

Supporting Information for
An Umpolung Mechanism of B(pin)-
Mediated Cu/B Rearrangement and Origin
of Regioselectivity for NHC-Cu Catalyzed
Selective Allylation of Imine

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1. Results for the other possible paths

To prove the reliability of our results, we further re-optimize the geometries for the oxidation addition steps using dispersion-corrected functional M06-L (Fig. S2). we further re-optimized the geometries for the oxidation addition steps using M06-L (Figure S2). The energy barriers optimized by M06-L are decreased both for C(sp²)-Cu oxidation addition or C(sp³)-Cu one and the regioselectivity $\Delta\Delta G^\ddagger$ decreased by 0.6 kcal/mol. However, no change nearly in structures and there was no effect on the conclusion. In addition, we further re-calculated the single point energies for the oxidation addition steps by using M06-L and def2-TZVP base set for all atoms (Figure S3). According to the calculations, the energy barriers both for C(sp²)-Cu oxidation addition or C(sp³)-Cu one are increased slightly and little effect on regioselectivity. Therefore, the geometries are not sensitive to changes in base and functional.

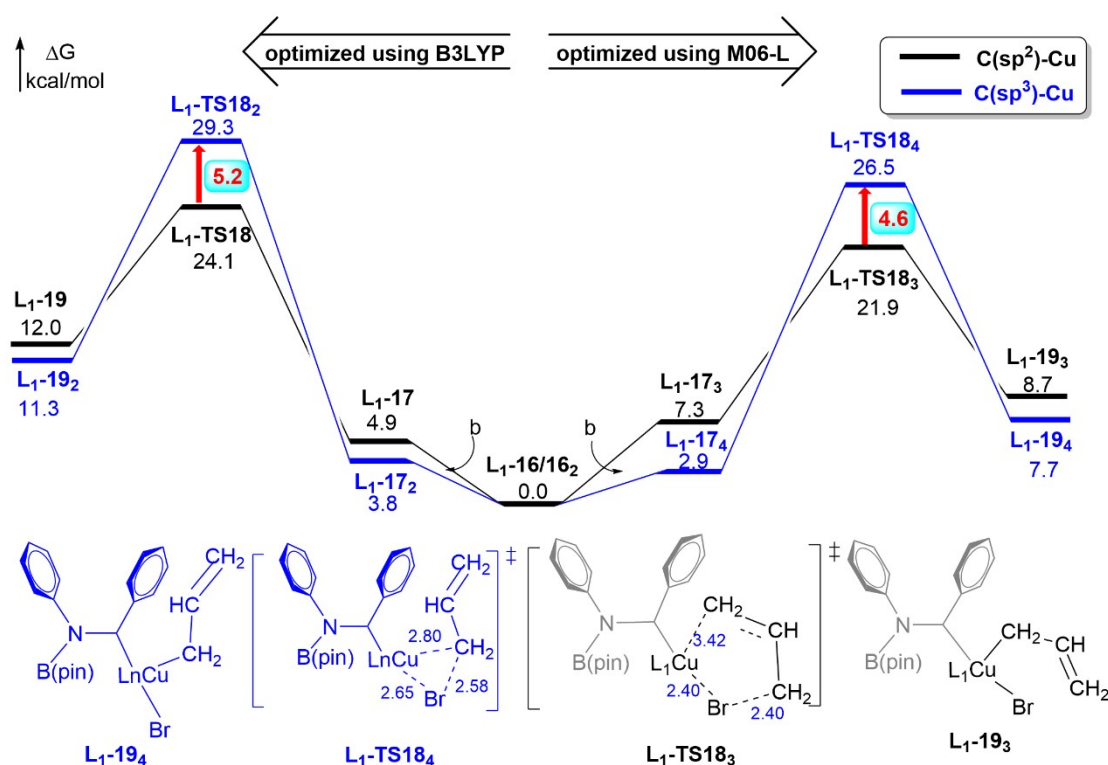


Fig. S1. Free energy profile and optimized structures of oxidation addition for L₁.

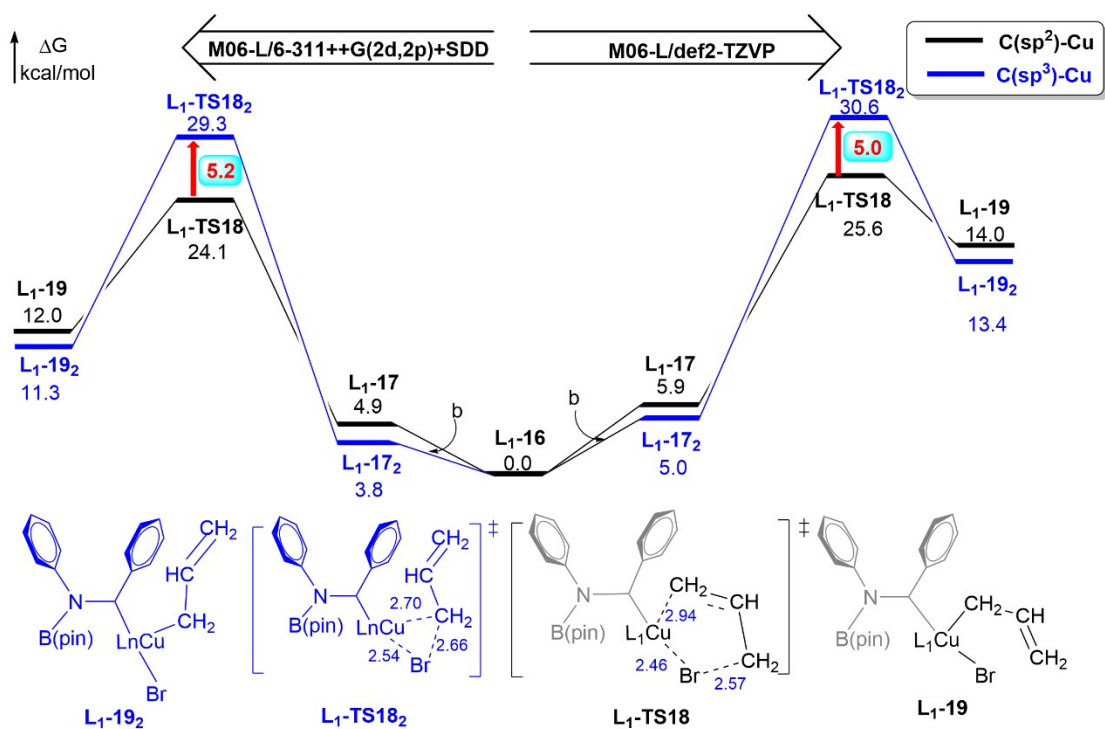


Fig. S2. Free energy profile and optimized structures of oxidation addition for L_1 .

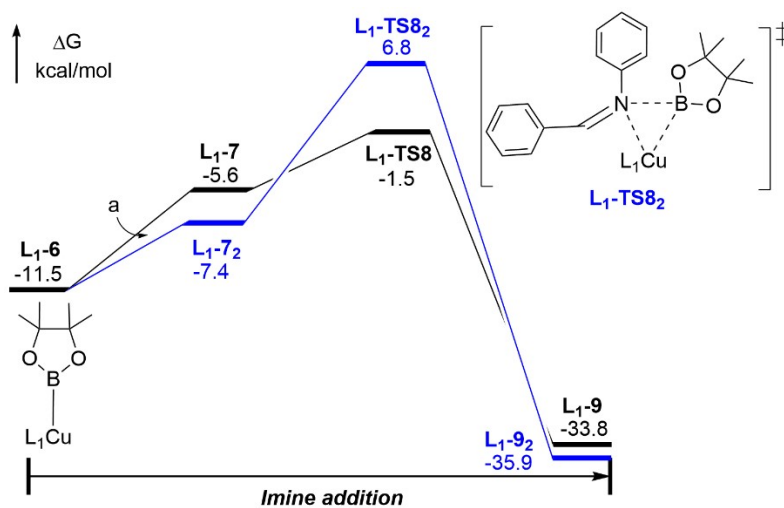


Fig. S3. Free energy profile for the generation of α -borylaminoalkyl copper, along with optimized structures

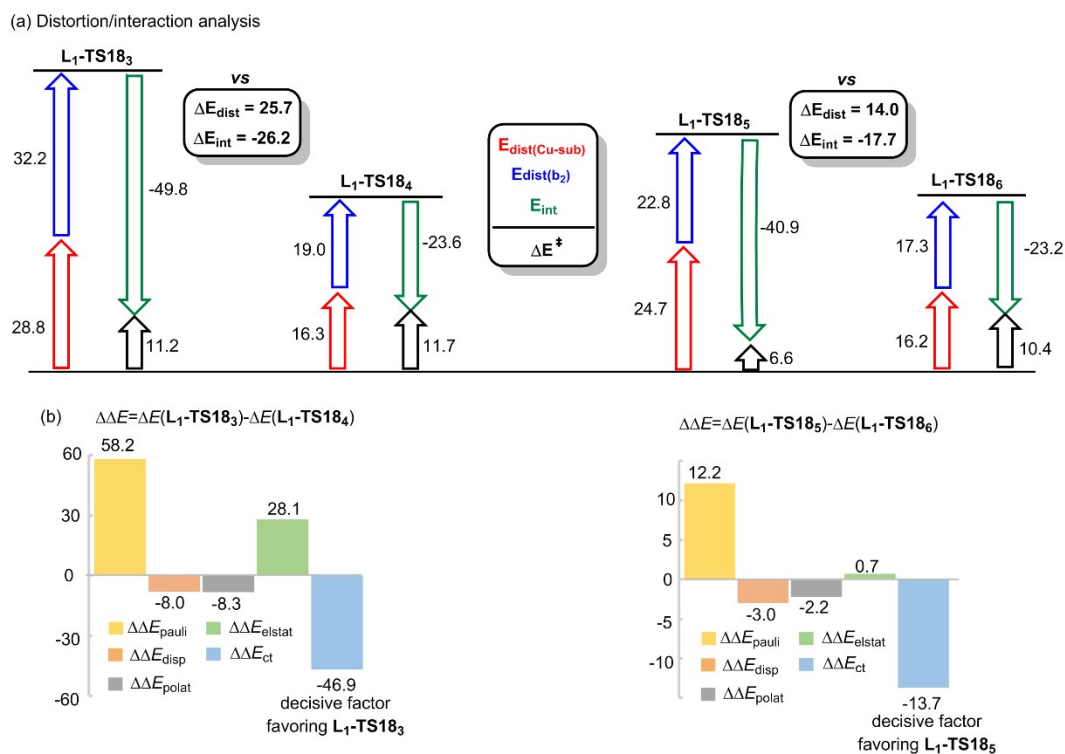


Fig. S4. DI and comparison of each energy term analysis for L₁-TS18₃, L₁-TS18₄, L₁-TS18₅ and L₁-TS18₆.

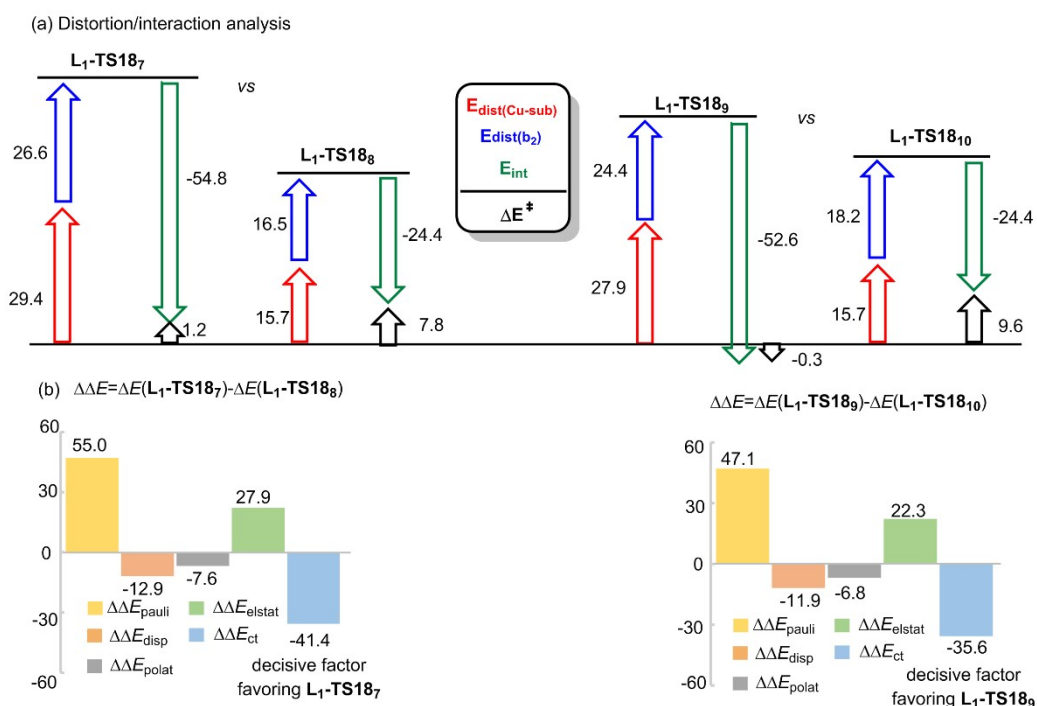


Fig. S5. DI and comparison of each energy term analysis for L₁-TS18₇, L₁-TS18₈, L₁-TS18₉ and L₁-TS18₁₀.

