	-1.61155500
C	2.06093800	-1.47684100	-0.26101400
C	3.01218900	-1.26415200	-1.27668700
H	2.69927000	-1.32018400	-2.30950300
C	4.31703900	-0.92983300	-0.92659400
C	4.67741000	-0.81469500	0.43729000

C	3.71548500	-1.03166600	1.44977200
C	2.40481000	-1.34924300	1.09933900
H	1.64232800	-1.49741800	1.85356100
C	2.79489600	2.35312900	-0.52056300
H	3.15628800	2.45918100	-1.54458200
H	3.55003100	1.81093300	0.06238900
H	2.68220500	3.34863200	-0.07624000
C	-4.34055300	-6.22634800	1.36506600
H	-5.13280900	-6.55767000	2.03854300
H	-3.36701500	-6.46166100	1.81267000
H	-4.43806700	-6.75397600	0.40839500
C	4.99774100	-0.69418100	-3.20502700
H	4.68459000	-1.69586800	-3.52215500
H	5.91935600	-0.42273500	-3.72162700
H	4.21383400	0.03093800	-3.45307700
C	6.95091200	-1.44346300	0.61971200
H	7.02786400	-1.75013100	-0.42751800
H	6.74122100	-2.31626200	1.24890600
H	7.88945000	-0.98490000	0.93668700
C	3.25133800	-1.14207900	3.79036400
H	2.86280100	-2.16687800	3.75306300
H	2.41562100	-0.43236500	3.78108800
H	3.82547800	-1.00738800	4.70821900
C	1.15696700	1.77420300	1.97639400
H	2.15323300	1.40435300	2.22753500
H	0.42652800	1.35807600	2.66927600
H	1.14036400	2.86376100	2.05023900
H	-2.14231400	0.42438500	1.02486100
C	-1.18576700	4.47299700	1.39619300
C	-2.17343700	3.49400900	1.31933700
C	-2.67975000	3.12411500	0.07009600
C	-2.19893700	3.72497600	-1.09333600
C	-1.20896200	4.70428700	-1.00234100
C	-0.68925300	5.09539700	0.23939500
H	-0.78885300	4.75711900	2.36735300
H	-2.53503400	3.00432200	2.21741200
H	-2.58470100	3.41043300	-2.05692600
H	-0.82666300	5.16299200	-1.91033200
S	-3.98481300	1.88813400	-0.02449500
O	-3.97122500	1.37534300	-1.41998800
O	-3.55024400	0.82780900	0.97983900
O	-5.24868300	2.53260400	0.39491800
C	0.36836400	6.16653300	0.33838400
H	-0.08572400	7.14600200	0.53482400

H	1.06608200	5.96437700	1.15742300
H	0.94151600	6.25161900	-0.58957000

TSB2

O	0.35307700	-2.02557400	-1.77877400
O	-1.10924600	0.29837200	1.26060100
O	-4.50184300	-4.89899400	1.14463700
O	5.35075400	-0.69291100	-1.81710100
O	5.98039500	-0.41138200	0.78409500
O	4.20193200	-0.79303600	2.71841000
N	0.81760200	1.43549700	0.64950000
N	0.93924000	1.10703800	-1.55589500
C	-0.17571900	0.42369200	-1.06541300
C	-0.28882500	0.70423300	0.32897800
C	1.52996000	1.65689000	-0.52572900
C	0.69238600	-1.58594700	-0.56910500
H	-0.00719100	-1.78500600	0.24281700
C	-1.15841700	-0.17551400	-2.02574500
H	-0.90417500	0.22057000	-3.01087400
H	-2.18157300	0.13524300	-1.80901900
C	-1.04485100	-1.73040900	-2.09483200
H	-1.14169500	-2.06319300	-3.13029400
C	-1.97229600	-2.54919500	-1.21066900
C	-3.12874100	-2.03290900	-0.61144800
H	-3.41192000	-0.99652200	-0.73593600
C	-3.94945100	-2.84235400	0.16732100
H	-4.83823900	-2.43404400	0.63769400
C	-3.63705700	-4.19406700	0.36448600
C	-2.48589800	-4.72822200	-0.23426300
H	-2.21741400	-5.76942500	-0.10282500
C	-1.67439300	-3.90482100	-1.01356600
H	-0.78222100	-4.32726300	-1.46730500
C	2.08255200	-1.39893700	-0.25110000
C	3.03724500	-1.23062800	-1.26933600
H	2.72308800	-1.30553500	-2.30064400
C	4.34995200	-0.91521800	-0.92684300
C	4.71373900	-0.77328600	0.43284100
C	3.74891400	-0.95033100	1.44805600
C	2.43053000	-1.24955900	1.10392100
H	1.66709800	-1.36694600	1.86262600
C	2.81500800	2.40152300	-0.53247600
H	3.16886000	2.49452200	-1.56026900
H	3.57371500	1.86495000	0.05105000
H	2.70404900	3.40128900	-0.09839200

C	-4.23699100	-6.28324600	1.36942300
H	-5.04663800	-6.64354200	2.00643900
H	-3.28033800	-6.43297900	1.88526300
H	-4.23745600	-6.85232900	0.43157400
C	5.03773100	-0.76360000	-3.21093600
H	4.70078100	-1.76713700	-3.49666000
H	5.96622000	-0.53189200	-3.73469200
H	4.27187400	-0.02826100	-3.48427900
C	6.97267100	-1.44459400	0.63668400
H	7.04550100	-1.78170200	-0.40170200
H	6.74276300	-2.29622400	1.28789800
H	7.92147500	-1.00028300	0.94384300
C	3.28386900	-1.01979500	3.79025800
H	2.88346300	-2.04046500	3.76682400
H	2.45586700	-0.30128200	3.77240900
H	3.85944200	-0.87956100	4.70648400
C	1.18017600	1.89663900	1.98175500
H	2.17294700	1.52630200	2.24557700
H	0.44581900	1.51337400	2.68912600
H	1.17445700	2.98819900	2.01368500
H	-2.13160100	0.42604300	1.03857300
C	-1.29207200	4.47997600	1.33466600
C	-2.25794300	3.47755900	1.29324900
C	-2.75932000	3.05629500	0.05802400
C	-2.29579100	3.62965000	-1.12600700
C	-1.32765700	4.63317500	-1.07006800
C	-0.81387700	5.07638900	0.15640200
H	-0.89945300	4.80435500	2.29476900
H	-2.60680500	3.01198200	2.20907500
H	-2.68027300	3.27835000	-2.07721200
H	-0.95980400	5.07176800	-1.99376200
S	-4.03335400	1.78652500	0.00818900
O	-4.06637100	1.28418800	-1.39053700
O	-3.52552400	0.72674200	0.98172800
O	-5.29362000	2.38830400	0.49336300
C	0.21382100	6.17882600	0.21510600
H	-0.26889100	7.15239100	0.36787900
H	0.91321700	6.03200700	1.04434100
H	0.78884800	6.24113200	-0.71352300

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O	-1.17857900	-0.62978200	-0.06788300
O	0.16076700	3.08022200	1.56004000
O	-7.55045400	-0.94893700	0.43149000

O	3.10149200	-3.03332300	-1.49555400
O	5.06013800	-2.04613600	0.03974700
O	4.57915500	-0.16482000	1.88885600
N	1.41072800	3.13975800	-0.40249700
N	0.47668100	1.47297900	-1.62284600
C	-0.22569500	1.53094900	-0.33919300
C	0.41981900	2.67556300	0.43558200
C	1.37786000	2.39016600	-1.59184500
C	-0.13655700	0.19225400	0.45933200
H	-0.36080000	0.44405500	1.50644600
C	-1.74309900	1.62525100	-0.52391000
H	-2.03241600	2.30775700	-1.32530500
H	-2.20076000	1.95501200	0.41398400
C	-2.11870200	0.16285500	-0.82629600
H	-1.94890200	-0.03658600	-1.89270300
C	-3.54190400	-0.19228000	-0.46822000
C	-4.56036300	-0.06714300	-1.42421900
H	-4.31098900	0.23298500	-2.43917100
C	-5.88667500	-0.32116200	-1.09461400
H	-6.67756400	-0.22609000	-1.83214800
C	-6.22452500	-0.71912600	0.20831000
C	-5.21576800	-0.85939100	1.17145800
H	-5.44880000	-1.17374400	2.18189800
C	-3.88893300	-0.59225000	0.82408900
H	-3.10736700	-0.71078800	1.56790900
C	1.21398100	-0.47889100	0.38777600
C	1.46322800	-1.48474000	-0.54517800
H	0.65341500	-1.82394000	-1.17582900
C	2.74874600	-2.03350300	-0.64017000
C	3.78500800	-1.54984300	0.17809300
C	3.51702700	-0.54391700	1.12345700
C	2.22729100	-0.00934200	1.23057200
H	2.00360900	0.76291200	1.95695000
C	2.34852300	2.68940500	-2.68161800
H	2.16996300	2.01693400	-3.52161500
H	3.37589500	2.55518100	-2.32604100
H	2.24891600	3.72675200	-3.01882400
C	-7.95478400	-1.35236900	1.73856800
H	-9.03906500	-1.47037700	1.69512000
H	-7.70528800	-0.59436200	2.49144300
H	-7.50091300	-2.30931600	2.02490500
C	2.09829100	-3.55182100	-2.36765700
H	1.26576200	-3.99691300	-1.80893500
H	2.58905200	-4.32839100	-2.95742000

H	1. 70938600	-2. 77912100	-3. 04225100
C	5. 35125600	-3. 13244100	0. 92756300
H	4. 67873700	-3. 98097200	0. 75003900
H	5. 27266400	-2. 81872200	1. 97573100
H	6. 37958200	-3. 43982600	0. 72062500
C	4. 36997100	0. 85996400	2. 85865400
H	3. 63131200	0. 56057200	3. 61237600
H	4. 04825900	1. 79939100	2. 39160600
H	5. 33532000	1. 01332200	3. 34439600
C	2. 34897200	4. 19273400	-0. 05709700
H	3. 37033100	3. 80315400	-0. 01779600
H	2. 06899600	4. 56790200	0. 92865500
H	2. 30183900	5. 01072700	-0. 78084100

INTB2

O	1. 46275500	-0. 74281800	-0. 83535000
O	-1. 12503700	-0. 21379400	1. 37294400
O	7. 80415100	-0. 99420800	-0. 93987900
O	-2. 91984800	1. 72570200	-1. 89798100
O	-2. 37696700	4. 30657300	-1. 31586000
O	-0. 01404000	5. 08570300	-0. 41562700
N	0. 12833000	1. 32398100	2. 57667500
N	2. 16429000	0. 40707700	2. 60902400
C	1. 31710500	-0. 41541600	1. 86533300
C	0. 02491300	0. 14839600	1. 88247200
C	1. 44473400	1. 43248900	3. 00186500
C	1. 55786600	0. 47768400	-0. 37352100
H	2. 50502000	0. 81295400	0. 04331000
C	1. 68942100	-1. 76765200	1. 35687000
H	0. 80720200	-2. 40961000	1. 36835400
H	2. 44515900	-2. 21560100	2. 00640300
C	2. 23397100	-1. 76769700	-0. 10865600
H	1. 91971600	-2. 68292400	-0. 60929900
C	3. 71931700	-1. 57208300	-0. 29552200
C	4. 53065500	-0. 87538400	0. 61697000
H	4. 10150200	-0. 46460600	1. 52586400
C	5. 88689900	-0. 69895100	0. 37041000
H	6. 51721700	-0. 16399500	1. 07376500
C	6. 47076400	-1. 21742700	-0. 79615500
C	5. 67498900	-1. 91621400	-1. 71585500
H	6. 09993000	-2. 33313600	-2. 62060300
C	4. 31524800	-2. 08341500	-1. 45483200
H	3. 70622200	-2. 62765500	-2. 17232100
C	0. 56990200	1. 44900100	-0. 73467000

C	-0.67336600	1.04446000	-1.25770900
H	-0.85361100	-0.00607200	-1.43939700
C	-1.66556300	2.00080700	-1.45935700
C	-1.40724400	3.36146100	-1.17333300
C	-0.14972400	3.75715900	-0.66099800
C	0.83728800	2.80076000	-0.43340400
H	1.80697500	3.07704500	-0.03944500
C	1.91764500	2.59516500	3.80220500
H	2.97667500	2.46565600	4.03150200
H	1.36005300	2.68378000	4.74165400
H	1.78773200	3.53652900	3.25542400
C	8.45892100	-1.51418800	-2.09823200
H	9.50706500	-1.22553000	-2.00401200
H	8.04936600	-1.08401400	-3.02027300
H	8.38878800	-2.60773000	-2.14317200
C	-3.31234900	0.34828000	-1.97971100
H	-2.74716200	-0.18799700	-2.75057100
H	-4.36809200	0.36048000	-2.25064600
H	-3.18452300	-0.15296300	-1.01666900
C	-2.73121500	4.63149400	-2.67369300
H	-3.12229000	3.75836000	-3.20384600
H	-1.86519500	5.03514400	-3.21130700
H	-3.50651600	5.39758700	-2.60950200
C	1.23053400	5.54366900	0.11381900
H	2.06262400	5.33056500	-0.56831500
H	1.44176000	5.09704800	1.09391100
H	1.12581200	6.62357300	0.22775500
C	-0.93818800	2.29814000	2.76078200
H	-1.13250200	2.45321700	3.82471700
H	-1.83810900	1.91470700	2.28111200
H	-0.66688700	3.24866800	2.29520400
H	-1.05530500	-1.02689300	0.72561300
C	-5.27599900	-1.31196000	1.09487700
C	-4.00799500	-1.88998400	1.15970800
C	-3.56062500	-2.68391100	0.10204500
C	-4.37339200	-2.90343600	-1.01187800
C	-5.63946500	-2.32306100	-1.06180500
C	-6.11031200	-1.51764300	-0.01299200
H	-5.62297700	-0.69214100	1.91744500
H	-3.36785000	-1.72048000	2.01888600
H	-4.01250200	-3.52530100	-1.82418500
H	-6.27412600	-2.49677400	-1.92733000
S	-1.87668500	-3.31403900	0.12559000
O	-1.79564000	-4.37854100	-0.89751400

O	-1.04109100	-2.09696100	-0.27474300
O	-1.58856300	-3.71583400	1.52341500
C	-7.48597600	-0.90259700	-0.08451600
H	-7.67111900	-0.22928200	0.75686300
H	-7.61688600	-0.33313100	-1.01161800
H	-8.26285800	-1.67650200	-0.07293300

TSB3

O	-1.48328700	0.73609700	-0.83453100
O	1.15313400	0.21466600	1.36161000
O	-7.81869600	1.04406900	-0.90966400
O	2.90605300	-1.72993600	-1.89010800
O	2.36580300	-4.31355600	-1.32356100
O	-0.00686500	-5.09901400	-0.44138100
N	-0.05542500	-1.36260400	2.54989500
N	-2.12578800	-0.51845400	2.55896400
C	-1.29924400	0.33105400	1.81382300
C	0.01894400	-0.18572000	1.86228100
C	-1.37772500	-1.51726900	2.95627000
C	-1.56900800	-0.48227900	-0.34717100
H	-2.52885800	-0.82885400	0.03033600
C	-1.68972800	1.70490300	1.37463400
H	-0.81479700	2.35552200	1.41259200
H	-2.44513900	2.11090200	2.05101000
C	-2.23735900	1.75443700	-0.08829800
H	-1.91558100	2.67855400	-0.56761200
C	-3.72649300	1.57938400	-0.27085600
C	-4.53732200	0.85997900	0.62434300
H	-4.10631600	0.41886200	1.51804700
C	-5.89598500	0.69850500	0.38054600
H	-6.52547800	0.14572300	1.07071300
C	-6.48300900	1.25523600	-0.76662900
C	-5.68798500	1.97663800	-1.66922200
H	-6.11509000	2.42249500	-2.55905400
C	-4.32570500	2.12796700	-1.41096100
H	-3.71719300	2.68887000	-2.11589000
C	-0.58292700	-1.45787200	-0.72401000
C	0.65927400	-1.05217300	-1.24545500
H	0.83967400	-0.00113000	-1.42332300
C	1.65153400	-2.00824400	-1.45240500
C	1.39295300	-3.36979700	-1.17536600
C	0.13368900	-3.76765400	-0.67213700
C	-0.85253000	-2.81064600	-0.43592500
H	-1.82317500	-3.08934700	-0.04637800

C	-1.81859000	-2.69899100	3.74649600
H	-2.88901400	-2.62043100	3.94313500
H	-1.28586400	-2.75791100	4.70248200
H	-1.62497000	-3.63330600	3.20693000
C	-8.47620300	1.60353800	-2.04775900
H	-9.52595700	1.31990600	-1.95612700
H	-8.07522800	1.19852000	-2.98488800
H	-8.39816700	2.69746600	-2.06041100
C	3.29681700	-0.35198300	-1.96577000
H	2.73114400	0.18738300	-2.73416000
H	4.35261800	-0.36145300	-2.23701500
H	3.16885600	0.14564100	-1.00057700
C	2.69754000	-4.64404100	-2.68476600
H	3.07913400	-3.77231800	-3.22482900
H	1.82384500	-5.05048100	-3.20796800
H	3.47497700	-5.40902100	-2.63142800
C	-1.25554700	-5.56035400	0.07474200
H	-2.08325600	-5.33683200	-0.60939900
H	-1.47242700	-5.12616900	1.05921000
H	-1.15424200	-6.64196300	0.17536100
C	1.03426900	-2.31256700	2.72667500
H	1.17458800	-2.53256900	3.78718400
H	1.94453900	-1.86785900	2.32592300
H	0.82189300	-3.23676500	2.18348800
H	1.06680100	1.04201200	0.71707700
C	5.29682900	1.36719300	1.07576500
C	4.02265900	1.92883900	1.15957300
C	3.54777900	2.71254600	0.10645200
C	4.33845100	2.93786300	-1.02215900
C	5.61097300	2.37382000	-1.09080900
C	6.10978900	1.57914800	-0.04662200
H	5.66570100	0.75559600	1.89488700
H	3.39963300	1.75622900	2.03059800
H	3.95668900	3.55227800	-1.83059400
H	6.22876200	2.55264500	-1.96741400
S	1.85784400	3.32315600	0.15711600
O	1.74960000	4.39763700	-0.85191000
O	1.03037200	2.10008900	-0.25122100
O	1.57925000	3.70041200	1.56313000
C	7.49294000	0.98381900	-0.13671600
H	7.69479200	0.30472100	0.69616200
H	7.62372200	0.42608600	-1.07084600
H	8.25899600	1.76853500	-0.12340300

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O	-0.99755400	-0.62000100	-1.37903300
O	1.39194000	1.74677500	-2.40975600
O	-6.61959800	-1.08933600	1.48960600
O	3.87436500	-2.11644400	-1.72026700
O	4.89593100	-1.80474500	0.74272400
O	3.44042600	-0.78424400	2.74252000
N	1.43448900	2.94573400	-0.41958500
N	-0.54867300	2.38678700	0.51968900
C	-0.40205300	1.58216400	-0.69550400
C	0.90542100	2.05452700	-1.33328200
C	0.51876700	3.10073300	0.62950600
C	-0.36244100	0.04758900	-0.30385300
H	-0.97045100	-0.02717300	0.60813600
C	-1.58055800	1.64156400	-1.69685300
H	-1.19650800	1.92884300	-2.67788100
H	-2.32893200	2.37333600	-1.39065800
C	-2.12595300	0.19781700	-1.77352000
H	-2.34187800	-0.08976800	-2.80603100
C	-3.34538700	-0.10191000	-0.92049500
C	-3.62930200	0.57320600	0.27961100
H	-2.98979700	1.38385100	0.61645200
C	-4.72439600	0.21882600	1.05954500
H	-4.94297500	0.73998500	1.98654200
C	-5.57284300	-0.82466600	0.65870800
C	-5.30796900	-1.50793000	-0.53576700
H	-5.94892400	-2.31309500	-0.87428900
C	-4.20130400	-1.13949500	-1.30387100
H	-4.00334400	-1.67841300	-2.22744100
C	1.00611600	-0.51928400	-0.02913000
C	1.75591100	-1.09140800	-1.05842900
H	1.32213200	-1.16010300	-2.04527600
C	3.05442000	-1.54174700	-0.79578300
C	3.60293100	-1.40910200	0.49258200
C	2.83264100	-0.84453000	1.52430600
C	1.53171900	-0.39618800	1.26127900
H	0.92448900	0.03939200	2.04519600
C	0.82659200	4.02568700	1.75695600
H	-0.00021000	4.02055700	2.46857300
H	0.98605900	5.04652800	1.39361600
H	1.74358300	3.71197700	2.26786000
C	-7.49627300	-2.16494900	1.15581600
H	-8.24059700	-2.20138300	1.95335700
H	-6.96264800	-3.12262200	1.11552300
H	-8.00447200	-1.99285500	0.19883900

C	3.39723100	-2.22001700	-3.06153200
H	2.50562000	-2.85575400	-3.12737800
H	4.20745400	-2.67904600	-3.63090500
H	3.17017500	-1.23372400	-3.48437900
C	5.02299800	-3.20454400	1.02215900
H	4.69981100	-3.81101000	0.16757600
H	4.44148500	-3.48602400	1.90921700
H	6.08277700	-3.39114100	1.21445800
C	2.73144000	-0.16432700	3.81285500
H	1.80596000	-0.70171500	4.05492300
H	2.49174200	0.88239300	3.58621400
H	3.40060700	-0.20005800	4.67452600
C	2.71706000	3.60926700	-0.57133100
H	2.59503700	4.69477700	-0.62182500
H	3.15721600	3.25366400	-1.50432100
H	3.38318000	3.35721300	0.25846500

TSC1

C	3.92248700	2.71688900	-0.09680300
C	3.73620900	1.34971900	-0.43132500
C	4.76692000	0.43210200	-0.11161600
C	5.93943100	0.84019600	0.49873700
C	6.10444300	2.20266900	0.82103600
C	5.08475600	3.13116700	0.51732000
H	3.13270900	3.43048900	-0.31844200
H	4.64201700	-0.61800200	-0.36004700
H	6.71282800	0.11641700	0.72102700
H	5.24268600	4.17229100	0.77879500
O	7.19467300	2.71458400	1.41390700
C	8.28617600	1.84458300	1.75118900
H	8.70161600	1.36833700	0.85678700
H	9.04121200	2.48555800	2.20691500
H	7.97341500	1.07969300	2.46978800
C	2.56825500	0.84848500	-1.08301300
C	1.59053700	1.62745700	-1.92556900
H	2.23311400	2.04354800	-2.72088300
H	0.93144300	0.90332300	-2.41109300
C	0.70639800	2.69620800	-1.35661400
C	-0.66794500	2.67672300	-1.42130600
C	0.02236600	4.54945200	-0.46286000
N	1.12064700	3.87450100	-0.76373100
N	-1.09791100	3.86812300	-0.85917900
C	-0.02460900	5.87433900	0.22280600
H	-0.57048200	5.81994800	1.17215100

H	0.99671900	6.20012600	0.43091500
H	-0.51356800	6.64023700	-0.39101600
C	-2.48619400	4.24259700	-0.64590200
H	-3.09662500	3.76444600	-1.41310600
H	-2.82444600	3.90141600	0.33507200
H	-2.59215100	5.32581400	-0.72901000
O	-1.52767200	1.79037900	-1.95697200
C	0.70702800	-1.86124300	0.41823900
C	-0.40098300	-2.67179200	0.71142100
C	-0.40794300	-4.01917700	0.35353400
C	0.71713600	-4.57991100	-0.29130200
C	1.83500400	-3.75884700	-0.56690200
C	1.83157100	-2.41706300	-0.21411700
H	-1.27103100	-2.25529000	1.20855500
H	2.72391000	-1.83867600	-0.40658000
O	2.95510400	-4.27456000	-1.17453500
O	0.66681700	-5.88416500	-0.68717600
O	-1.54517900	-4.71954500	0.62440300
C	2.77964300	-4.61014200	-2.56421400
H	2.02001300	-5.38646100	-2.69796400
H	2.49752500	-3.72170300	-3.14200100
H	3.74625200	-4.97937200	-2.91232800
C	1.65669300	-6.77510800	-0.13000500
H	1.60408700	-6.76640300	0.96423000
H	1.40153900	-7.76949500	-0.49924600
H	2.66560100	-6.50489600	-0.44945100
C	-1.43241400	-6.02054700	1.22623100
H	-2.38260900	-6.19375000	1.73710800
H	-1.27070700	-6.79816700	0.47673500
H	-0.62174800	-6.04533000	1.96342300
C	0.64673800	-0.47113700	0.85736300
O	1.34270700	0.48904400	0.48942400
H	-0.08450800	-0.26294000	1.64893500
H	2.64893200	-0.18584500	-1.39434600
H	-1.70895000	1.06099700	-1.28517300
C	-6.16452000	1.17218700	-0.96812600
C	-4.81702000	1.05542200	-0.64055800
C	-4.45478500	0.50023600	0.59173600
C	-5.43181400	0.06480200	1.48456900
C	-6.78040500	0.18709900	1.14219100
C	-7.16823800	0.74147200	-0.08386900
H	-6.44656900	1.60112500	-1.92653900
H	-4.05199000	1.38642900	-1.33549200
H	-5.13520900	-0.37140800	2.43244000

H	-7.54113500	-0.15596600	1.83861400
C	-8.62298200	0.86606800	-0.46407400
H	-8.86196200	1.88523700	-0.78791500
H	-8.86938600	0.19941800	-1.29947100
H	-9.28063300	0.61193700	0.37189700
S	-2.71709100	0.42246000	1.04956500
O	-2.60231300	-0.58155100	2.14096700
O	-2.31326100	1.79972700	1.43365000
O	-2.01203100	-0.04769200	-0.20806200