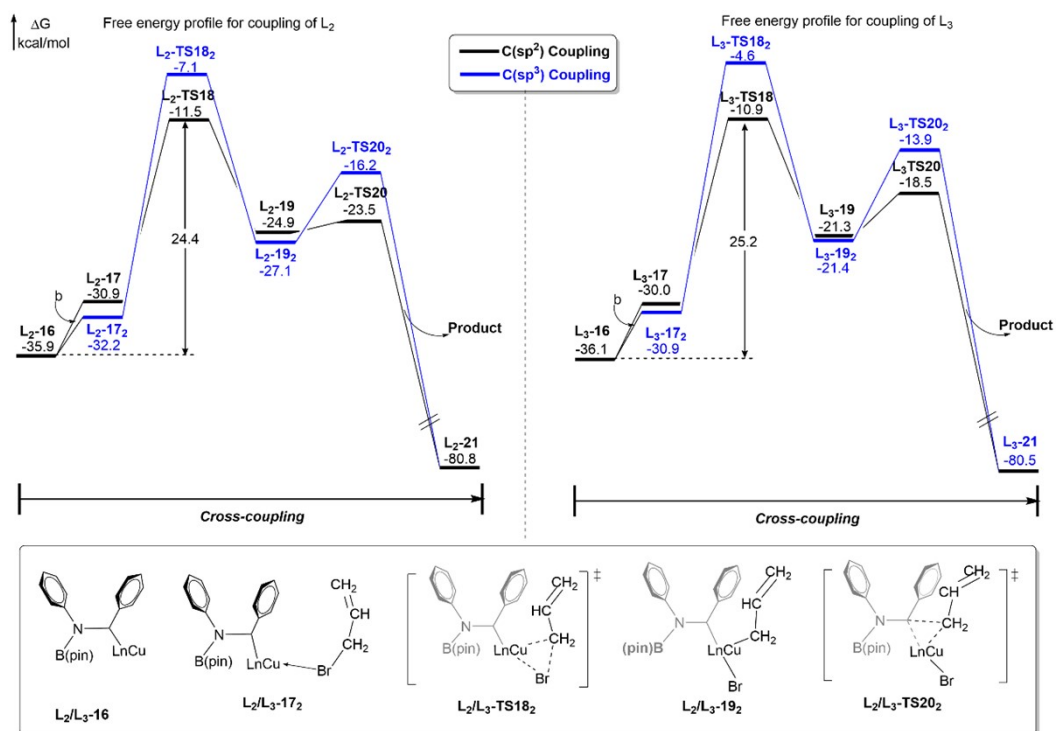


Fig. S6. Free energy profile and optimized structures of cross-coupling for L₂ and L₃ ligand.

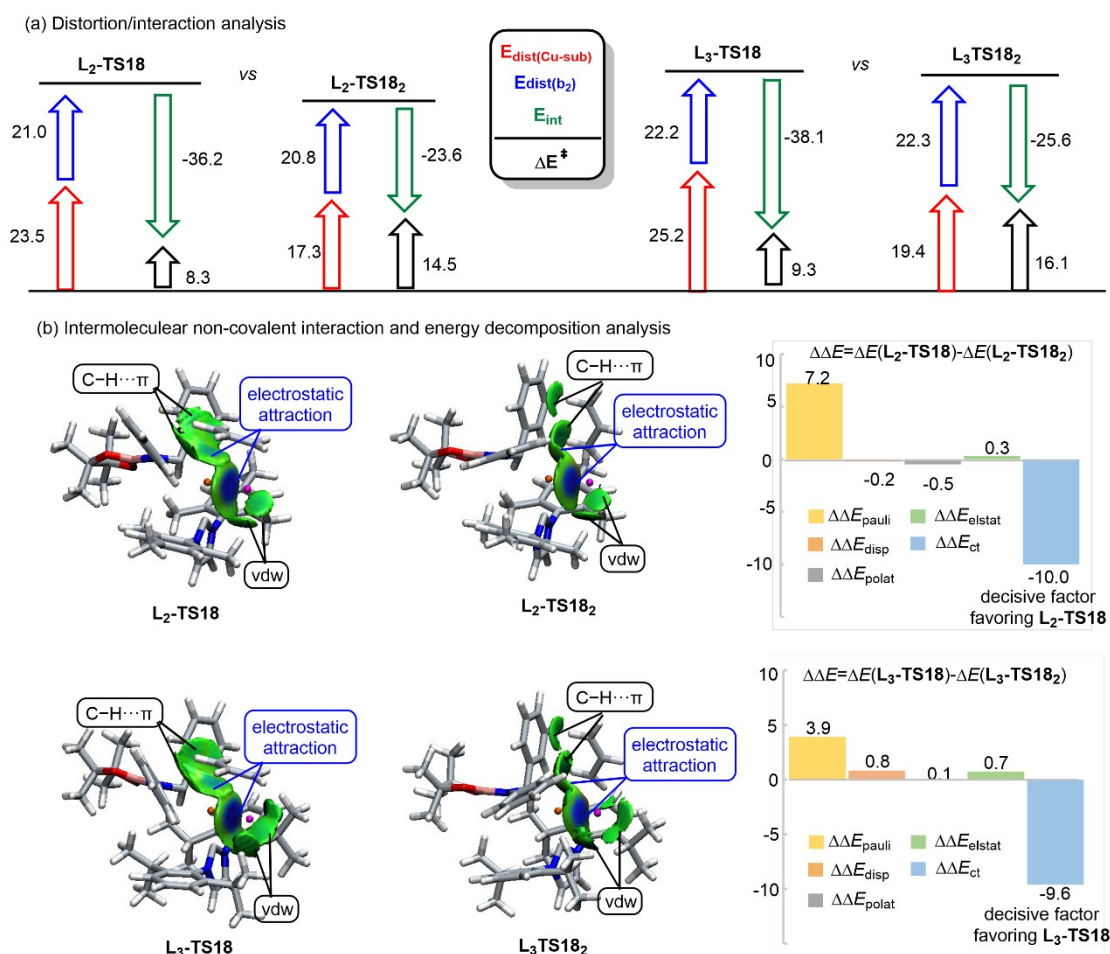


Fig. S7. (a) DI analysis. (b) NCIs and comparison of each energy term analysis for $L_2\text{-TS18}$, $L_2\text{-TS18}_2$, $L_3\text{-TS18}$ and $L_3\text{-TS18}_2$

We further explore the effect of the ligands on oxidation addition step by a visual analysis of noncovalent interactions (NCIs)¹ and energy decomposition analysis (EDA) according to your advice. The calculated results indicate the difference of charge transfer ($\Delta\Delta E_{ct} = -10.0/-9.6$ kcal/mol) is the most significant factor that stabilize the $L_2\text{-TS18}$ and $L_3\text{-TS18}$, and further confirm the charge transfer effects as the origin of regioselectivity.

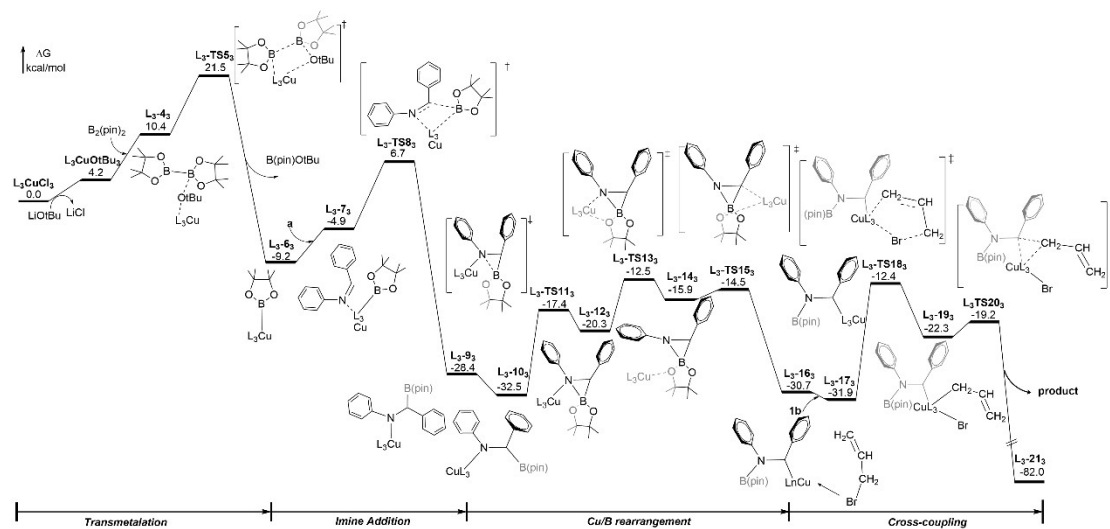


Fig. S8. Comparison of free energy profiles of solvent benzene effect on the catalytic reaction of ligand L_3 .

2. The tables of EDA calculation results

Table S1. EDA results of the computed transition states for **1b** (in kcal/mol)

	L₁-TS18	L₁-TS18₂	L₂-TS18	L₂-TS18₂	L₃-TS18	L₃-TS18₂
ΔE_{Pauli}	85.4	80.2	84.1	76.9	89.6	85.7
ΔE_{disp}	-17.1	-17.8	-16.8	-16.6	-20.4	-21.2
ΔE_{pol}	-15.0	-14.8	-14.8	-14.3	-15.4	-15.4
ΔE_{elstat}	-9.6	-10.4	-9.4	-9.7	-10.6	-11.3
ΔE_{ct}	-38.3	-28.1	-37.9	-27.9	-38.7	-29.1

Table S2. EDA results of the computed transition states for **2b** (in kcal/mol)

	L₁-TS18₃	L₁-TS18₄	L₁-TS18₅	L₁-TS18₆
ΔE_{Pauli}	137.8	79.6	88.9	76.7
ΔE_{disp}	-26.2	-18.2	-20.2	-17.2
ΔE_{pol}	-23.8	-15.4	-16.8	-14.6
ΔE_{elstat}	15.7	-12.4	-11.0	-11.7
ΔE_{ct}	-73.2	-26.4	-39.4	-25.7

Table S3. EDA results of the computed transition states for **3b** (in kcal/mol)

	L₁-TS18₇	L₁-TS18₈	L₁-TS18₉	L₁-TS18₁₀
ΔE_{Pauli}	128.9	74.0	121.6	74.5
ΔE_{disp}	-31.4	-18.5	-29.6	-17.8
ΔE_{pol}	-23.0	-15.3	-21.6	-14.8
ΔE_{elstat}	15.9	-12.0	11.4	-10.9
ΔE_{ct}	-66.0	-26.4	-61.2	-25.7

3 Cartesian coordinates of all optimized structures involved in this study

1a

C	-0.40144000	-0.40506700	-0.17067600
N	0.45621800	0.50277200	0.11412300
C	1.83173500	0.21421000	0.06745800
C	2.69492200	1.22832900	-0.37957000
C	2.38097500	-1.00868200	0.49263800
C	4.06753500	1.00781900	-0.44692400
H	2.26236000	2.17685800	-0.68114700
C	3.75840000	-1.21601700	0.43947500
H	1.72966900	-1.77781300	0.89668600
C	4.60636500	-0.21531000	-0.03831500
H	4.72125500	1.79625000	-0.80876900
H	4.17142500	-2.16085300	0.78157400
H	5.67885800	-0.38054000	-0.07631800
C	-1.84967900	-0.18169700	-0.08297500
C	-2.72859000	-1.22004100	-0.42687300
C	-2.37775600	1.05126200	0.33858000
C	-4.10826000	-1.03513700	-0.35195200
H	-2.32437700	-2.17503300	-0.75391500
C	-3.75385400	1.23420900	0.41081200
H	-1.68811200	1.84626100	0.60132400
C	-4.62307400	0.19243700	0.06683500
H	-4.77956700	-1.84554900	-0.61993700
H	-4.15562600	2.18929300	0.73655000
H	-5.69759500	0.33953500	0.12566400
H	-0.09548800	-1.40570600	-0.51167000