INTC1

C	4.38505200	-0.70044600	-0.45568500
C	3.66270200	0.06121000	0.48002800
C	4.24226800	1.22710800	0.98618300
C	5.51103300	1.64727700	0.57677100
C	6.21352500	0.88897600	-0.36766900
C	5.64025400	-0.28945700	-0.87801900
H	3.96402600	-1.62880300	-0.82742500
H	3.71061300	1.82095100	1.72578100
H	5.93062700	2.55479900	0.99282000
H	6.20472000	-0.86966100	-1.60111300
O	7.44639300	1.19968700	-0.84945800
C	8.08478500	2.38462400	-0.37185400
H	8.26193300	2.33958200	0.70967100
H	9.04331700	2.43661200	-0.89101200
H	7.49864400	3.28107200	-0.60842300
C	2.30647600	-0.37768600	0.96407700
C	2.26204200	-1.67576100	1.82177700
H	3.20358600	-1.71912800	2.37880900
H	1.45285500	-1.55920400	2.54910300
C	1.99986100	-2.94339500	1.07521700
C	0.79005100	-3.59582400	1.03363500
C	2.24962900	-4.60800100	-0.28971600
N	2.90152600	-3.58482100	0.24189300
N	0.95363200	-4.65813900	0.15752400
C	2.81792700	-5.60363500	-1.24591900
H	2.27820700	-5.60928300	-2.20060300
H	3.86146000	-5.34879800	-1.44335700
H	2.77971100	-6.62418300	-0.84618900
C	-0.07620300	-5.62436500	-0.18805100
H	-1.04824100	-5.17583000	0.01843300
H	-0.01772000	-5.86219700	-1.25229200
H	0.03886300	-6.54671500	0.39109500
O	-0.37005300	-3.38203400	1.68237600

C	0.08567000	1.35496700	-0.49378300
C	-1.17767800	1.65641700	-1.05698500
C	-1.76838500	2.89376000	-0.87311300
C	-1.07136000	3.90532900	-0.16110700
C	0.21894200	3.61705300	0.35826600
C	0.78548800	2.36496800	0.20474100
H	-1.70499800	0.89971600	-1.62753700
H	1.78207900	2.22024400	0.59378400
O	0.91421000	4.58588000	1.03800100
O	-1.70513200	5.07658600	0.00971800
O	-3.02868700	3.06358700	-1.36197400
C	0.56910900	4.67031800	2.43436000
H	-0.49640100	4.89016700	2.56996000
H	0.81293600	3.73441500	2.95107000
H	1.16572400	5.48430400	2.84980100
C	-0.98834800	6.33066800	-0.08333900
H	-0.20016000	6.27265700	-0.83757500
H	-1.73874200	7.06182700	-0.38821600
H	-0.56268400	6.61740600	0.87896400
C	-3.30768200	4.22428100	-2.17042000
H	-4.13913900	3.94025700	-2.81923300
H	-3.59587500	5.07751500	-1.55306200
H	-2.44433900	4.49183400	-2.78886600
C	0.52208500	0.02191400	-0.74175900
O	1.46891300	-0.67340600	-0.23544500
H	-0.00967600	-0.53540700	-1.51063300
H	1.82023400	0.42175800	1.52089500
H	-0.87014300	-2.65843800	1.20537400
C	-6.12907000	-1.68671000	1.05601200
C	-4.90524700	-2.15431000	0.58299800
C	-4.10006500	-1.31614600	-0.19313000
C	-4.51691700	-0.01873100	-0.49291400
C	-5.74413400	0.43751800	-0.01056100
C	-6.56900400	-0.38485500	0.76845900
H	-6.75661100	-2.34180800	1.65526400
H	-4.57575100	-3.16476800	0.80092700
H	-3.90344300	0.63361100	-1.10270400
H	-6.06316900	1.44925200	-0.24754200
C	-7.90619000	0.09737100	1.27329900
H	-8.72685900	-0.43577900	0.77792500
H	-8.01239600	-0.08210500	2.34888900
H	-8.04457000	1.16657300	1.09019000
S	-2.48674900	-1.90179800	-0.73609900
O	-2.20232500	-1.21610100	-2.02913300

0	-2.57697900	-3.37964900	-0.81490000
0	-1.52339700	-1.44074900	0.34430200

TAC2

C	-5.26550100	-1.53218700	0.23423200
C	-4.97317900	-1.07989900	-1.06373200
C	-5.98065200	-0.41468900	-1.77419200
C	-7.24428000	-0.19574700	-1.22653900
C	-7.52017700	-0.65571300	0.06969600
C	-6.52075000	-1.32394100	0.79350900
H	-4.50763100	-2.04136300	0.82057800
H	-5.77659700	-0.05777200	-2.78055100
H	-7.99752200	0.32023100	-1.80954800
H	-6.75049800	-1.67366600	1.79505200
O	-8.71239000	-0.50895700	0.70593900
C	-9.77364100	0.15606700	0.01901200
H	-10.05572600	-0.37497500	-0.89829700
H	-10.61995100	0.15681000	0.70791100
H	-9.50852700	1.19153600	-0.22677800
C	-3.62358800	-1.24106700	-1.72522700
C	-2.68136600	-2.35854000	-1.18716400
H	-2.00787600	-2.63271400	-2.00262500
H	-3.27288000	-3.23892900	-0.92520300
C	-1.85347000	-1.91032900	-0.02562500
C	-0.47162300	-1.60512500	-0.08533800
C	-1.13228500	-1.83996600	2.01969100
N	-2.20271500	-2.10188400	1.31511800
N	-0.04114900	-1.51738200	1.20892600
C	-1.04694300	-1.85089600	3.50661900
H	-0.27224400	-2.53847800	3.86233000
H	-0.81177600	-0.85570400	3.90153500
H	-2.01130300	-2.16562800	3.90864400
C	1.29268000	-1.11293700	1.64670600
H	2.01209100	-1.91291100	1.46237100
H	1.60934200	-0.22343700	1.10158800
H	1.26020800	-0.89002900	2.71221100
O	0.22685100	-1.38612200	-1.16023900
C	-1.34781100	1.22760500	-0.25088800
C	-0.55493600	1.63180700	-1.33203900
C	0.47460400	2.55691700	-1.14492800
C	0.73044300	3.06489400	0.14716700
C	-0.05702300	2.62249500	1.24323300
C	-1.09327800	1.71614300	1.04893700
H	-0.72493100	1.23416300	-2.32413500

H	-1.72255300	1.39868400	1.87028900
O	0.25271900	3.18831300	2.44199200
O	1.66134400	4.04720100	0.30736000
O	1.11841200	2.94690900	-2.27421000
C	-0.50853600	2.80293200	3.58565300
H	-0.09361400	3.36582600	4.42301800
H	-1.56888500	3.05686700	3.46878100
H	-0.41113000	1.72895500	3.78961100
C	2.80916700	3.74942200	1.13345000
H	2.53996600	3.75014900	2.19235300
H	3.24006000	2.78479800	0.85451600
H	3.52762200	4.54779200	0.93599700
C	2.50953600	3.32131600	-2.25111500
H	2.85177000	3.20107800	-3.28152800
H	2.63135300	4.36218300	-1.94256300
H	3.08330500	2.65923400	-1.60296500
C	-2.40661900	0.26739500	-0.41629700
O	-2.82364600	-0.01208600	-1.64006200
H	-3.76662500	-1.36159900	-2.79978500
H	-3.09816400	0.11735900	0.40969800
H	1.26817700	-1.35865100	-1.07019500
C	6.61204700	-1.34829200	1.37105800
C	5.42279400	-0.82692200	0.86392100
C	5.16863500	-0.90508500	-0.50645600
C	6.09692400	-1.49214700	-1.36763600
C	7.28152300	-2.01073800	-0.84694000
C	7.55631800	-1.95275000	0.52754000
H	6.81397600	-1.28109500	2.43704900
H	4.70207800	-0.34814900	1.51845700
H	5.89713700	-1.52716000	-2.43347900
H	8.00729600	-2.46261700	-1.51798200
S	3.61401900	-0.28697800	-1.16075800
O	3.87689100	0.17712300	-2.53994600
O	2.70397700	-1.50969000	-1.11847900
O	3.14702200	0.76233000	-0.21326300
C	8.82510800	-2.54584900	1.08788700
H	8.66973900	-3.59315800	1.37685800
H	9.63451700	-2.52813300	0.35190700
H	9.15838400	-2.00819700	1.98081000

3cc

C	3.70198600	0.58088000	0.15196400
C	3.45757600	-0.33321100	-0.88841800
C	4.37549100	-1.37207000	-1.07402900

C	5.50371300	-1.51612300	-0.26322200
C	5.72673900	-0.59854500	0.77210600
C	4.81659800	0.45091300	0.97252400
H	3.01752900	1.40541200	0.32745500
H	4.21051700	-2.09219500	-1.87200200
H	6.19173500	-2.33320400	-0.44483900
H	5.00516300	1.15648800	1.77585300
O	6.78746300	-0.63490800	1.62693900
C	7.76158200	-1.66240300	1.45009100
H	8.23791200	-1.60236300	0.46366000
H	8.51581300	-1.49757100	2.22170900
H	7.32575300	-2.66043200	1.58272100
C	2.22168500	-0.27583300	-1.76807000
C	1.61953100	1.12659000	-2.00591900
H	1.19440500	1.16354600	-3.01131400
H	2.34596700	1.93426800	-1.90572100
C	0.47362900	1.26109700	-0.97621400
C	-0.86149500	1.58948300	-1.64721900
C	-0.41364400	3.02004600	0.04098600
N	0.65313100	2.29752000	0.04420100
N	-1.36489700	2.65142300	-0.91893700
C	-0.67729700	4.16794400	0.95488500
H	-0.83504400	5.09069200	0.38619500
H	-1.58180300	3.99048400	1.54686100
H	0.17191600	4.30037700	1.62652200
C	-2.67000600	3.24778900	-1.13963600
H	-3.07715100	2.81097600	-2.05320300
H	-3.34493000	3.02745900	-0.30682200
H	-2.58829400	4.33028400	-1.26420300
O	-1.38767600	1.06194700	-2.61322100
C	-0.90569600	-0.68663400	0.07604200
C	-1.58842000	-1.56845200	-0.75209300
C	-2.89507100	-1.96646800	-0.43778100
C	-3.52594500	-1.47473400	0.71679100
C	-2.82154600	-0.57542200	1.55253800
C	-1.51998100	-0.18653000	1.23390900
H	-1.13165800	-1.94184800	-1.65951900
H	-0.97052800	0.48925100	1.87714800
O	-3.49155200	-0.17136400	2.67018300
O	-4.76803400	-1.94531800	1.07505600
O	-3.46094500	-2.87974300	-1.28444300
C	-2.84778700	0.75404000	3.54381000
H	-3.56042100	0.95173400	4.34638700
H	-1.92968600	0.33468800	3.97265100

H	-2.61085900	1.69503400	3.03124500
C	-5.83797800	-0.98698600	1.04718700
H	-5.69223100	-0.20171700	1.79402500
H	-5.93492900	-0.53262900	0.05343600
H	-6.74970800	-1.54340500	1.27703000
C	-4.82911100	-2.71196100	-1.67801700
H	-4.94415400	-3.28136000	-2.60413700
H	-5.51919000	-3.09695500	-0.92394200
H	-5.05661000	-1.65839900	-1.87893600
C	0.46138900	-0.16677700	-0.28515700
O	1.12590600	-1.02585400	-1.19154000
H	2.44361700	-0.77572800	-2.71460400
H	1.05227000	-0.04336600	0.63335500

INTC2

C	0.78621500	1.88084300	1.56265200
C		0.36598500	1.07031600
C		0.48567900	-0.31298900
C		1.02243200	-0.89804200
C		1.44571600	-0.08229100
C		1.31169100	1.31332900
H		0.71797800	2.96024900
H		0.18063400	-0.94431000
H		1.11814800	-1.97481200
H		1.64372000	1.93364300
O		1.99583500	-0.54366800
C		2.22445000	-1.94954600
H		2.88626000	-2.31329200
H		2.70530800	-2.09787800
H		1.28333400	-2.51264500
C		-0.11896400	1.66134700
C		0.98326900	2.15915600
H		1.26117600	1.27846500
H		0.52282100	2.87071800
C		2.19456200	2.73985500
C		3.32699000	2.05783700
C		3.44865000	4.17182200
N		2.28825700	4.05912000
N		4.12840200	2.97128100
C		4.00166000	5.41146200
H		4.92979700	5.73866300
H		3.26504800	6.21206000
H		4.22317700	5.27372400
C		5.40876100	2.67472100