1b

C	2.76408100	-0.33578200	-0.28882300
H	2.86297300	0.03435600	-1.30617400
H	3.56583400	-0.96655200	0.08161800
C	1.71070700	-0.02886900	0.46980000
H	1.62903800	-0.42103900	1.48138900
C	0.60623400	0.85975000	0.02247700
H	0.75255500	1.24406800	-0.98587200
H	0.40948200	1.67722000	0.71600900
Br	-1.13445700	-0.12967600	-0.03450600

LiOtBu

O	1.27086700	0.00080300	-0.00007600
C	-0.11639100	0.00000100	-0.00005800
C	-0.63022300	-1.21893100	-0.79633400
H	-0.25695800	-2.14330000	-0.34204800
H	-1.72543800	-1.26727200	-0.82694300
H	-0.25848200	-1.17355500	-1.82583000
C	-0.63105400	-0.08070800	1.45341000
H	-0.25883200	0.77503400	2.02725200
H	-1.72633200	-0.08382500	1.50986000
H	-0.25900900	-0.99475500	1.92907000
C	-0.63197400	1.29867900	-0.65707100
H	-0.26060500	1.36788700	-1.68541100
H	-1.72726400	1.34843000	-0.68176100
H	-0.25986600	2.16791800	-0.10378700
Li	2.87456800	0.00092200	0.00017600

L₁CuCl

C	0.00114300	-0.43284900	-0.00008100
C	0.77658600	-2.66412100	0.00706700
C	-0.76531300	-2.66728300	0.00502700
N	-1.08921600	-1.22321300	0.00308900
N	1.09465100	-1.21876000	0.00075700
C	-3.10208100	-0.54635400	-1.22562000
C	-2.44925000	-0.75797800	0.00163700
C	-3.10575100	-0.55051100	1.22769500
C	-4.43775800	-0.12773600	1.20029300
C	-5.11860300	0.09415500	-0.00085600
C	-4.43419800	-0.12360500	-1.20068500
H	-4.95310500	0.03948000	2.14314500
H	-4.94675600	0.04676800	-2.14448500
C	3.10929900	-0.54466600	-1.22509600
C	4.43953700	-0.11368700	-1.19852000
C	5.11887200	0.11438400	0.00138900
C	4.43154300	-0.09319200	1.20233000
C	3.10284400	-0.52393200	1.22814200
C	2.45323800	-0.74941800	0.00073400
H	4.95306600	0.05680200	-2.14162000
H	4.93916700	0.09410700	2.14568900
Cu	-0.00448600	1.46377000	-0.00483600

H	-1.18701500	-3.15423400	-0.88022200	H	5.17815900	-2.62061700	0.86817800
H	1.20266900	-3.15274300	-0.87508300	C	-3.03539700	-2.39949500	0.02185400
C	-6.54522700	0.58942500	-0.00203500	C	-4.35830500	-2.19684600	0.42373700
H	-7.09067400	0.24363000	0.88108100	C	-5.02271000	-0.98843700	0.18807500
H	-6.57766700	1.68583100	0.00309000	C	-4.32923700	0.03414900	-0.46588300
H	-7.08631200	0.25197500	-0.89101400	C	-3.00301200	-0.11548300	-0.88739600
C	6.56236700	0.55858400	0.00648600	C	-2.36983100	-1.34605600	-0.63083100
H	7.23528400	-0.28551600	0.20283300	H	-4.87963800	-3.00106200	0.93748500
H	6.85061500	0.99206800	-0.95503900	H	-4.82942800	0.98139800	-0.65308800
H	6.74620900	1.30644200	0.78405100	Cu	0.04697400	-0.42720400	1.39345600
C	-2.39226200	-0.74668200	2.54403900	C	6.54310800	-0.27184900	0.62023200
H	-1.99649000	-1.76292600	2.65357700	H	7.00733600	0.49528500	-0.00630800
H	-1.54569100	-0.05832100	2.63989400	H	6.53957900	0.10661900	1.64986300
H	-3.07017400	-0.56351500	3.38111700	H	7.18204600	-1.15988800	0.60235800
C	-2.38466500	-0.73763000	-2.54054200	C	-6.46247400	-0.80134100	0.60462000
H	-1.97893200	-1.75009800	-2.64796400	H	-7.14493400	-1.01854900	-0.22667600
H	-3.06280600	-0.56174200	-3.37899900	H	-6.73009000	-1.46726800	1.42991700
H	-1.54450000	-0.04127500	-2.63573900	H	-6.65541500	0.22783900	0.92164800
C	2.38160700	-0.70323000	2.54266700	C	2.23195700	1.21345300	-1.54726500
H	3.05702900	-0.51858600	3.38144400	H	1.66779100	0.84226300	-2.40898400
H	1.54010100	-0.00728400	2.62879400	H	1.50490100	1.67444700	-0.86417900
H	1.97705000	-1.71527600	2.65820600	H	2.88887200	2.01163300	-1.90273100
C	2.39659900	-0.74491200	-2.54125600	C	2.69883200	-3.52910800	0.25874800
H	2.00035400	-1.76131800	-2.64725600	H	2.40665700	-4.04354500	-0.66427600
H	1.55040900	-0.05647900	-2.64018400	H	3.42833600	-4.16109400	0.77087200
H	3.07519200	-0.56522500	-3.37853700	H	1.80495900	-3.46812200	0.88895200
Cl	-0.01394800	3.58860500	-0.00913600	C	-2.28971400	1.02985400	-1.56493900
H	-1.18942000	-3.15267300	0.88989800	H	-3.01613300	1.74827900	-1.95425600
H	1.20041400	-3.14425400	0.89504900	H	-1.62708400	1.57955900	-0.88021700
L₁-1				H	-1.67432400	0.69339300	-2.40558800
C	0.07318200	-1.20194000	-0.33901600	C	-2.34074400	-3.70951600	0.31126200
C	-0.67042100	-2.06151100	-2.40025600	H	-1.99118800	-4.20209400	-0.60356500
C	0.87204400	-2.00393900	-2.40302900	H	-1.46446900	-3.56475700	0.95264800
N	1.17592700	-1.45680800	-1.06093500	H	-3.01752400	-4.40057100	0.81953000
N	-1.00956500	-1.53916400	-1.05669000	Cl	0.00374200	0.66942600	3.26397700
C	3.27700700	-2.15987600	-0.01181800	O	-0.19848300	3.22705000	0.30448600
C	2.51815400	-1.15593200	-0.64092900	C	-0.30318100	4.45363100	-0.33949900
C	3.04430100	0.12570800	-0.88625700	C	-0.07529300	4.28893900	-1.86150000
C	4.35905200	0.37954400	-0.47768100	H	-0.80880900	3.59189100	-2.28080900
C	5.14065900	-0.58906700	0.15809700	H	-0.16377400	5.24090400	-2.39975500
C	4.58320300	-1.85358000	0.37789900	H	0.92408200	3.88327000	-2.05172100
H	4.77914100	1.36526600	-0.66270700	C	-1.71098500	5.05260300	-0.10970800
				H	-1.88487600	5.19300700	0.96388000
				H	-1.84642900	6.02161800	-0.60708600

H	-2.47559400	4.36374500	-0.48542900
C	0.75694700	5.43442300	0.21510100
H	1.75873100	5.01154200	0.07981800
H	0.72747400	6.41603300	-0.27516000
H	0.59724000	5.58646500	1.28969900
Li	-0.12574700	2.43739700	1.78967600
H	-1.05678100	-3.07821800	-2.52269900
H	-1.12046000	-1.43287000	-3.17474500
H	1.33211500	-2.98938100	-2.52617200
H	1.27139500	-1.34451500	-3.17981200

L₁-TS2

C	-0.06903600	-0.93605400	-0.35980100
C	-0.84909800	-2.15413200	-2.22121000
C	0.66936600	-2.36022500	-2.08769900
N	1.01738300	-1.43789800	-0.98177200
N	-1.16657700	-1.37094500	-1.00657900
C	2.79778200	-2.02434800	0.61142200
C	2.37207500	-1.30663900	-0.52337400
C	3.26285300	-0.49506700	-1.25024600
C	4.58371200	-0.39408700	-0.80248100
C	5.03490700	-1.07392000	0.33214400
C	4.12833700	-1.88736900	1.01872500
H	5.27436300	0.24004500	-1.35347300
H	4.46441400	-2.43541500	1.89587900
C	-3.27396400	-1.96381400	0.08601000
C	-4.60074400	-1.65114000	0.38924300
C	-5.18809100	-0.45054800	-0.02622200
C	-4.41300500	0.44428900	-0.76738100
C	-3.07787400	0.17937700	-1.09873800
C	-2.52269300	-1.03625400	-0.66147300
H	-5.18735500	-2.36004200	0.96906500
H	-4.85450000	1.38008500	-1.10214900
Cu	-0.14517800	0.18288100	1.18130100
C	6.45589100	-0.91470000	0.81824200
H	7.14145500	-0.70553800	-0.00831200
H	6.53617600	-0.08154000	1.52730000
H	6.80652000	-1.81428500	1.33292100
C	-6.61551900	-0.12215900	0.34301900
H	-7.24659900	-1.01642300	0.34027800
H	-6.67086500	0.31035100	1.34965100
H	-7.05119400	0.60424500	-0.34895400
C	2.82653300	0.24999700	-2.48905900

H	2.82835100	-0.40102000	-3.37332700
H	1.81886900	0.65789200	-2.37991800
H	3.50569000	1.07965200	-2.69912800
C	1.86148300	-2.92017000	1.38816300
H	1.25156900	-3.54661500	0.72924100
H	2.42548900	-3.57945900	2.05300800
H	1.17000600	-2.33521500	2.00527500
C	-2.26943300	1.19970100	-1.85907400
H	-2.92990000	1.90197700	-2.37564400
H	-1.62565800	1.77768100	-1.17938400
H	-1.62001500	0.73728500	-2.60922600
C	-2.66504300	-3.25654800	0.57548000
H	-2.35678900	-3.90940400	-0.24999500
H	-1.77722400	-3.06945500	1.18839100
H	-3.38239200	-3.81381900	1.18287900
Cl	-0.54053500	0.94010600	3.22889300
O	-0.26134800	2.92400600	0.31494300
C	0.61694800	3.78131100	-0.34871400
C	0.42520400	3.67637500	-1.87901000
H	-0.60164800	3.94460000	-2.14961100
H	1.10830900	4.33520700	-2.42931200
H	0.60198000	2.64751300	-2.21044800
C	0.34441400	5.24472200	0.07699300
H	0.49777200	5.35559800	1.15870100
H	1.00105300	5.96455500	-0.42815500
H	-0.69439100	5.51044400	-0.14934800
C	2.07888100	3.42341400	0.00450500
H	2.28507900	2.38237700	-0.26490700
H	2.80630200	4.06603200	-0.50831300
H	2.23851600	3.52356300	1.08466600
Li	-0.77748300	2.76195900	1.93272200
H	1.21492500	-2.10240300	-2.99845300
H	0.93361800	-3.38809900	-1.81101400
H	-1.11945500	-1.58103800	-3.11579800
H	-1.40895000	-3.09276900	-2.23731700

LiCl

Cl	0.00000000	0.00000000	0.30819100
Li	0.00000000	0.00000000	-1.74641300

L₁-3

C	0.22456500	-0.89167000	0.00284900
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C	1.19706900	-3.04729400	-0.00376400	H	2.20409600	-1.92416900	-2.64188500
C	-0.33499700	-3.18803000	0.07886500	H	1.69539500	-0.23630300	-2.59610100
N	-0.78948500	-1.78297500	-0.00183900	H	3.22110500	-0.67891800	-3.37629700
N	1.38464400	-1.58134700	0.03097600	O	0.09271400	2.77721900	-0.04076400
C	-2.88751100	-1.40151400	-1.20765700	C	-0.96934100	3.69270400	-0.02589300
C	-2.18632100	-1.44985400	0.00995800	C	-1.86035900	3.51521700	-1.27433400
C	-2.83139900	-1.20844200	1.23654000	H	-1.25228800	3.61637900	-2.17957500
C	-4.19928900	-0.92053300	1.21863800	H	-2.30869400	2.51459700	-1.27520800
C	-4.92992700	-0.87122000	0.02688700	H	-2.67043700	4.25473000	-1.31660900
C	-4.25494000	-1.11084800	-1.17387400	C	-0.35228100	5.10673500	-0.03435900
H	-4.70461400	-0.72397100	2.16140600	H	-1.11720300	5.89279800	-0.02583700
H	-4.80308400	-1.06237900	-2.11182100	H	0.28988800	5.23600200	0.84281700
C	3.29869500	-0.68973100	-1.22359900	H	0.26834400	5.23437500	-0.92711400
C	4.58726300	-0.14765300	-1.21319700	C	-1.82563600	3.51576000	1.24679500
C	5.27903100	0.09272600	-0.02208800	H	-2.27770700	2.51679800	1.25834400
C	4.64558000	-0.21531100	1.18596500	H	-1.19167900	3.61329600	2.13455800
C	3.35838400	-0.75836400	1.22734300	H	-2.63190000	4.25766500	1.31321100
C	2.69611100	-0.99517900	0.00971400	H	-0.75234600	-3.77812900	-0.74248900
H	5.05758200	0.10127300	-2.16156700	H	1.60851000	-3.46186900	-0.93116400
H	5.16151100	-0.01907300	2.12294500				
Cu	0.06935600	0.97962400	-0.02145400	B₂(pin)₂			
H	-0.66677900	-3.64101800	1.02013500	B	-0.85316000	-0.00022700	0.00030400
H	1.71392900	-3.52383400	0.83482400	O	-1.61574000	-1.08126500	0.37271300
C	-6.41299800	-0.58560800	0.04071800	O	-1.61538900	1.08102400	-0.37224100
H	-6.99127800	-1.50327100	0.20716800	C	-3.00462500	0.78754100	-0.04605900
H	-6.67707000	0.11362200	0.83970900	C	-3.00479200	-0.78750800	0.04599000
H	-6.74630100	-0.15725500	-0.90882500	C	-3.29226000	-1.47938000	-1.29329100
C	6.68177500	0.65253800	-0.04022500	H	-3.07495700	-2.54618900	-1.19361200
H	7.42823100	-0.15111800	-0.07636700	H	-4.33916900	-1.36643500	-1.59047100
H	6.84646800	1.28932600	-0.91424300	H	-2.65953000	-1.08004400	-2.09055700
H	6.88626600	1.24637200	0.85543000	C	-3.89178100	-1.37819400	1.14029100
C	-2.06922300	-1.21724100	2.53996300	H	-4.94563400	-1.14045600	0.96069800
H	-1.51207100	-2.14903100	2.68744000	H	-3.78710500	-2.46673300	1.14684400
H	-1.34222400	-0.39823600	2.57281700	H	-3.61451100	-1.00858500	2.12893000
H	-2.74997600	-1.09803900	3.38640000	C	-3.89110900	1.37845700	-1.14066800
C	-2.18394700	-1.62102100	-2.52555900	H	-3.61355100	1.00886100	-2.12922700
H	-1.38243000	-0.88926600	-2.67083400	H	-4.94507700	1.14091400	-0.96148700
H	-1.72812500	-2.61599600	-2.59006900	H	-3.78621500	2.46697500	-1.14712300
H	-2.88503400	-1.52472000	-3.35817900	C	-3.29243400	1.47940300	1.29314800
C	2.68869100	-1.04129600	2.55078700	H	-4.33949600	1.36675200	1.58989200
H	1.79303800	-0.42347900	2.67667000	H	-2.66015000	1.07977000	2.09062200
H	2.37422900	-2.08740500	2.64074500	H	-3.07475300	2.54615400	1.19367400
H	3.36646700	-0.82609100	3.38054100	B	0.85317300	-0.00020600	0.00031600
C	2.56717400	-0.89658400	-2.52824600				

C	3.00462100	0.78754600	-0.04638800	C	-7.09133600	-2.19205400	0.76494200
O	1.61541700	1.08085400	-0.37275000	H	-7.71652400	-1.90989100	1.61761500
C	3.00480100	-0.78750900	0.04634800	H	-7.74599800	-2.37195200	-0.09275400
O	1.61574200	-1.08108500	0.37317200	H	-6.61165200	-3.14616700	1.01566600
C	3.29241300	1.48009400	1.29245400	C	4.32852400	4.42202100	-0.59824800
H	4.33947500	1.36766300	1.58926100	H	4.45381400	5.42099300	-0.16899900
H	3.07465200	2.54677600	1.19240500	H	4.96323100	3.73856800	-0.02141900
H	2.66011900	1.08088000	2.09012400	H	4.71414800	4.44097100	-1.62166600
C	3.89111400	1.37793900	-1.14129800	C	-4.22310800	0.27622400	-2.58230100
H	3.78611700	2.46644400	-1.14833000	H	-4.54981500	1.25413000	-2.95754000
H	4.94509700	1.14057500	-0.96198500	H	-3.13476400	0.23780700	-2.68549900
H	3.61359200	1.00777500	-2.12965500	H	-4.65291600	-0.48441800	-3.23850000
C	3.29228900	-1.47999300	-1.29259200	C	-3.91986500	1.39553700	2.37207300
H	4.33920400	-1.36724200	-1.58979200	H	-2.84703800	1.20928100	2.48508600
H	3.07490600	-2.54674100	-1.19244200	H	-4.04365200	2.47280700	2.21228200
H	2.65957900	-1.08099100	-2.09003800	H	-4.40832400	1.14175600	3.31604700
C	3.89176300	-1.37774400	1.14095100	C	0.49265800	1.88604800	-2.67876200
H	3.78684700	-2.46625700	1.14810000	H	1.12714400	1.97369300	-3.56479500
H	4.94565900	-1.14031900	0.96120400	H	0.49446100	0.83500900	-2.36591200
H	3.61460400	-1.00752600	2.12938700	H	-0.53131400	2.14273600	-2.96765400
L₁-4				C	-0.14602500	4.34939700	1.73815600
C	-1.76645400	1.66076400	-0.20102000	H	-0.89781200	5.09899400	1.46047800
C	-2.16955300	3.84241100	-1.01480200	H	-0.68344800	3.49152500	2.15318300
C	-3.51629300	3.16199700	-0.73594200	H	0.46585200	4.78412300	2.53245200
N	-3.10194200	1.78529700	-0.38843800	O	0.07279300	-1.36396700	1.26213200
N	-1.20202200	2.85523800	-0.48530600	C	0.15057600	-1.60081400	2.68601700
C	-4.50344400	0.58799500	1.23680700	C	0.73377000	-0.35580300	3.37164600
C	-4.08437200	0.78127700	-0.09306600	H	1.74827000	-0.17332400	3.01088000
C	-4.65314300	0.05121700	-1.15197200	H	0.11607700	0.52349300	3.15283500
C	-5.63490300	-0.89825100	-0.85051700	H	0.76661700	-0.48727200	4.45964000
C	-6.05892300	-1.13258100	0.46063700	C	1.01390800	-2.83444600	2.98932100
C	-5.48501500	-0.37516600	1.48730200	H	0.97047000	-3.05528600	4.06206600
H	-6.07448800	-1.47225500	-1.66283200	H	0.65353500	-3.69997700	2.43046500
H	-5.81146800	-0.53447200	2.51239400	H	2.05632900	-2.65936900	2.71719200
C	0.71581600	3.94547300	0.56498900	C	-1.28872900	-1.85037200	3.16018100
C	2.05403100	4.34061000	0.50756800	H	-1.32686200	-1.98444400	4.24714100
C	2.88378000	3.98195500	-0.56106500	H	-1.93258100	-1.00477900	2.89580800
C	2.34549800	3.19075100	-1.57894900	H	-1.69461300	-2.74861100	2.68507000
C	1.01073500	2.76683000	-1.56829400	B	1.03616000	-1.83615500	0.13753000
C	0.20134000	3.16456000	-0.48887800	O	0.29304400	-1.32519000	-1.07147300
H	2.45704000	4.94652900	1.31591900	O	1.01942600	-3.29268000	-0.01011900
H	2.97600600	2.89580300	-2.41408300	C	0.63868900	-3.63393800	-1.33823100
Cu	-0.83613900	0.08174000	0.27041600	C	-0.31557800	-2.44964600	-1.74543900
				C	-1.74437300	-2.65885200	-1.21620400

H	-2.31408700	-1.73121300	-1.33010900	C	0.46754600	-4.26799000	-1.12300700
H	-2.27160400	-3.44541000	-1.76752100	C	1.96001400	-3.98062500	-0.89465700
H	-1.72893500	-2.91993200	-0.15643900	N	1.94248900	-2.60504900	-0.34557000
C	-0.36171400	-2.14275500	-3.24406300	N	-0.17633200	-3.02132600	-0.64845900
H	-0.72647900	-3.00536600	-3.81344000	C	3.87462800	-2.23042500	1.11422600
H	-1.04363300	-1.30608700	-3.43390300	C	3.18611600	-1.93762900	-0.07749600
H	0.62453300	-1.86679500	-3.62150300	C	3.73004700	-1.07621500	-1.04728400
C	-0.03268700	-5.01236400	-1.31302600	C	4.98875700	-0.51819100	-0.79872800
H	-0.85256600	-5.04548600	-0.59295600	C	5.70600400	-0.79390100	0.36901800
H	-0.41881600	-5.28961900	-2.30101400	C	5.13084200	-1.65111000	1.31283800
H	0.70259100	-5.76656100	-1.01553500	H	5.41855200	0.14836800	-1.54259400
C	1.89953200	-3.70621900	-2.22341900	H	5.66856800	-1.86879200	2.23290200
H	1.67480000	-4.06050500	-3.23575800	C	-2.42742600	-3.49266200	0.19121200
H	2.39267400	-2.73381800	-2.28642100	C	-3.81396700	-3.42309400	0.01362200
H	2.60066600	-4.41054600	-1.76474800	C	-4.38543300	-2.76218700	-1.07721500
B	2.65678900	-1.22354400	0.25517000	C	-3.53183200	-2.15405200	-2.00326700
C	4.71683700	-0.56178200	1.09851500	C	-2.14111300	-2.19529100	-1.87298500
O	3.42005800	-1.12539600	1.41593200	C	-1.60032600	-2.87395100	-0.76330100
C	4.82478800	-0.82907500	-0.44978700	H	-4.46020500	-3.90005300	0.74705200
O	3.43443500	-0.89517200	-0.85075900	H	-3.95834100	-1.63283100	-2.85706700
C	5.77151300	-1.25926300	1.95846600	Cu	0.25852000	-0.26503300	0.23061700
H	6.77930300	-0.90830400	1.70979300	C	7.04938900	-0.15265800	0.62472000
H	5.58774500	-1.03740500	3.01408000	H	7.71059300	-0.81738900	1.18919500
H	5.73869000	-2.34292400	1.83411600	H	7.55075100	0.11343800	-0.31034900
C	4.65754600	0.92955800	1.45938100	H	6.93763100	0.76867300	1.20945500
H	4.38892700	1.02767500	2.51530900	C	-5.88457600	-2.68578400	-1.24587400
H	5.62371700	1.42237600	1.30630600	H	-6.39697900	-3.41972200	-0.61743100
H	3.89834300	1.44919300	0.86922500	H	-6.26116500	-1.69343900	-0.97016600
C	5.51286000	0.27167500	-1.25732600	H	-6.17901700	-2.86437600	-2.28526600
H	6.55910100	0.39025000	-0.95401000	C	2.98492000	-0.74005300	-2.31576900
H	5.49785200	0.00744100	-2.31910200	H	2.57290500	-1.63301500	-2.79852800
H	5.00395500	1.23052800	-1.14349000	H	2.14852100	-0.06063100	-2.11331500
C	5.45293700	-2.18975300	-0.78791800	H	3.65050200	-0.24953200	-3.03108800
H	5.31826700	-2.38573200	-1.85537700	C	3.28155400	-3.13683200	2.16723300
H	6.52485200	-2.21182300	-0.56608000	H	2.22538700	-2.91081800	2.34046400
H	4.96439600	-2.99715200	-0.23598500	H	3.34714800	-4.19546400	1.88491100
H	-4.05222600	3.61836400	0.10546000	H	3.81339400	-3.02337600	3.11523800
H	-4.18376000	3.16291400	-1.60171100	C	-1.26462500	-1.51320700	-2.89442200
H	-2.06330600	4.80564400	-0.50965900	H	-1.83721500	-1.28870000	-3.79836700
H	-1.99068600	3.99881700	-2.08578500	H	-0.86557400	-0.56830600	-2.50629500
				H	-0.40986600	-2.13434900	-3.18311700
L₁- TS5				C	-1.85385800	-4.22211000	1.38358800
				H	-1.49847000	-5.22583200	1.11698800
C	0.70354100	-2.08295400	-0.24202300	H	-1.00891400	-3.68105600	1.81841900