H	5.84458900	1.80346500	0.05906300
H	6.08452000	3.52411200	0.43197700
H	5.28921500	2.45711200	1.61657500
O	3.74348100	0.78561500	-0.82592700
C	-3.16822800	1.80497600	-0.10896600
C	-4.51135700	2.25126200	0.02885800
C	-5.55150600	1.34971200	0.07619900
C	-5.30423700	-0.04958900	-0.01971800
C	-3.94916100	-0.51029300	-0.08796500
C	-2.91533600	0.40544800	-0.13146200
H	-4.74631500	3.30947100	0.06779700
H	-1.90781000	0.03287700	-0.13117000
O	-3.76838600	-1.85140200	-0.09509400
O	-6.39682200	-0.80547200	-0.00597300
O	-6.83696900	1.81057700	0.12933500
C	-2.43247700	-2.36497200	-0.22784300
H	-1.94751000	-1.99319100	-1.13733300
H	-1.82693700	-2.10680600	0.64750200
H	-2.54668000	-3.44766300	-0.28436600
C	-6.43398300	-2.21024900	-0.35675500
H	-5.97269100	-2.81576400	0.42316800
H	-7.49756100	-2.43733900	-0.43428300
H	-5.94063000	-2.38305600	-1.31392200
C	-7.50714400	1.61521500	1.38978900
H	-8.50197700	2.04874900	1.27316200
H	-7.59948500	0.55313300	1.63540800
H	-6.97433800	2.13515200	2.19494600
C	-2.22144600	2.84512400	-0.23094500
O	-0.95986200	2.85758200	-0.49368100
H	-2.59421100	3.86185700	-0.10836300
H	-0.74337000	0.96374400	-1.36199800
H	3.19745600	0.27734200	-1.48525200
C	1.18299900	-4.40998800	0.33184900
C	0.91165200	-3.62540900	-0.78574100
C	1.88720800	-2.74700200	-1.27117200
C	3.13110200	-2.67174200	-0.64785400
C	3.39384600	-3.46667900	0.47071700
C	2.42723400	-4.34078400	0.98235000
H	0.41945500	-5.08476200	0.71121900
H	-0.05690400	-3.68178900	-1.27202100
H	3.88178500	-1.98502100	-1.02142300
H	4.36289500	-3.39606500	0.95765700
C	2.68929400	-5.16467600	2.21843000
H	3.73407500	-5.09571400	2.53333100

H	2.06507700	-4.82613300	3.05429100
H	2.45315100	-6.22135100	2.05068700
S	1.50842300	-1.71827500	-2.70484300
O	0.14208800	-1.17024800	-2.44672300
O	1.58831200	-2.59465200	-3.89790700
O	2.57258100	-0.64913100	-2.70760200

TSC3

3'cc

C	3.71620700	0.53666900	0.29161000
C		3.47571700	-0.18513800
C		4.40330400	-1.16478800
C		5.53903000	-1.43481400
C		5.75901100	-0.70866600
C		4.83852900	0.27931000
H		3.02352200	1.30860300
H		4.23959800	-1.73737900
H		6.23443500	-2.19861800
H		5.02410600	0.83521500
O		6.82604100	-0.87755800
C		7.76802100	-1.90428900
H		8.26888600	-1.72229000
H		8.51021000	-1.87991400
H		7.29387000	-2.89325500
C		2.22797700	0.00101800
C		1.65352900	1.44316300
H		1.43639300	1.74209900
H		2.34014100	2.17433300
C		0.32849200	1.38104600
C		0.16760400	2.44940000
C		-1.58368200	2.43625800
N		-0.84920400	1.51399300
N		-1.05237000	3.02955200
C		-2.90622100	2.88316100
H		-3.69129600	2.69398300
H		-2.90344300	3.95802900
H		-3.13948900	2.33548000
C		-1.66017900	4.07000200
H		-0.99055000	4.26229000
H		-1.78874000	4.99138800
H		-2.63215700	3.74348600

O	0.91879800	2.71594400	1.02010400
C	-0.92228000	-0.65433100	0.01264800
C	-1.53471400	-1.55553100	-0.84872800
C	-2.81524100	-2.04826200	-0.56324900
C	-3.49273200	-1.62930000	0.59376600
C	-2.86017400	-0.70881600	1.46291000
C	-1.58168600	-0.22877400	1.17438000
H	-1.04056400	-1.87601800	-1.75741500
H	-1.08744400	0.46310200	1.84572700
O	-3.57042000	-0.37677400	2.57878000
O	-4.70781300	-2.18657900	0.91800500
O	-3.31058100	-2.97529300	-1.43958200
C	-3.00522300	0.57667000	3.47723300
H	-3.74019000	0.71020100	4.27272700
H	-2.06586600	0.21482000	3.91223600
H	-2.82832900	1.54059400	2.98319900
C	-5.83605300	-1.29726200	0.89424800
H	-5.76315400	-0.53673900	1.67661500
H	-5.93264700	-0.80778100	-0.08277100
H	-6.71639200	-1.91927700	1.07169400
C	-4.67506100	-2.86647700	-1.86576400
H	-4.74270100	-3.43252700	-2.79855700
H	-5.36556500	-3.28802000	-1.13190600
H	-4.94481500	-1.82244800	-2.06463800
C	0.41308300	-0.03997500	-0.31349700
O	1.14288100	-0.82067200	-1.24012900
H	2.43063500	-0.37071400	-2.74441900
H	0.98775600	0.09235800	0.61601600

TSD1

C	2.17312800	4.30913600	-1.09886800
C	2.19721800	2.96796400	-0.61729900
C	3.14138300	2.62653500	0.39122900
C	4.02909900	3.55817300	0.89007500
C	3.99067500	4.87857000	0.39111600
C	3.05373300	5.24162300	-0.60886800
H	1.45474900	4.60373900	-1.85541800
H	3.15239200	1.60628400	0.76633600
H	4.74028700	3.27194600	1.65428800
H	3.05124700	6.26687100	-0.96246100
O	4.79470600	5.86456100	0.79844400
C	5.77306200	5.60991500	1.82281200
H	6.49111700	4.85112000	1.49682100
H	6.28624900	6.55924500	1.97555500

H	5.29032400	5.29675400	2.75378500
C	1.32957900	1.95791400	-1.07296900
C	0.48235100	2.02421300	-2.30191200
H	0.15158400	3.04407800	-2.50907600
H	1.20964000	1.76659600	-3.09476900
C	-0.69693400	1.10170600	-2.38315700
C	-0.73796300	-0.26718700	-2.56589100
C	-2.79513600	0.55007300	-2.37034800
N	-1.98954600	1.59016600	-2.25997200
N	-2.08055300	-0.61139100	-2.54432200
C	-4.28276200	0.57030700	-2.27179800
H	-4.63471400	-0.02134400	-1.41923100
H	-4.61774900	1.59995300	-2.13179200
H	-4.76136400	0.16634000	-3.17219700
C	-2.60647200	-1.96402800	-2.60766300
H	-3.28402700	-2.07953900	-3.45843300
H	-1.76796100	-2.65123600	-2.72098400
H	-3.14080800	-2.20773000	-1.68474800
O	0.17713700	-1.20646500	-2.84313400
C	-2.10126000	0.45029600	0.92532900
C	-2.38878000	-0.91936000	0.95937800
C	-3.69849100	-1.36007200	1.16187900
C	-4.72547500	-0.41198900	1.36226300
C	-4.41371000	0.97146200	1.34211800
C	-3.11769500	1.40058600	1.10795300
H	-1.60290500	-1.65104200	0.79469300
H	-2.89766600	2.46101400	1.06829400
O	-5.40400600	1.90890600	1.51494200
O	-5.99141500	-0.84616700	1.64026800
O	-3.88773400	-2.71030900	1.18968700
C	-5.93319200	1.99061600	2.85118700
H	-6.39052700	1.04599200	3.16148600
H	-5.14375400	2.26587700	3.56086300
H	-6.69267800	2.77472700	2.83039400
C	-7.01464900	-0.50095600	0.68322200
H	-6.84106900	-1.02291600	-0.26438300
H	-7.95649500	-0.84223900	1.11618100
H	-7.05467700	0.57664200	0.51107100
C	-5.03220800	-3.27484000	0.53068800
H	-4.77374600	-4.31735100	0.33031300
H	-5.92354200	-3.23125700	1.15997800
H	-5.23108400	-2.76962000	-0.42124600
C	-0.73309500	0.84412500	0.61220700
O	-0.35801200	2.01107700	0.44861700

H	-0.02410100	0.01209600	0.52429900
H	1.52479100	0.96423000	-0.68836200
H	0.96271300	-1.16430200	-2.22112000
C	4.50794700	-4.84902100	-0.45184400
C	3.55405400	-3.85545800	-0.64828400
C	3.36154900	-2.88364500	0.33891900
C	4.11611900	-2.90338500	1.50990100
C	5.07194800	-3.90544300	1.69297500
C	5.28158100	-4.89145600	0.72091400
H	4.66086000	-5.60352800	-1.21947000
H	2.97063600	-3.82367000	-1.56287900
H	3.95951700	-2.13743200	2.26173500
H	5.66279700	-3.91903800	2.60501600
C	6.31036600	-5.97818200	0.91365500
H	5.84644100	-6.97053700	0.87514500
H	7.06827700	-5.94946900	0.12193000
H	6.82298600	-5.88180400	1.87473900
S	2.08794800	-1.63891400	0.10829700
O	2.36289100	-0.55485600	1.09194900
O	0.77312700	-2.30930300	0.30030000
O	2.27580200	-1.16337300	-1.31764300

INTD1

O	0.21262800	1.36579100	-0.85429200
O	0.25075600	-2.71494100	-0.51957800
O	-5.16818500	4.78950200	-0.62461900
O	4.81891700	2.74573300	1.09160400
O	6.49931900	0.84467700	0.20541600
O	5.69410100	-1.14185100	-1.36081300
N	1.92936200	-2.13097000	0.95381600
N	1.20674400	-0.22668900	1.86521700
C	0.27345600	-0.64704600	0.92218500
C	0.71444000	-1.87980100	0.37778300
C	2.18368200	-1.10194700	1.85234700
C	1.09520700	0.40690500	-1.06658900
H	0.78874700	-0.41980400	-1.70793000
C	-1.01440800	0.08624900	0.76524100
H	-1.06814200	0.82527000	1.56792400
H	-1.88174800	-0.57009300	0.85030900
C	-1.12524400	0.82292500	-0.60277100
H	-1.33797100	0.08921000	-1.38375100
C	-2.14511800	1.91997400	-0.62566300
C	-3.35578900	1.72323400	-1.30747700
H	-3.52640100	0.79685700	-1.85150900

C	-4.34733100	2.69689300	-1.27994500
H	-5.28873100	2.55190200	-1.80050000
C	-4.13982100	3.89816100	-0.58373700
C	-2.92832800	4.10926500	0.09214800
H	-2.74298400	5.02895000	0.63351400
C	-1.94949200	3.11463500	0.07318500
H	-1.01718100	3.27809700	0.60655500
C	2.48691600	0.61996300	-0.82352000
C	2.92709000	1.68993400	-0.02176000
H	2.20245100	2.39795600	0.35500500
C	4.27639400	1.78122600	0.30671300
C	5.18825600	0.80422500	-0.16069900
C	4.73740800	-0.26285200	-0.96880300
C	3.38476700	-0.36062300	-1.28995000
H	3.00794200	-1.17835100	-1.89102400
C	3.45294400	-1.01944700	2.62005800
H	3.65450200	-1.94328700	3.17267400
H	3.39282600	-0.18622700	3.32199400
H	4.30172600	-0.84308100	1.94662100
C	-5.00645400	6.04429100	0.03605100
H	-5.93545700	6.59255300	-0.12997900
H	-4.17004700	6.61626900	-0.38432200
H	-4.85344200	5.91715200	1.11481800
C	3.93726800	3.71844200	1.66034100
H	3.44408200	4.31516100	0.88400000
H	4.56708700	4.36740700	2.27040000
H	3.18005600	3.24341900	2.29518300
C	7.28815900	1.84705000	-0.46426800
H	6.90131200	2.85175800	-0.26852100
H	7.31034200	1.66106200	-1.54434800
H	8.29821500	1.75906700	-0.05937800
C	5.31214900	-2.19702700	-2.24670600
H	4.89973100	-1.80281300	-3.18321700
H	4.58373500	-2.87202700	-1.78251600
H	6.22810500	-2.75015600	-2.45948500
C	2.80569300	-3.25092800	0.63849600
H	2.79522800	-3.98854400	1.44547600
H	3.82378700	-2.88706400	0.48993400
H	2.45142900	-3.72074100	-0.27847600
H	-0.61015400	-2.41165400	-1.01652600
C	-3.04120400	-3.03499000	2.18974600
C	-2.82718200	-3.18525000	0.82365000
C	-3.50871000	-2.35631700	-0.07521000
C	-4.41156100	-1.40200800	0.38890700

C	-4.61948700	-1.26465000	1.76371100
C	-3.93655500	-2.06986600	2.68307800
H	-2.50532400	-3.67239700	2.88854200
H	-2.12641800	-3.92930200	0.45870300
H	-4.92947800	-0.76420300	-0.31820700
H	-5.31756700	-0.51399700	2.12435900
S	-3.12687700	-2.46924300	-1.82671500
O	-4.02489400	-1.52214800	-2.52778100
O	-1.67595500	-1.99041000	-1.91173000
O	-3.25545500	-3.89464600	-2.20134400
C	-4.14894200	-1.92012300	4.16868600
H	-4.58345500	-2.83104100	4.59735600
H	-3.19914100	-1.74498500	4.68678500
H	-4.81943500	-1.08743700	4.39749600