H	-2.61300200	-4.34758800	2.15991200	H	-2.67628600	2.77862900	3.72494100
O	1.41090200	1.68517400	0.44535100	C	-2.90736600	-0.59752200	2.97825000
C	2.08560500	2.39867000	1.50198800	H	-2.15537600	-0.87414500	3.72330500
C	2.91370700	1.35105800	2.25779000	H	-3.89719700	-0.80708700	3.39711400
H	2.25324200	0.60678900	2.71536000	H	-2.76161300	-1.22523000	2.09614300
H	3.59425500	0.83490700	1.57635500	C	-4.84608400	0.54736400	1.11744400
H	3.50446700	1.81962300	3.05325000	H	-5.55828500	0.66136800	1.94248000
C	1.12740600	3.09885000	2.47988500	H	-5.32464800	0.91893600	0.20623200
H	1.70909500	3.59147400	3.26799500	H	-4.63398500	-0.51390700	0.97883600
H	0.52768000	3.85094800	1.96481700	C	-3.89095700	2.85001600	1.38692400
H	0.45146100	2.37855800	2.94388300	H	-4.33749800	3.12336500	0.42756800
C	3.02136600	3.43676000	0.85917000	H	-4.59996600	3.10789200	2.18001300
H	3.62176000	3.94842400	1.62100600	H	-2.98248900	3.44412200	1.51339700
H	3.70187000	2.95032300	0.15297800	H	0.22159700	-4.43627200	-2.17687800
H	2.43844500	4.19035000	0.32358400	H	0.10995400	-5.12931500	-0.55118700
B	0.10999400	1.96287500	-0.19952900	H	2.54660300	-4.00705400	-1.81881600
O	0.12304500	1.56164500	-1.60987200	H	2.42065800	-4.67194000	-0.18248500
O	-0.33044900	3.34069700	-0.17130400				
C	-0.63069600	3.79049300	-1.50461800				
C	0.11733100	2.74320300	-2.42471100				
C	1.57090100	3.13838600	-2.74345700	tBuOBPin			
H	2.05800700	2.30063500	-3.25218400	O	-1.56557800	-0.83748400	-0.31031900
H	1.62516500	4.01144700	-3.40318300	C	-2.73239400	-0.03587100	0.00419800
H	2.13493500	3.34837700	-1.83406600	C	-3.92162700	-0.93655200	-0.34320200
C	-0.60514500	2.42166100	-3.73720700	H	-3.89668700	-1.20813000	-1.40246000
H	-0.69918400	3.31268400	-4.36838800	H	-3.88573400	-1.85757500	0.24572000
H	-0.03185600	1.67516200	-4.29697900	H	-4.86753200	-0.42675100	-0.13577300
H	-1.60159300	2.01529200	-3.55525700	C	-2.74003900	1.23048700	-0.86138500
C	-0.12332500	5.23115600	-1.63790500	H	-3.65305700	1.80773200	-0.68367400
H	0.94026900	5.30967800	-1.40545700	H	-1.87959600	1.86243700	-0.63082300
H	-0.28814500	5.61672900	-2.65061200	H	-2.70589900	0.96340000	-1.92228600
H	-0.66770600	5.87478300	-0.93984800	C	-2.73085800	0.30561800	1.50013200
C	-2.15469400	3.77981000	-1.70267200	H	-3.64379300	0.84677800	1.76896200
H	-2.43634800	4.17053600	-2.68628000	H	-2.69022200	-0.61146200	2.09623200
H	-2.56043800	2.77423900	-1.58218300	H	-1.87092200	0.92862500	1.75670700
H	-2.61062400	4.42037100	-0.94218100	B	-0.27494600	-0.45388900	-0.17735500
B	-1.34926200	1.11247900	0.78701200	O	0.75059600	-1.29857200	-0.54812400
C	-2.73993900	0.88976000	2.63669100	O	0.17777500	0.75702800	0.32142400
O	-1.37362300	1.06941900	2.17943800	C	1.60898700	0.81325100	0.06657600
C	-3.57153700	1.34845500	1.38083300	C	1.98300200	-0.71670400	-0.05441300
O	-2.64292900	1.11128300	0.28638600	C	2.27792000	-1.37300300	1.30140400
C	-2.93924500	1.73368100	3.89605000	H	2.31616300	-2.45719700	1.16675500
H	-3.97748100	1.68491800	4.24270000	H	3.23548200	-1.04181500	1.71434100
H	-2.29852300	1.35198700	4.69669900				

H	1.49133200	-1.15061300	2.02799700	C	-6.56471200	-0.69976700	0.02642400
C	3.10013000	-1.03519800	-1.04586600	H	-7.06270500	-0.96685800	0.96351700
H	4.03919700	-0.55919200	-0.74466500	H	-6.62073100	0.39143800	-0.07151500
H	3.26362900	-2.11612500	-1.07671300	H	-7.13874200	-1.13097400	-0.79905200
H	2.84808400	-0.70543100	-2.05501000	C	2.24673800	-1.60560100	-2.47929900
C	2.27577700	1.55961700	1.21959000	H	1.70132400	-2.54215100	-2.63720100
H	2.03812600	1.10689400	2.18367600	H	1.50663700	-0.79693100	-2.47431200
H	3.36387700	1.57311900	1.09789700	H	2.90672900	-1.45204500	-3.33677900
H	1.92569700	2.59578500	1.23783000	C	2.53069600	-2.31728800	2.54790200
C	1.79989000	1.58591400	-1.24517500	H	1.64413400	-1.70257700	2.73434900
H	2.85876800	1.73067800	-1.47905500	H	2.20906000	-3.36528900	2.57755100
H	1.32875100	1.06544000	-2.08366700	H	3.22875700	-2.16516900	3.37481500
H	1.33200700	2.56972000	-1.15021900	C	-2.52990400	-2.31799300	-2.54794000
L₁-6				H	-3.22823300	-2.16659100	-3.37476000
C	0.00034100	-1.65435300	-0.00006200	H	-1.64391200	-1.70252400	-2.73461600
C	-0.76619900	-3.89114100	0.05699200	H	-2.20733800	-3.36570600	-2.57750600
C	0.76764400	-3.89087700	-0.05703400	C	-2.24594000	-1.60643700	2.47927700
N	1.08815400	-2.44873500	0.05298200	H	-1.69998500	-2.54269400	2.63702800
N	-1.08720100	-2.44910100	-0.05308400	H	-1.50629600	-0.79734900	2.47435000
C	3.17613500	-1.95390800	1.23186100	H	-2.90596700	-1.45336300	3.33681500
C	2.44860100	-1.98747400	0.02898900	B	-0.00046200	2.31614800	-0.00015800
C	3.03671500	-1.61306400	-1.19273600	C	0.42601100	4.50264200	-0.65964700
C	4.37549900	-1.21014300	-1.18494500	O	0.32259400	3.12342800	-1.09388900
C	5.13013300	-1.16894200	-0.00861000	C	-0.42783000	4.50235200	0.65974800
C	4.51246000	-1.54595800	1.18782600	O	-0.32385400	3.12308700	1.09373800
H	4.83825100	-0.91735900	-2.12463000	C	-0.09515500	5.40512500	-1.77875000
H	5.08148700	-1.51481200	2.11412900	H	-0.08111500	6.45917900	-1.47829200
C	-3.03598300	-1.61417700	1.19275600	H	0.54304500	5.29763300	-2.66122900
C	-4.37493600	-1.21175700	1.18505800	H	-1.11315500	5.13851000	-2.06861800
C	-5.12965100	-1.17080800	0.00878900	C	1.91768500	4.78428900	-0.41861800
C	-4.51189900	-1.54755100	-1.18771600	H	2.47026700	4.56512400	-1.33691300
C	-3.17543900	-1.95498700	-1.23184400	H	2.10036400	5.82965400	-0.14746500
C	-2.44781300	-1.98833500	-0.02900100	H	2.31386600	4.14267700	0.37307500
H	-4.83774700	-0.91918200	2.12477500	C	0.09300200	5.40484400	1.77900000
H	-5.08099500	-1.51659700	-2.11398700	H	0.07875300	6.45892500	1.47864900
Cu	-0.00004400	0.31985900	-0.00016400	H	-0.54524900	5.29712300	2.66141500
H	1.25584300	-4.46257800	0.73676300	H	1.11103800	5.13842900	2.06892600
H	-1.11702100	-4.28169800	1.01990900	C	-1.91961000	4.78344000	0.41877900
C	6.56502200	-0.69737200	-0.02624000	H	-2.47209400	4.56391000	1.33704400
H	7.13802800	-1.12472600	0.80192800	H	-2.10270800	5.82878000	0.14779800
H	7.06448700	-0.96835900	-0.96144700	H	-2.31555400	4.14180700	-0.37301600
H	6.62044200	0.39427900	0.06692000	H	1.11860400	-4.28137300	-1.01992600
				H	-1.25421300	-4.46304600	-0.73677000

L₁-7

C	-0.40096800	-1.14063200	-1.27432100	H	0.81094400	-4.34961800	-1.13364200
C	-0.02026000	-2.36847300	-3.26751500	H	2.08176900	-4.74683500	0.03059300
C	-1.52117700	-2.05621800	-3.15286000	C	2.25487100	0.33202300	-3.09419800
N	-1.59339000	-1.28535200	-1.89074700	H	1.60039300	0.02273600	-3.91697900
N	0.52821300	-1.75062300	-2.03926000	H	1.67350000	1.00165700	-2.45096500
C	-3.25883000	0.51635300	-1.89700100	H	3.07661400	0.90899800	-3.52716400
C	-2.85161600	-0.75410000	-1.44681900	C	0.70817200	0.01681500	2.29777300
C	-3.68489500	-1.54629800	-0.63806300	N	0.37261900	-1.26769500	2.10230900
C	-4.92409000	-1.02414800	-0.25261600	C	-0.87768200	-1.72088700	2.58189000
C	-5.35042800	0.24339600	-0.65822300	C	-0.97890700	-3.09568700	2.87265700
C	-4.50787800	0.99228500	-1.48643800	C	-2.00851900	-0.90863700	2.81281700
H	-5.57021100	-1.62755900	0.38042600	C	-2.15142400	-3.63644100	3.39466100
H	-4.83151800	1.97299600	-1.82822100	H	-0.10437700	-3.71716000	2.70544500
C	2.79316100	-0.84958700	-2.32244800	C	-3.18232400	-1.45935100	3.32695600
C	4.16848500	-0.99343100	-2.12036900	H	-1.97624500	0.15068000	2.57804100
C	4.70427200	-2.06530300	-1.39796600	C	-3.26294900	-2.82110700	3.62738600
C	3.82444200	-3.01005400	-0.86348300	H	-2.19628100	-4.69750800	3.62632100
C	2.43890900	-2.90968200	-1.03549900	H	-4.04195300	-0.81513000	3.49289100
C	1.93720600	-1.82393000	-1.77290400	H	-4.17715500	-3.24042400	4.03768900
H	4.83847300	-0.24626400	-2.53988000	B	0.04836100	1.97221600	0.14164500
H	4.22199500	-3.84915700	-0.29704500	C	-0.34874300	4.23531100	0.49751000
Cu	0.02881200	-0.04228000	0.33349100	O	-0.32102100	2.91119500	1.09964600
H	-2.13755800	-2.95863400	-3.08425300	C	0.57237000	4.05062000	-0.76448000
H	0.19145200	-3.44283100	-3.27950000	O	0.44957300	2.62249600	-1.02714900
C	-6.67865700	0.79937800	-0.20123600	C	-1.81460900	4.53484600	0.15068800
H	-6.55980500	1.41270000	0.70074500	H	-2.41470700	4.45523100	1.06159400
H	-7.13196000	1.43617900	-0.96734500	H	-1.94106200	5.54317400	-0.25702100
H	-7.38628500	0.00049300	0.03938500	H	-2.20583400	3.81307800	-0.57117900
C	6.19612200	-2.18173000	-1.19049300	C	0.15616200	5.24736600	1.52558800
H	6.74269000	-2.05199000	-2.13088100	H	1.14832400	4.98412900	1.89635300
H	6.55829100	-1.41058300	-0.49993000	H	0.20132300	6.25463300	1.09664200
H	6.46842300	-3.15529800	-0.77340400	H	-0.52703000	5.27525000	2.37979800
C	-3.26680100	-2.92739200	-0.19649400	C	0.12809700	4.81456200	-2.01145400
H	-4.01970100	-3.36668700	0.46111600	H	0.15456600	5.89629400	-1.83897500
H	-3.13521400	-3.60238300	-1.05114000	H	0.80616600	4.59036800	-2.84045500
H	-2.32224100	-2.90503900	0.35274700	H	-0.88192500	4.53737500	-2.31855800
C	-2.38436700	1.35288600	-2.80038000	C	2.05739200	4.32435100	-0.48729200
H	-1.45987200	1.65812500	-2.30018300	H	2.40853000	3.76654100	0.38466700
H	-2.09660300	0.80984000	-3.70793200	H	2.64338800	3.99719800	-1.35108900
H	-2.91634300	2.25510000	-3.11541000	H	2.25154900	5.38979100	-0.32645300
C	1.51267400	-3.92307400	-0.40838400	C	2.13852600	0.41815800	2.29955000
H	0.92032200	-3.45356100	0.38395000	C	3.16234000	-0.48111500	1.96303600
				C	2.48778300	1.71353800	2.71962000
				C	4.49783600	-0.08686500	2.03099700