TSD2

O	0.18837500	1.35449300	-0.86442200
O	0.27858300	-2.75012100	-0.42295100
O	-5.14240600	4.84813000	-0.57470600
O	4.81658000	2.80560600	0.98497800
O	6.48903000	0.86242500	0.17685400
O	5.66460400	-1.19332200	-1.29222800
N	1.91881800	-2.11321200	1.06574000
N	1.19414500	-0.15516300	1.86082400
C	0.28570500	-0.60851900	0.90014700
C	0.72575800	-1.88704700	0.44677500
C	2.15951300	-1.03448100	1.91663500
C	1.06050300	0.36356600	-1.00961300
H	0.75820000	-0.46223100	-1.65551600
C	-1.03336300	0.07552400	0.75083200
H	-1.11609200	0.79995800	1.56405300
H	-1.87255000	-0.61661300	0.82515000
C	-1.15167900	0.82873300	-0.60854300
H	-1.37867800	0.10411000	-1.39385100
C	-2.15889500	1.93759300	-0.61450700
C	-3.37293100	1.76610700	-1.29693500
H	-3.55344600	0.84988100	-1.85467900
C	-4.35113900	2.75274200	-1.25637000
H	-5.29493000	2.62786900	-1.77782800
C	-4.12608900	3.94246400	-0.54592200
C	-2.91076600	4.12903100	0.13035300
H	-2.71203600	5.03980800	0.68197100
C	-1.94571400	3.12131000	0.09771900
H	-1.00984000	3.26520500	0.63053900

C	2.46312900	0.59127700	-0.79874400
C	2.91189000	1.69592500	-0.05406300
H	2.19163800	2.42169300	0.29648800
C	4.26574400	1.80245900	0.25482000
C	5.17233800	0.80458900	-0.17407000
C	4.71266700	-0.29592600	-0.92838000
C	3.35519300	-0.40790400	-1.23014900
H	2.97264200	-1.25356700	-1.78779100
C	3.41406500	-0.92312300	2.70420200
H	3.60533200	-1.82692700	3.29190000
H	3.34119300	-0.06479700	3.37375400
H	4.27270600	-0.77003200	2.03751700
C	-4.96252600	6.09366700	0.09856300
H	-5.88395800	6.65637300	-0.06132300
H	-4.11846900	6.65816700	-0.31658300
H	-4.81079100	5.95327300	1.17586400
C	3.94105000	3.80261100	1.51877300
H	3.43760700	4.36313900	0.72215000
H	4.57726800	4.47991700	2.09027900
H	3.19201300	3.35831300	2.18499600
C	7.26934600	1.82424700	-0.55704900
H	6.88987200	2.83985800	-0.40677700
H	7.27234900	1.58500800	-1.62702900
H	8.28655200	1.75335200	-0.16654300
C	5.27185900	-2.28568900	-2.12612800
H	4.85423500	-1.93342500	-3.07703400
H	4.54376900	-2.93583300	-1.62731100
H	6.18376900	-2.85242800	-2.31987900
C	2.79921300	-3.25047500	0.83503100
H	2.80614800	-3.91214200	1.70501100
H	3.81220200	-2.89457900	0.63885700
H	2.43366300	-3.80102900	-0.03123700
H	-0.56497300	-2.45015000	-0.97081500
C	-3.11009200	-3.08940200	2.13643300
C	-2.83935100	-3.22823400	0.77920500
C	-3.47721000	-2.38614200	-0.13922900
C	-4.39432100	-1.43165500	0.29532200
C	-4.65954300	-1.30626500	1.66126100
C	-4.01992400	-2.12346100	2.60092900
H	-2.60878200	-3.73756900	2.85082600
H	-2.12977500	-3.97486000	0.43735100
H	-4.87948400	-0.78501300	-0.42668300
H	-5.36853500	-0.55544200	1.99932400
S	-3.02672500	-2.48603700	-1.87462500

O	-3.87693500	-1.51477500	-2.60023400
O	-1.56378400	-2.02871400	-1.89635200
O	-3.16008500	-3.90414900	-2.27238900
C	-4.29024600	-1.98267000	4.07795700
H	-4.70515400	-2.90899300	4.49227000
H	-3.36596600	-1.77236800	4.62851300
H	-4.99762300	-1.17441800	4.28219200

3dd

O	-0.96938800	-0.22591600	-1.66853100
O	1.37732200	-3.72163800	-0.87684600
O	-6.75273700	1.28276600	0.38404900
O	1.71764300	3.51464000	0.49270800
O	4.27030000	2.67788300	0.52520600
O	4.97143000	0.29090800	-0.45766900
N	1.36136100	-2.79293700	1.25746800
N	-0.27298400	-1.23368400	1.09053700
C	-0.14705200	-1.88050800	-0.21651300
C	0.93573800	-2.94057200	-0.04568900
C	0.60143500	-1.77657800	1.86196200
C	0.25101200	-0.86326900	-1.33731900
H	0.61870100	-1.46894300	-2.18197200
C	-1.48606900	-2.38869900	-0.77074700
H	-2.16333500	-2.68675400	0.03053200
H	-1.29816600	-3.25329300	-1.41301500
C	-2.03957600	-1.19657800	-1.61275600
H	-2.24491000	-1.54710600	-2.63270000
C	-3.27721200	-0.52847800	-1.06282000
C	-4.47409300	-0.51929100	-1.79036100
H	-4.51265400	-0.99190800	-2.76877200
C	-5.61907100	0.08693000	-1.28166900
H	-6.54793800	0.09635600	-1.84343500
C	-5.58488400	0.70986300	-0.02569200
C	-4.39235700	0.71118800	0.71421100
H	-4.34104000	1.18398700	1.68782400
C	-3.25510700	0.09534300	0.19027300
H	-2.33413700	0.08540000	0.76547800
C	1.30738400	0.13055700	-0.92633200
C	0.95013300	1.39096800	-0.44709400
H	-0.09361700	1.67082300	-0.43849900
C	1.94714700	2.25896500	0.01456300
C	3.29376500	1.85321300	0.01794800
C	3.64150900	0.58474000	-0.47946600
C	2.64489700	-0.27775100	-0.95376800

H	2.89638400	-1.25803900	-1.34050500
C	0.85283900	-1.40133600	3.28169000
H	0.72382800	-2.26319000	3.94491600
H	0.15975700	-0.61191000	3.57517500
H	1.87981000	-1.04037300	3.40459100
C	-6.78364700	1.91730300	1.66110700
H	-7.79983200	2.29710500	1.78250700
H	-6.07917700	2.75672800	1.71468800
H	-6.56534300	1.20998900	2.47089100
C	0.37061200	3.98637400	0.51116800
H	-0.06101900	4.01651500	-0.49675500
H	0.41578500	5.00036200	0.91265300
H	-0.26497200	3.36928200	1.15796200
C	4.72818300	3.66733700	-0.40497600
H	3.91534600	4.34220800	-0.69823300
H	5.15572200	3.20109200	-1.30167700
H	5.50587500	4.24154300	0.10531000
C	5.37834600	-0.99784600	-0.91297300
H	5.13924300	-1.14976000	-1.97292300
H	4.91934400	-1.80029400	-0.32179500
H	6.46154400	-1.03165000	-0.78260700
C	2.45318800	-3.54153000	1.85430700
H	2.11349900	-4.09524100	2.73355500
H	3.26869900	-2.87170800	2.14175000
H	2.81469100	-4.24609000	1.10336900

INTD2

O	-0.17945000	-1.32922800	-1.00420600
O	1.51668800	-0.73688700	2.11693600
O	-6.38342900	-2.06151000	-1.65843200
O	2.07588800	3.21777900	0.22307800
O	4.61702100	2.89297600	-0.58062000
O	5.47576000	0.65823200	-1.70735400
N	3.17594400	-2.21115400	1.46506100
N	2.05928800	-3.83942700	0.42125700
C	1.14740800	-2.87002400	0.83974600
C	1.85348700	-1.85469800	1.51823700
C	3.24840400	-3.41871700	0.78689900
C	1.12238800	-1.40980300	-1.12406900
H	1.53977500	-2.31813200	-1.55595400
C	-0.32709300	-3.03098900	0.70174000
H	-0.84054700	-2.42344300	1.44538600
H	-0.60863300	-4.07773800	0.85072200
C	-0.82012700	-2.62734300	-0.71570500

H	-0.41816500	-3.33925600	-1.44476300
C	-2.30274800	-2.48728800	-0.90071600
C	-2.89984600	-2.96204200	-2.07979400
H	-2.28808400	-3.45391900	-2.83182000
C	-4.26206500	-2.81255400	-2.30377300
H	-4.72721200	-3.18082000	-3.21262400
C	-5.06486000	-2.17071300	-1.34610800
C	-4.48359800	-1.69457000	-0.16252100
H	-5.07475500	-1.19025600	0.59195500
C	-3.11525600	-1.86029900	0.05104100
H	-2.68844800	-1.46783100	0.96508600
C	1.95347300	-0.24947300	-1.03559700
C	1.49045500	0.95243000	-0.46416500
H	0.47422800	1.00825200	-0.09937500
C	2.37931500	2.01836300	-0.32854600
C	3.72027400	1.88520000	-0.76008400
C	4.17246400	0.67352900	-1.32845000
C	3.29060600	-0.39552300	-1.46418400
H	3.61087700	-1.33208400	-1.90195100
C	4.54360800	-4.10499000	0.52096800
H	5.22039800	-3.47166700	-0.06423500
H	4.35040100	-5.02203800	-0.03825000
H	5.06264400	-4.36394900	1.45086500
C	-7.24972600	-1.41917000	-0.72089200
H	-8.24543300	-1.44682500	-1.16656300
H	-6.95835300	-0.37559600	-0.55144200
H	-7.26933700	-1.95173100	0.23755800
C	0.74649100	3.40809600	0.72602300
H	0.00389800	3.28941000	-0.06845100
H	0.71662000	4.43269200	1.09914300
H	0.53014300	2.71809700	1.54769800
C	4.45407700	4.03057200	-1.44909200
H	3.48288600	4.51099900	-1.29886900
H	4.56263900	3.73177200	-2.49830500
H	5.25246500	4.72730500	-1.18649700
C	5.99849900	-0.55615900	-2.24641800
H	5.47982700	-0.84818800	-3.16763400
H	5.93910400	-1.37589000	-1.51921400
H	7.04631000	-0.35377200	-2.47297000
C	4.28303300	-1.39859200	1.95048600
H	4.70524200	-0.79822600	1.13953900
H	5.05612600	-2.04416700	2.36938300
H	3.91291800	-0.73152700	2.72886000
H	0.53158300	-0.47941100	1.98504700

C	-2.98961800	4.22567000	0.40642500
C	-2.59607600	3.33442900	1.40560800
C	-2.26197300	2.02373900	1.06497700
C	-2.31948000	1.60121300	-0.26623200
C	-2.71363600	2.50179000	-1.25335400
C	-3.05734000	3.82565500	-0.93523000
H	-3.24137400	5.24888300	0.67244900
H	-2.52293700	3.65912300	2.43829100
H	-2.02858600	0.58991200	-0.52523000
H	-2.74961900	2.17430000	-2.28947000
S	-1.76594000	0.88073800	2.36183700
O	-2.99590700	0.20898600	2.84895600
O	-0.86173200	-0.09940500	1.62906900
O	-1.03128900	1.68338400	3.36895000
C	-3.48622100	4.78434900	-2.01850600
H	-4.43463000	4.46826200	-2.46912300
H	-3.62073300	5.79748700	-1.62962300
H	-2.74715600	4.82508100	-2.82651300

TSD3

O	-0.19947200	-1.31609400	-1.06638400
O	1.47356200	-0.74065100	2.12267000
O	-6.43257700	-2.00804200	-1.57892500
O	2.09589900	3.19437100	0.23202100
O	4.64078000	2.86226500	-0.54881400
O	5.49161000	0.61924200	-1.68450000
N	3.15522200	-2.18579900	1.50509500
N	2.10307100	-3.75455800	0.30602100
C	1.16633800	-2.78355900	0.69555900
C	1.84172700	-1.82397700	1.50344600
C	3.26199100	-3.36449100	0.76574900
C	1.11760600	-1.43964700	-1.11796600
H	1.51575600	-2.30641100	-1.64451300
C	-0.30722600	-3.02027100	0.61005000
H	-0.82059600	-2.44919900	1.38172800
H	-0.52707500	-4.08164200	0.75480400
C	-0.84736200	-2.60407600	-0.78506400
H	-0.47241200	-3.31357200	-1.53213200
C	-2.33454900	-2.45792000	-0.92851700
C	-2.96024200	-2.89756500	-2.10653400
H	-2.36690700	-3.36911300	-2.88584500
C	-4.32692100	-2.74000600	-2.29525600
H	-4.81315900	-3.08183600	-3.20341300
C	-5.10674000	-2.12584100	-1.30120800