H	2.89609200	-1.48714900	1.66097300	H	6.35088500	-2.67461100	0.31582600
C	3.82390300	2.10239500	2.79137500	C	-3.06942000	-2.52381300	0.98130100
H	1.69844100	2.41317700	2.97921500	H	-3.83558500	-2.81246300	1.70435900
C	4.83676900	1.20390000	2.44354400	H	-2.72336500	-3.42919800	0.47130000
H	5.27864000	-0.79716600	1.77254600	H	-2.22497200	-2.12435900	1.55067200
H	4.07681000	3.10520100	3.12562700	C	-2.79680400	0.03376700	-3.41507700
H	5.87908600	1.50491400	2.50290400	H	-1.71310300	0.11901000	-3.29603000
H	0.05828400	0.68519500	2.86846000	H	-2.98096500	-0.75497600	-4.15639800
H	0.43939900	-1.92596000	-4.15758800	H	-3.17038800	0.96732000	-3.84359200
H	-1.89567100	-1.45715800	-3.98916400	C	1.42885100	-3.95154800	0.63772600
L₁- TS8				H	0.84974000	-3.26184300	1.26118500
C	-0.49291300	-1.54066900	-1.01924600	H	0.71607600	-4.58123400	0.09396500
C	-0.20038100	-3.33969200	-2.52806900	H	2.01075500	-4.59856600	1.29895000
C	-1.70304800	-3.03638800	-2.39188100	C	2.09769900	-0.69733900	-3.21370700
N	-1.71394200	-1.84859000	-1.51069500	H	1.32572700	-1.18095400	-3.82089000
N	0.40208800	-2.39069900	-1.56996800	H	1.64759500	0.18851600	-2.75114900
C	-3.48302000	-0.26573000	-2.10277600	H	2.89043800	-0.35984800	-3.88670900
C	-2.94454200	-1.18610400	-1.18445900	C	0.72572300	1.05235100	1.74092900
C	-3.61581100	-1.50656300	0.01022200	N	0.50104800	-0.26647800	2.23939800
C	-4.82066000	-0.85093300	0.28365100	C	-0.62616300	-0.48405800	3.03335000
C	-5.37088000	0.08900100	-0.59281500	C	-0.65794100	-1.68726400	3.78544800
C	-4.69187400	0.36028700	-1.78457600	C	-1.74109700	0.38270700	3.17164200
H	-5.33956600	-1.08518600	1.20994600	C	-1.72480200	-2.00015800	4.61835200
H	-5.11161400	1.07744000	-2.48651500	H	0.19766400	-2.35223400	3.70592800
C	2.65717800	-1.61741000	-2.15463800	C	-2.80512300	0.05927400	4.01581500
C	4.03773700	-1.68437800	-1.93787000	H	-1.78884100	1.30772900	2.60494100
C	4.59058600	-2.47978200	-0.92993300	C	-2.81499900	-1.12909600	4.74694400
C	3.72349800	-3.21258700	-0.11191100	H	-1.70302200	-2.92864500	5.18492700
C	2.33745600	-3.18392600	-0.29134200	H	-3.64196600	0.75033000	4.09473700
C	1.81765900	-2.38552200	-1.32788200	H	-3.64493000	-1.37068600	5.40454700
H	4.69534800	-1.09236500	-2.57007300	B	0.23688200	1.82033200	-0.03331200
H	4.13406700	-3.82027000	0.69102700	C	-0.62803000	3.76605900	-0.92353600
Cu	0.00961500	-0.26110500	0.28381800	O	-0.71870100	2.79770100	0.15854900
H	-2.25768100	-3.85704900	-1.92232900	C	0.82486800	3.51121300	-1.49587400
H	0.05163800	-4.36993900	-2.25863100	O	1.09949700	2.14252600	-1.06312100
C	-6.65576900	0.80559500	-0.25064400	C	-1.74950200	3.43035600	-1.91396300
H	-6.46184500	1.67752900	0.38626600	H	-2.70611200	3.44762200	-1.38493700
H	-7.16716700	1.16395900	-1.14892400	H	-1.79451600	4.15242100	-2.73551200
H	-7.34419300	0.15380400	0.29604200	H	-1.61787700	2.43074600	-2.33241900
C	6.08708000	-2.56454600	-0.74044100	C	-0.85725400	5.15742900	-0.33335400
H	6.50365900	-3.43063000	-1.27013700	H	-0.15450800	5.37478500	0.47259300
H	6.59066700	-1.67357000	-1.12656500	H	-0.75778200	5.93134100	-1.10204000
				H	-1.86961500	5.21644600	0.07665400
				C	0.93559400	3.56027700	-3.01947800

H	0.69010300	4.55898500	-3.39655100	H	4.96424300	-3.14482700	1.43921900
H	1.96278400	3.33146500	-3.31786500	Cu	-0.17330500	-0.52048800	0.46051300
H	0.27480100	2.83609900	-3.49940100	H	-1.00934600	-4.84676100	-1.53243100
C	1.90416500	4.40288300	-0.87136900	H	1.37570000	-4.71467000	-1.59344800
H	1.88397000	4.35627000	0.21909000	C	-6.55222600	-1.51714100	-0.05887500
H	2.88672100	4.04947900	-1.19530200	H	-6.58521700	-0.69829600	0.67012100
H	1.79215700	5.44600500	-1.18399200	H	-7.08637600	-1.18238800	-0.95301400
C	2.18183200	1.45498900	1.79587700	H	-7.09953900	-2.36168200	0.37076800
C	3.20479200	0.61178500	1.33937100	C	6.57418600	-1.31067600	0.22220800
C	2.53189700	2.68425200	2.36923800	H	7.12048000	-0.95202600	-0.65531500
C	4.53906100	0.99748300	1.44499500	H	6.59222500	-0.50980200	0.97115500
H	2.95017700	-0.35322200	0.91446300	H	7.11910000	-2.16311700	0.63914600
C	3.87042100	3.07027200	2.48064700	C	-2.35900200	-4.08277000	1.09325800
H	1.74899400	3.33828400	2.74705200	H	-3.01802300	-4.43687700	1.88972300
C	4.87961200	2.22884200	2.01416500	H	-2.00099400	-4.96325500	0.54668800
H	5.31875800	0.33160300	1.08476900	H	-1.48542000	-3.61629900	1.56077000
H	4.12084100	4.02381800	2.93810100	C	-2.38045800	-0.84687000	-2.82665600
H	5.92187600	2.52425500	2.09826000	H	-1.54662400	-0.24106500	-2.45589700
H	0.10686100	1.82602400	2.20387200	H	-1.96429500	-1.55914100	-3.54883200
H	0.17821400	-3.15462600	-3.54023900	H	-3.06602200	-0.18925600	-3.36692300
H	-2.17894000	-2.81377300	-3.35100400	C	2.40223000	-3.98504200	1.18883900
L₁-9				H	1.50205500	-3.55727800	1.64244000
C	0.00708900	-2.08154300	-0.60916700	H	2.08501400	-4.85613500	0.60294200
C	0.88938600	-3.80694200	-1.96292800	H	3.04564200	-4.34854300	1.99389600
C	-0.64693900	-3.90852400	-1.96610000	C	2.44341000	-0.55582200	-2.57193700
N	-1.04240500	-2.76066700	-1.12242000	H	1.75559500	-1.18642000	-3.14304900
N	1.13699000	-2.67258500	-1.04527800	H	1.85987100	0.27271700	-2.15316600
C	-3.09341900	-1.54236800	-1.69190700	H	3.17237600	-0.13200100	-3.26867900
C	-2.42338500	-2.46050500	-0.86489200	C	0.49387400	2.15507400	1.42463100
C	-3.08379100	-3.10936400	0.19432300	N	-0.49639800	1.05434000	1.43755100
C	-4.43024200	-2.80822700	0.41737200	C	-1.74374600	1.29129700	1.99525600
C	-5.12117300	-1.88218700	-0.37040600	C	-2.58981800	0.18554600	2.28471000
C	-4.43785700	-1.26900200	-1.42453400	C	-2.26405200	2.57305300	2.31874200
H	-4.94690200	-3.29739900	1.23987900	C	-3.84625900	0.34479200	2.85315300
H	-4.96050200	-0.54941800	-2.05021800	H	-2.22196500	-0.81377900	2.06272900
C	3.14339100	-1.31741500	-1.47260000	C	-3.52404100	2.71776100	2.90137100
C	4.47646900	-1.03007800	-1.16070700	H	-1.70385600	3.46651200	2.07250900
C	5.15018700	-1.67468800	-0.12104800	C	-4.33403600	1.61672100	3.17828800
C	4.45826500	-2.63773300	0.62098500	H	-4.44631000	-0.53889900	3.06087400
C	3.12780700	-2.96167800	0.34807800	H	-3.87936900	3.72078700	3.12961500
C	2.48128800	-2.29345600	-0.70908800	H	-5.31213800	1.74145900	3.63352100
H	4.99729900	-0.27490300	-1.74480100	B	0.32804700	2.88139600	0.02882100
				C	-0.71362000	4.20055000	-1.52467500
				O	-0.43930100	4.01668100	-0.11123000

C	0.49158700	3.43553200	-2.19223600	C	1.12389500	4.98839800	-0.40209500
O	0.81718700	2.43426100	-1.18631500	C	0.67551700	4.40414100	-1.59036500
C	-2.07569800	3.54710900	-1.79719100	H	0.74227800	5.17904900	1.70722100
H	-2.82212500	4.00200700	-1.14099500	H	1.23475900	4.56827900	-2.50844300
H	-2.39328100	3.68713100	-2.83524500	C	-4.31517700	-1.27795800	-1.44473000
H	-2.05018400	2.47673400	-1.57519700	C	-4.79581300	-2.58295200	-1.30026300
C	-0.77831300	5.69836000	-1.81677500	C	-5.11614700	-3.11834200	-0.04872200
H	0.12900400	6.21285500	-1.49525400	C	-4.95121500	-2.30962500	1.08021500
H	-0.92613300	5.88299300	-2.88628900	C	-4.47432500	-0.99895400	0.98750300
H	-1.62275000	6.13797000	-1.27842700	C	-4.16116600	-0.49406400	-0.28740600
C	0.16160800	2.72814100	-3.50515700	H	-4.91527700	-3.19839000	-2.18884200
H	-0.15194900	3.45034600	-4.26668700	H	-5.19155500	-2.71075900	2.06190800
H	1.04928300	2.20982300	-3.87988400	Cu	-0.92283800	0.14502500	0.01648000
H	-0.63318500	1.99110600	-3.37814400	H	-3.92512500	3.96701100	0.03398300
C	1.74152700	4.30926400	-2.36789500	H	-5.33767600	2.05026900	0.22864600
H	1.98889900	4.83676100	-1.44240800	C	2.34995400	5.87044800	-0.38322100
H	2.58846400	3.66883000	-2.62989000	H	2.07397300	6.93180900	-0.41921700
H	1.61091700	5.04940600	-3.16332700	H	2.93556600	5.71911700	0.52865700
C	1.89413500	1.68925900	1.81623700	H	2.99880400	5.67145100	-1.24071500
C	2.05908500	0.73862300	2.83599000	C	-5.59267500	-4.54513200	0.08485600
C	3.04353000	2.27302700	1.26751800	H	-6.10043400	-4.88534300	-0.82243400
C	3.32856400	0.39405400	3.29883300	H	-4.74820300	-5.22257700	0.26126800
H	1.17274100	0.28144800	3.26488400	H	-6.28257900	-4.66077000	0.92618100
C	4.31733200	1.93487800	1.73171800	C	-1.49214600	3.68966900	2.06595100
H	2.94526000	3.00182900	0.46777800	H	-1.02374000	4.22264700	2.89667900
C	4.46567300	0.99568400	2.75251600	H	-2.54026300	4.00659800	2.01511400
H	3.43086500	-0.33649600	4.09755500	H	-1.48777000	2.62120700	2.30632700
H	5.19296400	2.40857400	1.29466600	C	-0.89937300	2.95425600	-2.92913700
H	5.45462300	0.73900400	3.12364500	H	-0.81803700	1.86331000	-2.86690500
H	0.21465200	2.88338800	2.20200300	H	-1.93930700	3.18618900	-3.18474400
H	1.30178400	-3.58528100	-2.95368300	H	-0.27079500	3.29160000	-3.75692900
H	-1.07662100	-3.81379500	-2.96841800	C	-4.27088300	-0.16933800	2.23271000
L₁-10				H	-3.20861500	0.05011500	2.38737000
C	-2.41608300	1.25645400	-0.31099800	H	-4.79463500	0.79184900	2.18168600
C	-4.64472500	1.98180400	-0.61708400	H	-4.63584200	-0.70091100	3.11483100
C	-3.70291900	3.19869600	-0.71313300	C	-3.94286100	-0.74572200	-2.80802200
N	-2.37589400	2.59639900	-0.46156200	H	-4.49811800	0.16397900	-3.06394500
N	-3.70076600	0.86068600	-0.41712000	H	-2.87724200	-0.49676600	-2.85550900
C	-0.47041100	3.60319900	-1.63464900	H	-4.14963700	-1.48883500	-3.58198900
C	-1.17979500	3.39175300	-0.43947500	C	1.85577800	-0.15385200	0.58620100
C	-0.75364600	3.95718400	0.77650600	N	0.59091600	-0.87380100	0.37585500
C	0.39829400	4.74836000	0.76987900	C	0.59130300	-2.25163700	0.47107500
				C	1.67841300	-3.01609000	0.97211500
				C	-0.55147400	-2.98768400	0.05511100

C	1.61984300	-4.41040300	1.03169800
H	2.56085300	-2.51735800	1.35743900
C	-0.59959600	-4.37225600	0.12833800
H	-1.40135300	-2.43850100	-0.34556000
C	0.48892100	-5.11004000	0.61341500
H	2.47523300	-4.95200200	1.43066900
H	-1.49689000	-4.88715500	-0.20949700
H	0.45013400	-6.19399100	0.66580800
B	3.01737600	-0.69830700	-0.36571900
C	4.06296500	-1.15989600	-2.34999400
O	2.78419600	-0.96726800	-1.69311600
C	5.02903300	-1.47396200	-1.13833500
O	4.34071500	-0.84385900	-0.02135000
C	3.91392200	-2.28743600	-3.37062100
H	3.20136900	-1.98646400	-4.14420000
H	4.87062300	-2.50664800	-3.85709200
H	3.53766200	-3.19973700	-2.90540600
C	4.39117600	0.15735900	-3.06688500
H	4.48161600	0.98369000	-2.35607500
H	5.32095100	0.08837000	-3.63999300
H	3.57738300	0.39493900	-3.75787000
C	5.13145300	-2.96911100	-0.80769000
H	5.68515700	-3.51476000	-1.57813500
H	5.66189200	-3.08318600	0.14205200
H	4.14262800	-3.42037900	-0.69588800
C	6.42699800	-0.86551200	-1.24311800
H	6.39100800	0.22083900	-1.34421700
H	6.99440800	-1.10019300	-0.33794300
H	6.97051700	-1.27873100	-2.09954900
C	2.25176200	0.09470700	2.04749200
C	3.37954500	0.87508200	2.34991000
C	1.47895600	-0.38581400	3.11187300
C	3.72302300	1.16499200	3.66951700
H	3.99997100	1.25198600	1.54131500
C	1.82353200	-0.10055000	4.43625600
H	0.60583600	-0.98999800	2.89189600
C	2.94517800	0.67700300	4.72291700
H	4.60163400	1.77122400	3.87656500
H	1.21155000	-0.49190500	5.24541600
H	3.21356900	0.89865500	5.75247600
H	1.68888600	0.85642200	0.17329200
H	-3.72596500	3.67320300	-1.70031700
H	-5.23704700	1.83035200	-1.52477200

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C	1.91053300	1.51740400	-0.16169400
C	3.11442800	3.52513100	0.13058200
C	4.10982100	2.36499600	-0.04811700
N	3.21550500	1.18621500	-0.08938300
N	1.81175300	2.85964600	-0.09128500
C	3.91608000	-0.71827500	-1.47735200
C	3.73910500	-0.14700200	-0.20401700
C	4.09678100	-0.83942800	0.96653400
C	4.63869800	-2.12177200	0.83753900
C	4.82645600	-2.72230300	-0.41134000
C	4.46072600	-2.00366600	-1.55374000
H	4.91618500	-2.66585500	1.73734100
H	4.59666600	-2.45542700	-2.53339600
C	0.15384000	4.21888000	-1.27165500
C	-1.02357400	4.96997500	-1.24414400
C	-1.77771400	5.11741900	-0.07461000
C	-1.32375800	4.49126500	1.08881800
C	-0.15167600	3.72631300	1.11391500
C	0.58063000	3.60147300	-0.08030400
H	-1.36272600	5.44701000	-2.16072200
H	-1.89725100	4.59486700	2.00704800
Cu	0.43995600	0.33657300	-0.32933900
H	4.67870100	2.43838000	-0.98252400
H	3.14699100	3.95752700	1.13778900
C	5.38139400	-4.12249600	-0.52391100
H	6.01048600	-4.37514200	0.33460700
H	4.57277600	-4.86250300	-0.56608000
H	5.97909000	-4.24432000	-1.43231600
C	-3.06491000	5.90768800	-0.07824300
H	-3.26344500	6.35419800	0.90055200
H	-3.04039000	6.71052900	-0.82110900
H	-3.91921300	5.26402500	-0.32153400
C	3.88779200	-0.23142700	2.33315400
H	4.49245100	0.67163400	2.48003300
H	2.84199800	0.05320400	2.48722000
H	4.16499900	-0.94068600	3.11698500
C	3.50763500	0.01201200	-2.73439900
H	2.41774400	0.10395400	-2.79800700
H	3.92112500	1.02551500	-2.77717600
H	3.84880400	-0.52703600	-3.62138900
C	0.26305400	3.02915600	2.38744200
H	-0.15566600	3.54266900	3.25760800

H	-0.10768700	1.99654800	2.39697000	H	-3.50423400	-2.80204900	-0.34093400
H	1.34972100	2.99170700	2.50707900	C	-5.71562200	-0.10652600	-2.03018300
C	0.92608400	4.05813000	-2.55970500	H	-4.19324800	1.29135100	-1.43167400
H	1.92224100	4.51388800	-2.50567000	C	-6.12295600	-1.44087800	-2.03909000
H	1.06723000	3.00130700	-2.80830300	H	-5.62354700	-3.44814100	-1.43187800
H	0.39494000	4.53234500	-3.38857900	H	-6.33417200	0.65746400	-2.49457900
C	-2.42321100	-0.25460400	-0.13448300	H	-7.06011400	-1.72611900	-2.50954200
N	-1.04631800	-0.81334600	-0.52556100	H	-2.38170300	0.83719100	-0.14049900
C	-0.89668000	-1.79517300	-1.53146700	H	3.26737400	4.33364700	-0.58918200
C	0.00116800	-2.86304900	-1.32054600	H	4.82342200	2.28442900	0.77614300
C	-1.54726200	-1.73108300	-2.78304200				
C	0.24682100	-3.81041500	-2.31284200	L₁-12			
H	0.50309700	-2.93253300	-0.36112600	C	1.91888800	1.55688900	-0.11242600
C	-1.30651200	-2.68986000	-3.76616300	C	3.09461700	3.55000800	0.34326300
H	-2.23700500	-0.91917300	-2.98173100	C	4.10516900	2.40127600	0.15542600
C	-0.40807100	-3.73654900	-3.54452200	N	3.22271900	1.23185400	-0.05703000
H	0.94637700	-4.61966100	-2.11579700	N	1.80057400	2.88508400	0.07049300
H	-1.82337800	-2.61117800	-4.71974700	C	4.13425900	-0.54376700	-1.48661600
H	-0.22429300	-4.48001300	-4.31500300	C	3.75306100	-0.09504500	-0.20916600
B	-1.88807000	-0.94112100	1.15781600	C	3.90962700	-0.90199600	0.93122700
C	-1.56084300	-2.47697000	2.83926500	C	4.47064100	-2.17268500	0.76754500
O	-2.25829300	-2.21763900	1.60516800	C	4.86611500	-2.65056000	-0.48536100
C	-1.32330000	-1.02142400	3.39449900	C	4.68956300	-1.82138000	-1.59816300
O	-1.19340100	-0.24595900	2.18476500	H	4.59757500	-2.80523300	1.64291400
C	-2.44716400	-3.36878100	3.70985800	H	4.98563800	-2.17947300	-2.58134300
H	-2.56422900	-4.34589600	3.23135900	C	0.14109000	4.32507000	-1.01036500
H	-2.00065400	-3.52762800	4.69779900	C	-1.05301400	5.04714900	-0.93554900
H	-3.44222600	-2.93906000	3.83887600	C	-1.83238400	5.06607900	0.22581700
C	-0.24925200	-3.20702700	2.51210800	C	-1.38742000	4.33956900	1.33406900
H	0.41349500	-2.57255200	1.91821800	C	-0.20004800	3.59951900	1.31135700
H	0.28131100	-3.51557000	3.41904600	C	0.55716500	3.60449400	0.12475000
H	-0.47912600	-4.10056400	1.92517200	H	-1.38472600	5.60345400	-1.80905800
C	-2.53794900	-0.47359000	4.16202700	H	-1.98058500	4.34345400	2.24554600
H	-2.66800500	-0.96349900	5.13255300	Cu	0.46636900	0.35972000	-0.32763700
H	-2.39362000	0.59710800	4.33479600	H	4.74189700	2.24623300	1.03136700
H	-3.45545700	-0.60156400	3.58135800	H	3.09932800	3.95573900	1.36111800
C	-0.05891400	-0.84826900	4.23689100	C	5.44031000	-4.03881600	-0.64083500
H	0.83842500	-1.10515800	3.67055000	H	5.90364500	-4.38723700	0.28669700
H	0.02999700	0.19382900	4.56075200	H	4.65696700	-4.75927600	-0.90627200
H	-0.09458700	-1.47470600	5.13519700	H	6.19443300	-4.07389100	-1.43301000
C	-3.68302600	-0.70760200	-0.81431000	C	-3.13661100	5.82639700	0.27317100
C	-4.11221200	-2.04728800	-0.82527800	H	-3.31512100	6.25336000	1.26477800
C	-4.50750300	0.24968600	-1.42851700	H	-3.15312300	6.64071800	-0.45691500
C	-5.31411200	-2.40609600	-1.43406600				

H	-3.98318500	5.16638700	0.04765900	H	-2.82525800	-1.21975900	4.75830900
C	3.45625700	-0.43349300	2.29326600	H	-2.29769500	0.32166700	4.05648700
H	3.86760000	0.54873300	2.55094500	H	-3.33650100	-0.76276100	3.11864400
H	2.36451500	-0.34870500	2.33722100	C	-0.11731200	-1.34210600	4.26942100
H	3.76988000	-1.13855700	3.06719600	H	0.82782300	-1.68346400	3.84239500
C	3.92501200	0.31001400	-2.71465900	H	0.02456500	-0.31853800	4.63239900
H	2.86307200	0.53496700	-2.86165900	H	-0.35513500	-1.97295300	5.13330300
H	4.45326400	1.26831500	-2.64958600	C	-3.65331600	-0.56129700	-0.77691500
H	4.28493300	-0.20540800	-3.60825200	C	-4.10896200	-1.88579500	-0.92772000
C	0.21249300	2.79678400	2.52187400	C	-4.45568300	0.46888100	-1.30056600
H	-0.27784100	3.18297900	3.41974000	C	-5.30906100	-2.15705500	-1.58304500
H	-0.07614500	1.74351200	2.41075800	H	-3.52480500	-2.69622300	-0.50808100
H	1.29353600	2.82578300	2.68964000	C	-5.66457300	0.19830200	-1.94223700
C	0.94205400	4.30914500	-2.29110800	H	-4.12234600	1.49947700	-1.19600600
H	1.90295600	4.82769700	-2.18507500	C	-6.09543700	-1.12050600	-2.09239300
H	1.16078300	3.28588600	-2.61256800	H	-5.63785000	-3.18792800	-1.68819300
H	0.39255800	4.80559200	-3.09461900	H	-6.26490500	1.01714100	-2.33128500
C	-2.40802800	-0.20606200	-0.04544600	H	-7.03283000	-1.33846900	-2.59713500
N	-1.03074000	-0.82689600	-0.47026100	H	-2.29787600	0.87350200	0.05480000
C	-0.93752100	-1.71176900	-1.58656400	H	4.75568100	2.54926100	-0.71328100
C	-0.36038500	-2.98271500	-1.43555600	H	3.25926000	4.37832800	-0.35145400
C	-1.36498800	-1.31422500	-2.86569600				
C	-0.19666100	-3.82166200	-2.53868400	L₁- TS13			
H	-0.04952800	-3.30256100	-0.44836200	C	-1.74754000	1.63425200	0.04877000
C	-1.20551800	-2.16040400	-3.96148100	C	-3.55136000	2.84490900	0.96425700
H	-1.83011100	-0.34133300	-2.98773600	C	-2.33959500	3.78507600	0.80982400
C	-0.61661600	-3.41837400	-3.80751500	N	-1.29630900	2.87990700	0.27642700
H	0.25324000	-4.80182400	-2.40095600	N	-3.04060400	1.56945400	0.41201700
H	-1.54517400	-1.83453700	-4.94132300	C	0.31819100	3.83753400	-1.30380400
H	-0.49376000	-4.07629900	-4.66317500	C	0.03161000	3.35013700	-0.01549200
B	-1.61653600	-1.14774300	0.96596700	C	1.00206400	3.34251900	1.00251700
C	-1.53567400	-2.79245800	2.61143000	C	2.27708500	3.82993100	0.69676200
O	-2.07039800	-2.45910700	1.32503500	C	2.60269100	4.31109100	-0.57525300
C	-1.24480300	-1.37411900	3.23629100	C	1.60830200	4.31082200	-1.55896700
O	-0.84713800	-0.61716000	2.08337000	H	3.03713200	3.82535000	1.47413600
C	-2.57276700	-3.63051200	3.36384100	H	1.84145400	4.68709700	-2.55220600
H	-2.71308700	-4.58744700	2.85117100	C	-4.65044400	0.16664400	-0.79008900
H	-2.24825000	-3.84134300	4.38935400	C	-5.46819300	-0.96563800	-0.81849000
H	-3.54035500	-3.12650100	3.39752100	C	-5.52372700	-1.86278500	0.25457400
C	-0.25165500	-3.61792700	2.41507400	C	-4.73695000	-1.60024600	1.37901900
H	0.52036000	-3.02567600	1.91536600	C	-3.89641200	-0.48326700	1.45558200
H	0.15285000	-3.98517100	3.36470600	C	-3.86362300	0.39188900	0.35553500
H	-0.48178100	-4.48307500	1.78587100	H	-6.07845800	-1.15008400	-1.69959500
C	-2.50921700	-0.72849200	3.83214600				