C	-4.49747800	-1.68435300	-0.11846300
H	-5.06967900	-1.20056200	0.66349900
C	-3.12472000	-1.85737900	0.05833900
H	-2.67662500	-1.49106000	0.97278200
C	1.96365900	-0.27489800	-1.02195000
C	1.50680300	0.92640700	-0.45052800
H	0.48705400	0.99151300	-0.09786400
C	2.40095200	1.98982200	-0.31036000
C	3.74277500	1.85089400	-0.73074900
C	4.18794500	0.64082900	-1.30277600
C	3.29891100	-0.42418000	-1.44679400
H	3.61555500	-1.35724200	-1.89392800
C	4.56765200	-4.04908100	0.55710800
H	5.29426900	-3.38648100	0.07372100
H	4.41100100	-4.92391800	-0.07585000
H	5.00407100	-4.37616500	1.50755700
C	-7.27725200	-1.39960400	-0.60014100
H	-8.28388400	-1.41724600	-1.02118900
H	-6.98552000	-0.36062100	-0.40498100
H	-7.27101300	-1.96159800	0.34157800
C	0.76206800	3.39269400	0.71749800
H	0.02747800	3.27213500	-0.08429300
H	0.73113400	4.41969300	1.08435700
H	0.53278700	2.70890800	1.54091500
C	4.50338000	3.96675200	-1.46082400
H	3.53018300	4.45502600	-1.34949700
H	4.63353900	3.63247600	-2.49712900
H	5.29715800	4.67213100	-1.20615400
C	6.00757100	-0.59713000	-2.22400000
H	5.49114900	-0.88412500	-3.14813800
H	5.93865000	-1.41839600	-1.49918100
H	7.05793800	-0.40236400	-2.44584200
C	4.23524800	-1.39838700	2.08553000
H	4.63462600	-0.69559900	1.34840100
H	5.02811400	-2.06395800	2.42688400
H	3.84471400	-0.83956400	2.93612000
H	0.47559200	-0.48003200	1.97692000
C	-2.97806100	4.20389100	0.37025300
C	-2.59193400	3.31935400	1.37805100
C	-2.25035700	2.00801800	1.04693300
C	-2.29127400	1.57822800	-0.28238200
C	-2.67790000	2.47278800	-1.27793500
C	-3.03043800	3.79659400	-0.97005500
H	-3.23595100	5.22759000	0.62831400

H	-2.53097200	3.65002600	2.40965400
H	-1.99283200	0.56733000	-0.53352400
H	-2.70103200	2.13999800	-2.31267800
S	-1.76931900	0.87466100	2.35644900
O	-3.00470400	0.22114600	2.85137600
O	-0.87770500	-0.12842800	1.63226800
O	-1.01945200	1.67475900	3.35328800
C	-3.45320900	4.74764100	-2.06241100
H	-4.40316100	4.43236000	-2.51044000
H	-3.58272900	5.76503000	-1.68305400
H	-2.71348900	4.77657200	-2.87021100

3'dd

O	1.03496900	0.02140700	-1.28021300
O	0.42923600	0.64754700	1.89053400
O	6.85068800	-1.33657000	0.69174200
O	-2.10990000	-3.25676700	1.01568000
O	-4.59735300	-2.44385900	0.40517200
O	-5.02973500	-0.27053600	-1.09363900
N	-1.22127100	2.25804200	1.63311600
N	-0.85246300	3.00781100	-0.47176100
C	0.08025000	1.90716900	-0.23355500
C	-0.16139700	1.47823600	1.21514600
C	-1.55977000	3.13971200	0.59725300
C	-0.19002100	0.72553500	-1.23767600
H	-0.39506100	1.21086800	-2.20518500
C	1.56623700	2.21986700	-0.51327300
H	2.12408600	2.33758700	0.41735400
H	1.64876300	3.14647500	-1.08497400
C	2.08884600	1.00271600	-1.33736600
H	2.22001400	1.31460200	-2.38330100
C	3.36669400	0.38270900	-0.83502100
C	3.40976000	-0.21593600	0.43657700
H	2.51040800	-0.22391300	1.04546500
C	4.58408600	-0.77987900	0.91422400
H	4.62630300	-1.24654700	1.89375800
C	5.75165000	-0.75664400	0.13046300
C	5.72313700	-0.16197300	-1.13626400
H	6.60751700	-0.13319400	-1.76105500
C	4.52823600	0.39518900	-1.60618000
H	4.51195300	0.84769200	-2.59472100
C	-1.33956600	-0.17559600	-0.86768500
C	-1.11719500	-1.33399100	-0.12056000
H	-0.10425500	-1.60466300	0.13849700

C	-2.20878400	-2.10857700	0.28822200
C	-3.51893500	-1.71660500	-0.04067500
C	-3.72851800	-0.55649600	-0.80711300
C	-2.63505200	0.21568500	-1.22056200
H	-2.77792500	1.11480400	-1.80631700
C	-2.66536300	4.12155300	0.78334000
H	-3.61017600	3.60275200	0.97935400
H	-2.76843800	4.72715100	-0.11800000
H	-2.46590800	4.77508600	1.63915900
C	8.06358300	-1.34933000	-0.05921300
H	8.79918000	-1.85881100	0.56586100
H	8.41729500	-0.33318400	-0.27396300
H	7.94959100	-1.89932500	-1.00166300
C	-0.80884400	-3.67028500	1.43355800
H	-0.16022500	-3.89540900	0.57811700
H	-0.95897100	-4.57976300	2.01804400
H	-0.32779000	-2.91116100	2.06218100
C	-4.89491500	-3.58687100	-0.40619600
H	-4.05783600	-4.29503100	-0.41635200
H	-5.13402400	-3.29123800	-1.43565500
H	-5.76825200	-4.07008600	0.03960400
C	-5.30323300	0.90715300	-1.84974000
H	-4.85281300	0.86218200	-2.84916700
H	-4.95114500	1.81017800	-1.33513000
H	-6.38929700	0.95216100	-1.94921100
C	-1.83817200	2.16621800	2.94456700
H	-2.89363800	1.89413200	2.85705500
H	-1.75064500	3.11237100	3.48577100
H	-1.31209500	1.38618400	3.49715300

2b

C0.00000000	0.57566200	0.00000000	
C	1.33515500	0.14667300	0.00000000
C	1.62995300	-1.21642500	0.00000000
C	0.59029800	-2.15046100	0.00000000
C	-0.74495600	-1.72633300	0.00000000
C	-1.04119300	-0.36742100	0.00000000
H	2.13531600	0.88310700	0.00000000
H	-2.06781300	-0.01431800	0.00000000
C	-0.30062700	2.02145200	0.00000000
O	-1.42584300	2.49659700	0.00000000
H	0.59229900	2.68180700	0.00000000
H	2.66299300	-1.55073300	0.00000000
H	-1.54655000	-2.45907300	0.00000000

H	0.81872000	-3.21244800	0.00000000
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TSA1-2b

C	-3.88617300	-0.72005400	-0.31084500
C	-2.63341400	-0.31652500	0.20398800
C	-2.47766900	-0.21425300	1.60099400
C	-3.52234900	-0.50273200	2.46853600
C	-4.76135700	-0.90444700	1.93826400
C	-4.93221500	-1.01192600	0.54207700
H	-4.02784700	-0.81907500	-1.38029000
H	-1.51317900	0.08887100	1.99968100
H	-3.37211300	-0.42116900	3.53766600
H	-5.89763500	-1.33039600	0.16316000
O	-5.84627800	-1.21275500	2.67894700
C	-5.75893200	-1.12569500	4.10649000
H	-5.53311600	-0.10346800	4.42989500
H	-6.74196400	-1.41522800	4.47992600
H	-5.00360700	-1.81429400	4.50151900
C	-1.50261300	0.02199700	-0.62804700
C	-1.33620500	-0.41958000	-2.04930900
H	-2.23716400	-0.25482300	-2.64410800
H	-0.50770100	0.13036600	-2.50230400
C	-1.02616900	-1.88843800	-1.96435900
C	0.19533300	-2.50495000	-1.74752700
C	-1.42811500	-4.01526200	-1.83869500
N	-2.02507000	-2.85196600	-1.99583200
N	-0.06688000	-3.85768600	-1.67705100
C	-2.08728200	-5.35268700	-1.83654100
H	-1.95226900	-5.87314500	-0.88047800
H	-3.15738300	-5.21962800	-2.00768400
H	-1.68708000	-6.00543400	-2.62171000
C	0.92647200	-4.90601400	-1.50775100
H	1.11759100	-5.42177700	-2.45413500
H	1.85424700	-4.45373800	-1.15720100
H	0.58075900	-5.63122200	-0.76766600
O	1.46148200	-2.08578200	-1.65644900
C	-0.70961200	4.05689700	-0.97185900
C	0.53384000	4.71726600	-0.97651300
C	0.57169000	6.10886400	-0.98053800
C	-0.62259100	6.83575600	-0.98418800
C	-1.86239500	6.18009400	-0.97613000
C	-1.91110700	4.79293200	-0.96555100
H	1.44723000	4.13059200	-0.94635100

H	-2.85914200	4.26502200	-0.95794700
C	-0.70737600	2.60797600	-0.95856100
O	-1.74862200	1.92977400	-0.84204200
H	0.26061200	2.10453200	-1.05706700
H	-0.56741900	0.11690400	-0.08475100
H	1.52120800	-1.11587000	-1.39553200
C	5.06622400	-1.90693100	0.96621000
C	3.82957000	-1.33720800	0.67838400
C	3.66183800	0.04427900	0.82245600
C	4.71681600	0.84592500	1.25381800
C	5.95126900	0.25936100	1.54016200
C	6.14645400	-1.12057000	1.40062500
H	5.19948500	-2.97990700	0.85405700
H	3.00791000	-1.95823500	0.33670000
H	4.56771400	1.91459900	1.36278600
H	6.77327300	0.88473400	1.87857400
C	7.48666100	-1.75239200	1.68393800
H	7.37347800	-2.71856300	2.18636300
H	8.03623400	-1.93608000	0.75208100
H	8.11000900	-1.10957200	2.31215700
S	2.05723200	0.77587600	0.47752100
O	2.20335100	2.24691400	0.61249300
O	1.09126400	0.14823500	1.42124100
O	1.74623900	0.39401700	-0.96167700
H	1.52520800	6.62714700	-0.97759000
H	-2.78141800	6.75757300	-0.97702700
H	-0.59103000	7.92150300	-0.99013900

2c

C	1.31668300	0.20838800	0.00000000
C	0.52346800	1.36349100	0.00000000
C	-0.86354300	1.26016500	0.00000000
C	-1.45510600	-0.01452400	0.00000000
C	-0.66347200	-1.17979800	0.00000000
C	0.71860000	-1.06169100	0.00000000
H	0.99445800	2.34241600	0.00000000
H	1.35206700	-1.94252900	0.00000000
C	2.79361500	0.33784400	0.00000000
O	3.56128100	-0.60936900	0.00000000
H	3.17111400	1.38068000	0.00000000
H	-1.48723900	2.14726900	0.00000000
H	-1.13820500	-2.15486900	0.00000000
C	-2.88379400	-0.13155800	0.00000000

N	-4.04302100	-0.22741600	0.00000000
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TSA1-2c

C	1.79589700	-3.60847300	-0.24903800
C	1.23942100	-2.42287200	0.27622700
C	1.25548900	-2.22730600	1.66954400
C	1.80933100	-3.17103700	2.52610400
C	2.35878100	-4.34662500	1.98653500
C	2.34740300	-4.55610300	0.59236000
H	1.80628100	-3.77778000	-1.31946900
H	0.83241200	-1.31254100	2.07640600
H	1.81393400	-2.99036600	3.59359500
H	2.78395400	-5.46984900	0.20299000
O	2.92239500	-5.33354800	2.71660600
C	2.99724500	-5.18378600	4.13895000
H	1.99958000	-5.10712100	4.58604400
H	3.48961500	-6.08555000	4.50512000
H	3.59283800	-4.30638800	4.41560500
C	0.62713500	-1.39587100	-0.54897400
C	0.96790300	-1.18592100	-1.99750000
H	0.95710800	-2.12119400	-2.56121100
H	0.24226200	-0.50043400	-2.44356300
C	2.34436900	-0.58328800	-2.01086800
C	2.70584100	0.74433600	-1.85915600
C	4.51184800	-0.53361200	-2.02930800
N	3.49006900	-1.36233000	-2.09558900
N	4.08504500	0.76964100	-1.87678200
C	5.95486000	-0.90334500	-2.10852600
H	6.49991400	-0.61983700	-1.19993700
H	6.03552900	-1.98497100	-2.23420900
H	6.45596000	-0.41641200	-2.95380000
C	4.90701200	1.96658000	-1.80227300
H	5.21772600	2.29423200	-2.79973000
H	4.32691900	2.76164900	-1.33275700
H	5.79428600	1.76841200	-1.19796700
O	2.03766200	1.89994200	-1.76294600
C	-3.42464600	-1.38299300	-0.78525000
C	-4.33084300	-0.31352900	-0.89452400
C	-5.69717900	-0.56428200	-0.88067400
C	-6.14946100	-1.88959200	-0.76085300
C	-5.24467800	-2.96364400	-0.64317500
C	-3.88356000	-2.70676300	-0.65242500

H	-3.95675200	0.70270800	-0.96151200
H	-3.16728900	-3.51632600	-0.56591100
C	-2.00456200	-1.07764900	-0.81195100
O	-1.13774100	-1.95479500	-0.61295900
H	-1.70203800	-0.04573200	-1.01527800
H	0.43973700	-0.47023100	-0.01395400
H	1.10150300	1.76638900	-1.42454900
C	0.90971600	5.62225100	0.73053400
C	0.70774100	4.26938900	0.47649700
C	-0.49944300	3.67427600	0.86007900
C	-1.49129000	4.42204800	1.49067700
C	-1.27257000	5.77868700	1.74010600
C	-0.07315900	6.39820200	1.36893000
H	1.84404100	6.08900000	0.42908100
H	1.47507700	3.68647700	-0.02336800
H	-2.42346200	3.94607400	1.77492000
H	-2.04733300	6.36224600	2.23009700
C	0.17618900	7.85819600	1.65354900
H	0.93810400	7.97947800	2.43325900
H	0.54461700	8.37839000	0.76264000
H	-0.73231100	8.36342300	1.99306400
S	-0.74208300	1.91795700	0.58019100
O	-2.17623300	1.61956700	0.82788600
O	0.21096100	1.20450500	1.47390100
O	-0.39412800	1.69741800	-0.88442800
H	-6.41073900	0.24803000	-0.95937400
H	-5.61762500	-3.97713200	-0.54893000
C	-7.55867900	-2.15612400	-0.75748700
N	-8.70090100	-2.37353600	-0.75670000

2d

C	-0.61067200	-0.21829200	0.40866900
C	0.20024400	-1.23812600	-0.42501200
C	1.69851400	-1.17728900	-0.05131100
C	2.14643400	0.25007100	0.34686300
C	1.29491700	1.31116100	-0.36167200
C	-0.17949000	1.22917900	0.09191100
H	-0.18748700	-2.25326700	-0.28270900
H	-0.83849000	1.63589900	-0.68213200
C	-2.08738600	-0.46366900	0.22233600
O	-2.89168500	0.33812300	-0.21394800
H	-2.41817400	-1.48583500	0.51399900

H	1.90020300	-1.86855700	0.77539900
H	1.68715700	2.31605600	-0.17044300
H	2.04114500	0.38417000	1.43155200
H	3.20974700	0.38784800	0.12126800
H	2.28765600	-1.53088400	-0.90546500
H	0.06217900	-0.99779600	-1.48622200
H	-0.41636200	-0.45397600	1.46776200
H	-0.33154800	1.84726100	0.98408600
H	1.36208900	1.15588800	-1.44622200

TSA1-2d

C	-4.08743800	-0.37555700	-0.37815600
C		-2.77407900	-0.24977200
C		-2.57046100	-0.34327400
C		-3.63167500	-0.55185800
C		-4.93320700	-0.66411300
C		-5.15062900	-0.57640900
H		-4.26836800	-0.31031800
H		-1.55707200	-0.27796900
H		-3.44525000	-0.63225300
H		-6.16545400	-0.67292600
O		-6.04042900	-0.86063600
C		-5.90639500	-0.96801000
H		-5.49032200	-0.05050100
H		-6.91693700	-1.12033400
H		-5.28038000	-1.82351500
C		-1.62359700	-0.00680200
C		-1.51783200	-0.44528600
H		-2.44880000	-0.31304400
H		-0.72822500	0.13002900
C		-1.13455600	-1.89512800
C		0.14180600	-2.41095100
C		-1.36435100	-4.03588200
N		-2.06022000	-2.92411700
N		-0.00974900	-3.77598200
C		-1.91406500	-5.41874600
H		-1.61986800	-5.90733900
H		-3.00428900	-5.37073700
H		-1.56631300	-6.05582900
C		1.06665900	-4.74175600
H		1.18191100	-5.34072000
H		1.99399200	-4.20059500

H	0.86282500	-5.40506700	-0.81575700
O	1.36808600	-1.87068300	-1.97463000
H	-0.67434800	-0.05162700	-0.19568500
H	1.39274500	-0.98092400	-1.50963500
C	5.23089600	-1.87376500	0.47478300
C	3.92619500	-1.42273100	0.29643100
C	3.49042000	-0.29108600	0.99409400
C	4.35072000	0.38012500	1.86139900
C	5.65653100	-0.08456900	2.03007800
C	6.11747500	-1.21399000	1.34224600
H	5.57003900	-2.75264600	-0.06768400
H	3.25702400	-1.94200600	-0.38191000
H	3.99844500	1.25611500	2.39486500
H	6.32541200	0.43944900	2.70771200
C	7.53634700	-1.70043200	1.50216900
H	8.00008700	-1.29834200	2.40756800
H	7.58012400	-2.79353200	1.54982600
H	8.15309200	-1.39117000	0.64889400
S	1.79216400	0.26868200	0.80377800
O	1.69513600	1.58144900	1.49708100
O	0.91920400	-0.79431000	1.37475300
O	1.57436900	0.41041200	-0.69180700
C	-0.62421800	3.97148800	-0.35567400
C	0.89689300	4.08341400	-0.68807200
C	1.33619500	5.56241200	-0.61453100
C	0.21045200	6.53907200	-1.02677400
C	-0.73248000	5.88708300	-2.04581800
C	-1.48084800	4.68791500	-1.42135400
H	1.48784700	3.46261100	-0.01031700
H	-1.76352500	3.97602800	-2.20283000
C	-0.92445100	2.53040100	-0.16768900
O	-1.58132700	1.86750100	-0.98258800
H	-0.49721800	2.04659200	0.71961400
H	1.67130800	5.79446900	0.40271300
H	-1.45765600	6.61356900	-2.42802700
H	-0.37261400	6.83135600	-0.14332900
H	0.64130300	7.46192300	-1.43008900
H	2.20508600	5.69240000	-1.26996000
H	1.04242600	3.68296500	-1.69734200
H	-0.75886500	4.42676800	0.63633200
H	-2.40984000	5.02738700	-0.95036100
H	-0.14531400	5.55089900	-2.90965900

2e

C	-0.61067200	-0.21829200	0.40866900
C	0.20024400	-1.23812600	-0.42501200
C	1.69851400	-1.17728900	-0.05131100
C	2.14643400	0.25007100	0.34686300
C	1.29491700	1.31116100	-0.36167200
C	-0.17949000	1.22917900	0.09191100
H	-0.18748700	-2.25326700	-0.28270900
H	-0.83849000	1.63589900	-0.68213200
C	-2.08738600	-0.46366900	0.22233600
O	-2.89168500	0.33812300	-0.21394800
H	-2.41817400	-1.48583500	0.51399900
H	1.90020300	-1.86855700	0.77539900
H	1.68715700	2.31605600	-0.17044300
H	2.04114500	0.38417000	1.43155200
H	3.20974700	0.38784800	0.12126800
H	2.28765600	-1.53088400	-0.90546500
H	0.06217900	-0.99779600	-1.48622200
H	-0.41636200	-0.45397600	1.46776200
H	-0.33154800	1.84726100	0.98408600
H	1.36208900	1.15588800	-1.44622200

TSA1-2e

C	-4.08743800	-0.37555700	-0.37815600
C	-2.77407900	-0.24977200	0.12664700
C	-2.57046100	-0.34327400	1.51779000
C	-3.63167500	-0.55185800	2.38991200
C	-4.93320700	-0.66411300	1.87087600
C	-5.15062900	-0.57640900	0.47957000
H	-4.26836800	-0.31031800	-1.44546600
H	-1.55707200	-0.27796900	1.90533700
H	-3.44525000	-0.63225300	3.45342900
H	-6.16545400	-0.67292600	0.10839200
O	-6.04042900	-0.86063600	2.61677600
C	-5.90639500	-0.96801000	4.03896900
H	-5.49032200	-0.05050100	4.47018100
H	-6.91693700	-1.12033400	4.41997900
H	-5.28038000	-1.82351500	4.31606800
C	-1.62359700	-0.00680200	-0.71598000
C	-1.51783200	-0.44528600	-2.14436700
H	-2.44880000	-0.31304400	-2.69903200
H	-0.72822500	0.13002900	-2.63560200
C	-1.13455600	-1.89512800	-2.06241100

C	0.14180600	-2.41095100	-1.93530900
C	-1.36435100	-4.03588200	-1.84098600
N	-2.06022000	-2.92411700	-1.97902900
N	-0.00974900	-3.77598200	-1.80586500
C	-1.91406500	-5.41874600	-1.74198900
H	-1.61986800	-5.90733900	-0.80538600
H	-3.00428900	-5.37073700	-1.77828400
H	-1.56631300	-6.05582900	-2.56444200
C	1.06665900	-4.74175600	-1.65973700
H	1.18191100	-5.34072000	-2.56831700
H	1.99399200	-4.20059500	-1.47136600
H	0.86282500	-5.40506700	-0.81575700
O	1.36808600	-1.87068300	-1.97463000
H	-0.67434800	-0.05162700	-0.19568500
H	1.39274500	-0.98092400	-1.50963500
C	5.23089600	-1.87376500	0.47478300
C	3.92619500	-1.42273100	0.29643100
C	3.49042000	-0.29108600	0.99409400
C	4.35072000	0.38012500	1.86139900
C	5.65653100	-0.08456900	2.03007800
C	6.11747500	-1.21399000	1.34224600
H	5.57003900	-2.75264600	-0.06768400
H	3.25702400	-1.94200600	-0.38191000
H	3.99844500	1.25611500	2.39486500
H	6.32541200	0.43944900	2.70771200
C	7.53634700	-1.70043200	1.50216900
H	8.00008700	-1.29834200	2.40756800
H	7.58012400	-2.79353200	1.54982600
H	8.15309200	-1.39117000	0.64889400
S	1.79216400	0.26868200	0.80377800
O	1.69513600	1.58144900	1.49708100
O	0.91920400	-0.79431000	1.37475300
O	1.57436900	0.41041200	-0.69180700
C	-0.62421800	3.97148800	-0.35567400
C	0.89689300	4.08341400	-0.68807200
C	1.33619500	5.56241200	-0.61453100
C	0.21045200	6.53907200	-1.02677400
C	-0.73248000	5.88708300	-2.04581800
C	-1.48084800	4.68791500	-1.42135400
H	1.48784700	3.46261100	-0.01031700
H	-1.76352500	3.97602800	-2.20283000
C	-0.92445100	2.53040100	-0.16768900
O	-1.58132700	1.86750100	-0.98258800
H	-0.49721800	2.04659200	0.71961400

H	1.67130800	5.79446900	0.40271300
H	-1.45765600	6.61356900	-2.42802700
H	-0.37261400	6.83135600	-0.14332900
H	0.64130300	7.46192300	-1.43008900
H	2.20508600	5.69240000	-1.26996000
H	1.04242600	3.68296500	-1.69734200
H	-0.75886500	4.42676800	0.63633200
H	-2.40984000	5.02738700	-0.95036100
H	-0.14531400	5.55089900	-2.90965900

N-TSA1

C	-0.55849900	-2.24324800	0.67073400
C	-0.26428600	-2.35193500	-0.70772700
C	-0.06082300	-3.63534100	-1.24968100
C	-0.15407200	-4.77814300	-0.46597900
C	-0.46014400	-4.65148500	0.90134600
C	-0.65969600	-3.37532700	1.45978700
H	-0.72661800	-1.27676200	1.13071800
H	0.17040700	-3.73463600	-2.30673800
H	0.00139800	-5.75129700	-0.91477900
H	-0.90353800	-3.29789200	2.51406300
O	-0.58727200	-5.69123000	1.75493500
C	-0.42826900	-7.02158200	1.25035100
H	0.57766900	-7.17711400	0.84394900
H	-0.57887600	-7.68194800	2.10525600
H	-1.17527700	-7.24780900	0.48084400
C	-0.13502500	-1.18953800	-1.57569500
C	-0.77684000	0.13369500	-1.25395700
H	-0.39008000	0.89503200	-1.93685500
H	-0.57167200	0.45249600	-0.22769300
C	-2.23509100	-0.06516700	-1.48993300
C	-2.93878300	0.01553000	-2.70844800
C	-4.37037400	-0.52528500	-0.99522000
N	-3.14453400	-0.41909000	-0.49513400
N	-4.30081700	-0.27889300	-2.32188000
C	-5.60136700	-0.79518100	-0.21019200
H	-6.13082200	-1.67596400	-0.58952100
H	-5.33933700	-0.96553900	0.83606900
H	-6.29089000	0.05546100	-0.26055600
C	-5.41013700	-0.26608200	-3.25444700
H	-5.87100100	-1.25490200	-3.33731600
H	-6.16862100	0.46062300	-2.94937600
H	-4.99929200	0.02273200	-4.22357400

O	-2.60128700	0.27505800	-3.88205800
C	3.50586300	0.02291600	-0.30590300
C	4.00193900	0.19947800	0.99776100
C	5.27841100	0.70905800	1.18360600
C	6.07967000	1.05773400	0.07120100
C	5.54894000	0.92571800	-1.24733800
C	4.28162900	0.39175500	-1.42645200
H	3.41165200	-0.07609500	1.86574100
H	3.85921600	0.27294000	-2.41555900
O	6.34846800	1.36625300	-2.25082300
O	7.29874900	1.55321100	0.35256600
O	5.78647300	0.80144800	2.45080900
C	5.88219900	1.23542400	-3.59725500
H	5.70634300	0.18537700	-3.85827700
H	4.96483500	1.81380400	-3.75674100
H	6.67832700	1.63785400	-4.22456600
C	8.44403400	1.23435600	-0.46833900
H	8.51973500	1.91174300	-1.31959200
H	9.30630500	1.35930700	0.18900700
H	8.39718900	0.20025800	-0.81975200
C	5.89147700	2.13854800	2.97222500
H	6.31878100	2.04177500	3.97232300
H	6.54700700	2.76017900	2.35451900
H	4.90152700	2.60547100	3.04489800
C	2.18980200	-0.52174900	-0.46341600
O	1.66447300	-0.73106300	-1.58395100
H	1.62847300	-0.76254200	0.44813300
H	-0.12791400	-1.41845400	-2.63790000
H	-2.93972700	-0.48731900	0.51949800
C	-5.22956400	3.02321500	1.12704300
C	-4.41169000	2.20722900	1.90771900
C	-3.04833600	2.11460300	1.61746500
C	-2.50536800	2.84426500	0.55917700
C	-3.33372300	3.65328300	-0.21784700
C	-4.70752500	3.75022800	0.04652900
H	-6.29047000	3.09037900	1.35389900
H	-4.83432000	1.63813900	2.72989600
H	-1.44590700	2.76371000	0.34396000
H	-2.90887200	4.21052800	-1.04919900
S	-2.03343500	0.95038100	2.54861800
O	-2.15092800	1.31204700	3.98116200
O	-2.66789600	-0.38589300	2.23411300
O	-0.65541800	1.06001300	1.98534000
C	-5.59235200	4.61366000	-0.81835300

H	-5.55499900	4.28969800	-1.86505500
H	-6.63522900	4.57746500	-0.49113200
H	-5.26786100	5.66056000	-0.79669700

N-TSA2

C	0.94674400	-2.44253200	-0.50935500
C	0.39415200	-2.23122400	0.77290800
C	0.26275000	-3.33100800	1.63843900
C	0.67700700	-4.60423400	1.26358200
C	1.23591700	-4.79493100	-0.01200800
C	1.36511600	-3.70373800	-0.89225900
H	1.07159900	-1.61925200	-1.20358600
H	-0.16403300	-3.18216400	2.62682700
H	0.57122600	-5.42919700	1.95715200
H	1.80847200	-3.87041700	-1.86823200
O	1.68165300	-5.98162000	-0.48378800
C	1.61230100	-7.13145800	0.36494700
H	0.57533900	-7.37333300	0.62585600
H	2.03998200	-7.95238700	-0.21215300
H	2.19778300	-6.98781500	1.28036900
C	-0.05328300	-0.91759000	1.21701800
C	0.54599900	0.35005200	0.67346500
H	0.62786500	0.34349300	-0.41639900
H	-0.06144400	1.20846200	0.97500200
C	1.87798600	0.42230200	1.33731500
C	2.18312900	0.93778200	2.61420400
C	4.07602000	0.10870600	1.61524700
N	3.05296400	-0.08946500	0.79238500
N	3.60654000	0.72004300	2.72549000
C	5.49621500	-0.20069000	1.31421000
H	5.93968400	-0.83498100	2.08930900
H	5.56381000	-0.71555700	0.35377300
H	6.08790500	0.72024300	1.25532900
C	4.38638600	1.13421700	3.87475600
H	5.15728500	1.85425700	3.58514600
H	3.69099100	1.60738300	4.57026600
H	4.85898700	0.27649000	4.36223600
O	1.49746400	1.47517600	3.50842400
C	-3.88375100	0.25469700	0.69825800
C	-4.70037200	1.10683900	1.46379100
C	-5.98058300	1.43508700	1.03026300
C	-6.45306800	0.91455600	-0.20054500

C	-5.61562300	0.06564900	-0.97004900
C	-4.35032900	-0.26951300	-0.52355900
H	-4.35510300	1.50612700	2.41201900
H	-3.72140600	-0.91007200	-1.13107900
O	-6.05790100	-0.42088800	-2.17376200
O	-7.67659100	1.30726500	-0.61999700
O	-6.70156800	2.28758100	1.80801000
C	-6.00508800	0.54383600	-3.24330000
H	-6.61941600	1.42325100	-3.01930600
H	-4.97131100	0.85916500	-3.42620000
H	-6.39582300	0.04041300	-4.12930300
C	-8.61318200	0.31004900	-1.08960500
H	-8.50027300	-0.62144300	-0.52841900
H	-9.60305600	0.73193900	-0.90681700
H	-8.48604100	0.11332600	-2.15524500
C	-8.08344000	1.98220000	2.07764300
H	-8.30586600	2.44543900	3.04177600
H	-8.73950100	2.39676500	1.30968400
H	-8.24442100	0.90148200	2.15373000
C	-2.56767600	-0.05926900	1.18448800
O	-1.79205500	-0.83880300	0.58375300
H	-2.24004900	0.41388800	2.12068100
H	-0.30677000	-0.85650700	2.27422600
H	3.16229800	-0.47578200	-0.16689000
C	3.36282700	3.69305200	-0.59022300
C	2.80015400	2.61974300	-1.28548100
C	3.63025700	1.69861400	-1.92073500
C	5.01995400	1.85777100	-1.87829400
C	5.56956000	2.93171900	-1.18422400
C	4.75057100	3.86260500	-0.52161000
H	2.71183000	4.40264600	-0.08623500
H	1.72515200	2.48522300	-1.32478100
H	5.66458400	1.14042000	-2.37669000
H	6.64975200	3.05036700	-1.14787200
C	5.36285000	5.02169400	0.22553100
H	4.62424200	5.53191800	0.85030800
H	6.18423200	4.69002200	0.87027000
H	5.78026600	5.76096700	-0.46937500
S	2.94255300	0.22061100	-2.69279700
O	3.49988600	0.14922200	-4.06451100
O	1.45980400	0.36920300	-2.62126300
O	3.44266500	-0.89820000	-1.80619900

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C	-3.93004300	-0.16675500	0.12442100
C	-3.70456600	0.40107900	-1.16161400
C	-4.54652500	1.46016100	-1.58873200
C	-5.58305800	1.92197400	-0.80200100
C	-5.79715900	1.33592200	0.46519900
C	-4.95828400	0.29414900	0.91791200
H	-3.29246200	-0.96193600	0.49970500
H	-4.37165300	1.91115900	-2.56141200
H	-6.21676900	2.72445300	-1.15701900
H	-5.14169400	-0.12790500	1.90020900
O	-6.76865600	1.70406600	1.31168400
C	-7.66194300	2.76833100	0.94489700
H	-8.22682200	2.51585300	0.04135900
H	-8.34711300	2.87486200	1.78602600
H	-7.11613200	3.70577800	0.79545800
C	-2.65100800	-0.02179400	-2.01537400
C	-1.93782900	-1.34393900	-1.89510000
H	-2.10971400	-1.80623500	-0.92031200
H	-2.45284000	-1.97577100	-2.63719900
C	-0.47700000	-1.31060800	-2.19721100
C	0.19014600	-1.14501100	-3.42113700
C	1.67439700	-0.95004300	-1.66901100
N	0.45773400	-1.15855400	-1.17695200
N	1.57038500	-0.94463200	-3.01564800
C	2.90098600	-0.70525400	-0.86966800
H	3.26193600	0.32037600	-1.01449200
H	2.68347000	-0.84660600	0.19121200
H	3.70831000	-1.38842100	-1.15475400
C	2.64655800	-0.72894000	-3.96089500
H	2.20043600	-0.77651100	-4.95615700
H	3.10774200	0.25331000	-3.81802800
H	3.41475400	-1.50265500	-3.87062000
O	-0.17199100	-1.14897700	-4.61800700
C	0.47489400	2.06587000	-0.00093100
C	0.89118200	1.94338300	1.33191900
C	2.08568900	2.52887800	1.75323800
C	2.87882000	3.24023100	0.82564100
C	2.45285700	3.34289400	-0.52263200
C	1.26027300	2.76901200	-0.93151300
H	0.30762000	1.36938400	2.04311100
H	0.95705700	2.84238900	-1.96968700
O	3.21741000	4.01889900	-1.44254900

O	4.08136900	3.73451700	1.23596900
O	2.44665600	2.32613400	3.05155400
C	4.42767100	3.34032900	-1.82681200
H	5.06676500	3.13642200	-0.96194600
H	4.19365700	2.40045800	-2.34213400
H	4.94727100	4.00925800	-2.51553900
C	4.27910300	5.16007100	1.11736500
H	3.49459300	5.69950700	1.65912000
H	5.24718300	5.36344000	1.57759300
H	4.28819300	5.47810300	0.07288200
C	2.91968400	3.44482300	3.82153900
H	2.74581000	3.18020300	4.86721100
H	3.98442400	3.62349800	3.65857800
H	2.35420200	4.35343300	3.58514300
C	-0.74729300	1.39387000	-0.41408000
O	-1.13308100	1.36055900	-1.59225600
H	-1.31646000	0.87163300	0.36764500
H	-2.61748000	0.42197300	-3.00524400
H	0.22903200	-1.16676400	-0.16734900
C	1.29223600	-4.99349100	-0.11218600
C	0.25063700	-4.16461100	0.30076800
C	0.34435700	-3.49721100	1.52389000
C	1.46758000	-3.66703300	2.33556200
C	2.50125700	-4.50247700	1.91312500
C	2.43306100	-5.17462300	0.68379500
H	1.21950400	-5.50769100	-1.06720900
H	-0.62789500	-4.02905900	-0.32018700
H	1.52594800	-3.15137600	3.28870100
H	3.37498000	-4.63461500	2.54606500
C	3.54127400	-6.09653000	0.23900800
H	3.70190400	-6.03566300	-0.84219200
H	4.48492800	-5.86259500	0.74067800
H	3.29642800	-7.14101300	0.47027500
S	-0.91795600	-2.30197200	1.99213500
O	-0.99624300	-2.30984500	3.47095700
O	-2.16396400	-2.72265700	1.28669000
O	-0.38354500	-0.99304100	1.44699000

N-TSA4

C	-2.66806800	2.55613200	-0.13632000
C	-1.66009300	2.83259500	-1.10298000
C	-1.24758700	4.18031300	-1.27677700

C	-1.79999400	5.20847400	-0.54004400
C	-2.79925800	4.90903400	0.41261500
C	-3.22562900	3.57470300	0.60160700
H	-3.03611400	1.54943200	0.01943800
H	-0.47067100	4.40222000	-2.00277300
H	-1.46582000	6.22638700	-0.69425100
H	-4.00214600	3.37591100	1.33240300
O	-3.40594500	5.82211700	1.18122300
C	-3.05040000	7.20845800	1.04881200
H	-3.26476100	7.57365800	0.03912800
H	-3.67334300	7.73848500	1.76936400
H	-1.99422300	7.36859300	1.28877100
C	-1.04959700	1.83031900	-1.89254000
C	-1.46531100	0.37838200	-1.90635900
H	-2.55370800	0.31003100	-1.78817900
H	-1.20648000	-0.03613300	-2.88437600
C	-0.77871900	-0.45436000	-0.86858800
C	0.48318100	-1.04118200	-0.98217000
C	-0.40198900	-1.51583100	1.06160600
N	-1.26962400	-0.75743600	0.39089700
N	0.67924500	-1.69925400	0.27403800
C	-0.62630400	-2.10553400	2.40561600
H	0.16548200	-1.81297500	3.10395300
H	-1.58599900	-1.76564900	2.79973500
H	-0.64178800	-3.20023200	2.35670700
C	1.87557000	-2.45109300	0.60915600
H	2.55650100	-2.35416000	-0.23733000
H	2.35280800	-2.04385200	1.50367200
H	1.63922900	-3.50692200	0.76978900
O	1.35400700	-0.98504400	-1.89242400
C	3.13978300	0.99070300	-0.90936000
C	4.28907000	0.76850200	-1.67299600
C	5.47785000	0.36123600	-1.06449000
C	5.51690200	0.16439300	0.33280100
C	4.35129100	0.40709000	1.09446600
C	3.17766000	0.82400300	0.48229800
H	4.27224700	0.87914700	-2.75272900
H	2.29314800	1.00019500	1.08258200
O	4.34714200	0.20033500	2.45552400
O	6.69955600	-0.18979200	0.92787100
O	6.56537800	0.21294100	-1.87771000
C	5.11541100	1.15136600	3.21435300
H	6.17033600	1.13839300	2.92357300
H	4.71178400	2.16306200	3.08491700

H	5.02124100	0.85478100	4.26100000
C	6.71584000	-1.47388700	1.58297800
H	6.52149800	-2.27588100	0.86151100
H	7.72105300	-1.58962400	1.99248200
H	5.97945600	-1.51928300	2.38899000
C	7.35870200	-0.97840100	-1.75548500
H	7.88661900	-1.08481300	-2.70636200
H	8.08300100	-0.89983100	-0.94173900
H	6.72523300	-1.85923200	-1.59943400
C	1.87801400	1.34802700	-1.56824300
O	0.88498300	1.71701100	-0.91331400
H	1.87452300	1.37962600	-2.66546700
H	-0.46496500	2.17739700	-2.73869700
H	-2.21563500	-0.51278400	0.75039300
C	-2.79603600	-4.07294700	-1.34667900
C	-3.44624300	-2.84522800	-1.21622500
C	-4.04237200	-2.50595500	-0.00186300
C	-4.00565900	-3.39756200	1.07389900
C	-3.35505400	-4.62154600	0.93148200
C	-2.72956200	-4.97409100	-0.27518300
H	-2.32801400	-4.33203300	-2.29300300
H	-3.48833000	-2.14684900	-2.04437500
H	-4.48025100	-3.13631000	2.01463000
H	-3.32898000	-5.31420300	1.76883300
C	-1.98584600	-6.27988400	-0.40971300
H	-0.91629100	-6.14243600	-0.20508000
H	-2.35951300	-7.02956600	0.29414600
H	-2.07073500	-6.68673100	-1.42223300
S	-4.76038400	-0.86944300	0.23742200
O	-6.11593300	-1.06513200	0.80189600
O	-4.71417100	-0.19862400	-1.09206000
O	-3.81513100	-0.21847300	1.22933000