H	-4.77202500	-2.28339000	2.22426500	C	-0.00772500	-2.06376100	-2.52992600
Cu	-0.72872200	0.22416500	-0.68843100	O	0.32923200	-1.12345100	-1.47262100
H	-2.01693600	4.22383500	1.75833500	C	2.39975800	-2.10214200	-3.48741300
H	-3.85268100	2.70984600	2.00817800	H	3.36410700	-2.60009900	-3.35630400
C	4.00035800	4.79173000	-0.88475700	H	2.15568100	-2.09580800	-4.55516800
H	4.46430500	5.26204200	-0.01269800	H	2.51025400	-1.07044000	-3.14342200
H	4.64297400	3.95409700	-1.18219700	C	1.19372500	-4.28355300	-3.18555400
H	4.00393500	5.51452700	-1.70579600	H	0.56230800	-4.88704900	-2.53050500
C	-6.39449800	-3.09491700	0.18701000	H	0.76794600	-4.29089200	-4.19530400
H	-7.29841800	-2.91530400	-0.40282900	H	2.17772900	-4.75916500	-3.23024700
H	-5.85863200	-3.92811400	-0.28406000	C	-0.41892800	-1.28544600	-3.77839000
H	-6.69782300	-3.42575000	1.18439200	H	-0.56684800	-1.96384200	-4.62550500
C	0.70926200	2.79456100	2.37868200	H	-1.36651800	-0.76204700	-3.60473800
H	-0.24075800	3.16006100	2.78148200	H	0.33582300	-0.54610400	-4.05298200
H	0.65979700	1.69958200	2.37183800	C	-1.16433900	-2.94401600	-2.03931300
H	1.49825100	3.07869700	3.07925400	H	-0.86313700	-3.52089900	-1.16165800
C	-0.72299400	3.83380200	-2.39849500	H	-2.01556300	-2.31183000	-1.76339100
H	-1.00436900	2.81163500	-2.67588800	H	-1.49835700	-3.63807400	-2.81712100
H	-1.64227800	4.34916000	-2.09845600	C	3.93319600	-0.90402200	0.32388000
H	-0.34173800	4.32977500	-3.29433800	C	4.43768800	-2.15801500	0.71341900
C	-3.03543900	-0.26972900	2.67729000	C	4.85941700	0.12626000	0.08331300
H	-2.96085700	0.78452400	2.95861700	C	5.80883000	-2.36802500	0.85033400
H	-3.43900500	-0.81788800	3.53218500	H	3.74015800	-2.96722500	0.90424700
H	-2.01543700	-0.63713300	2.51439600	C	6.23195300	-0.08488600	0.21424800
C	-4.60929100	1.11032600	-1.96893600	H	4.48932800	1.10771300	-0.20893100
H	-4.94455700	2.11912100	-1.70053200	C	6.71745100	-1.33575300	0.60088800
H	-3.59478800	1.20685900	-2.37005100	H	6.17171300	-3.34683000	1.15516800
H	-5.25738100	0.75214100	-2.77243900	H	6.92414100	0.73182100	0.02136600
C	2.47792200	-0.65737100	0.12326900	H	7.78564100	-1.50287800	0.70978000
N	1.49443700	-1.50170100	0.80271500	H	2.23592300	0.41552200	0.11242900
C	1.13232800	-1.64657900	2.11269900	H	-2.52417700	4.60288800	0.10524200
C	0.12598200	-2.57195800	2.48329400	H	-4.42678500	3.18222600	0.40129700
C	1.73646300	-0.88166600	3.13771000				
C	-0.25335500	-2.71360700	3.81521900	L1-14			
H	-0.32756400	-3.18546500	1.70971600	C	-1.57640500	1.66195100	-0.36317100
C	1.34207700	-1.03597200	4.46540900	C	-3.31054300	3.25309300	-0.25125200
H	2.53428900	-0.19453900	2.87349500	C	-1.98304100	3.97254000	-0.54877700
C	0.34336600	-1.94626800	4.82230100	N	-0.99655200	2.87146400	-0.45801700
H	-1.02179400	-3.43991800	4.07187000	N	-2.91092400	1.82843100	-0.29107000
H	1.83143100	-0.44163200	5.23406600	C	0.99559900	2.97854300	-1.89609300
H	0.04661700	-2.06613700	5.85995000	C	0.41253000	3.11231100	-0.62342800
B	1.47458700	-1.70686500	-0.63123300	C	1.16774400	3.51512400	0.49362700
C	1.34989800	-2.85786000	-2.65070300	C	2.53101600	3.76121100	0.31132100
O	1.79227400	-2.92955800	-1.30089300				

C	3.15217900	3.61548200	-0.93377600	C	-0.54035600	-1.19285400	4.21774400
C	2.36515700	3.23346700	-2.02448200	H	-0.25904800	-2.67248400	2.67395100
H	3.12614900	4.06336500	1.16957700	C	0.98795000	0.66411400	4.18931700
H	2.82715900	3.12692700	-3.00295700	H	2.46584000	0.65136100	2.61548500
C	-4.56285200	0.29078500	-1.23994100	C	-0.09522000	0.00846400	4.78225700
C	-5.50316500	-0.72596100	-1.05344700	H	-1.37250200	-1.72807300	4.67030600
C	-5.76722100	-1.26429700	0.21101600	H	1.36328100	1.58831100	4.62386700
C	-5.05825700	-0.76194200	1.30598600	H	-0.57106200	0.41416700	5.67019400
C	-4.10618300	0.25552700	1.17339600	B	1.45367600	-2.08940200	0.04376200
C	-3.86742600	0.77038100	-0.11376700	C	0.91182700	-3.65284900	-1.59435900
H	-6.03929700	-1.10929200	-1.91846900	O	1.68227900	-3.42070000	-0.42402200
H	-5.24738900	-1.17152000	2.29537800	C	-0.41548500	-2.86139500	-1.29629200
Cu	-0.70721600	-0.01608800	-0.40109400	O	0.11906000	-1.69930600	-0.59345900
H	-1.75336200	4.76106400	0.17171100	C	1.66672200	-3.09663300	-2.81757200
H	-3.71270600	3.50136900	0.73767400	H	2.66416800	-3.54353700	-2.83516700
C	4.63871400	3.83092400	-1.08154100	H	1.16467300	-3.33355800	-3.76189500
H	4.98830300	4.65753800	-0.45527800	H	1.79127600	-2.01291900	-2.74460700
H	5.18599300	2.93197800	-0.77303900	C	0.71502700	-5.16276200	-1.75388200
H	4.91289900	4.04698000	-2.11807100	H	0.31256900	-5.60888700	-0.84249400
C	-6.81185600	-2.34008700	0.39133700	H	0.04656000	-5.39702900	-2.59018200
H	-7.80158100	-1.90156200	0.57028100	H	1.68323300	-5.63094100	-1.95348100
H	-6.89256900	-2.97239400	-0.49766800	C	-1.18754000	-2.39681100	-2.52986200
H	-6.58093100	-2.98221800	1.24599200	H	-1.48668600	-3.25579400	-3.14018400
C	0.54834800	3.64766000	1.86400200	H	-2.10158100	-1.87004400	-2.23254800
H	-0.34801700	4.27719000	1.85952200	H	-0.58596600	-1.72816200	-3.14953400
H	0.26428600	2.66928100	2.26563500	C	-1.34607600	-3.60640900	-0.33134100
H	1.26030800	4.09485400	2.56212700	H	-0.78677800	-3.98200700	0.52841200
C	0.18762600	2.54927900	-3.09851700	H	-2.12099500	-2.92247800	0.02993400
H	-0.09862200	1.49347500	-3.02822800	H	-1.84051000	-4.45034900	-0.82297800
H	-0.73750500	3.12615600	-3.20402700	C	3.98879200	-1.00033400	0.22932400
H	0.76696700	2.67565300	-4.01633800	C	4.73052600	-1.92074900	0.98812400
C	-3.34830100	0.74586500	2.38380200	C	4.68815800	-0.18770200	-0.68253600
H	-3.24349100	1.83501500	2.39451400	C	6.11398000	-2.02179900	0.84089300
H	-3.86133200	0.45021900	3.30222500	H	4.20114200	-2.55209100	1.69481500
H	-2.33797800	0.32336100	2.42631600	C	6.07077200	-0.29127200	-0.83227100
C	-4.29391100	0.83850600	-2.62195900	H	4.13172900	0.52873000	-1.28422700
H	-4.58956200	1.89079400	-2.71159600	C	6.79599900	-1.21007800	-0.06859500
H	-3.23089000	0.78076000	-2.87697100	H	6.66450000	-2.74064300	1.44345600
H	-4.85361200	0.27782800	-3.37447200	H	6.58463400	0.34576100	-1.54918800
C	2.50978700	-0.89589500	0.33172000	H	7.87360200	-1.29199900	-0.18193000
N	1.80862600	-1.63789100	1.39974400	H	2.14584300	0.12990500	0.17478200
C	1.17414100	-1.07077600	2.48002700	H	-1.95687600	4.41241600	-1.55250800
C	0.07509100	-1.72612800	3.08863900	H	-4.08510800	3.46028200	-0.99428800
C	1.61164300	0.14530600	3.05505300				

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C	0.96378100	1.93643600	0.10283500	H	-2.32963700	2.57950200	3.31445300
C	0.92110400	4.23813100	0.63698000	H	-0.67988900	2.36450100	2.71402600
C	2.36594000	3.71995000	0.76183800	C	-0.84609400	3.13149200	-2.41783900
N	2.24012200	2.31030300	0.32649500	H	-0.03673400	3.85855400	-2.29243400
N	0.16942700	3.00853700	0.30618800	H	-0.37863300	2.15704300	-2.59995500
C	4.12807700	1.47270200	-0.98778400	H	-1.40818900	3.40463200	-3.31440900
C	3.39543900	1.46411000	0.21454800	C	-1.11101500	-1.40143300	0.95306900
C	3.79592800	0.67990900	1.31141800	N	-2.00956900	-2.19993000	0.10352100
C	4.94553500	-0.10578300	1.17407000	C	-3.32785400	-1.87162500	-0.15544700
C	5.69541500	-0.12525300	-0.00556700	C	-3.93783900	-2.26096100	-1.36834400
C	5.26821700	0.66882100	-1.07514200	C	-4.11648100	-1.18544900	0.79161700
H	5.25880800	-0.72088400	2.01425200	C	-5.27535700	-1.97066600	-1.61784700
H	5.83508900	0.66235300	-2.00321300	H	-3.34716600	-2.80051400	-2.10207200
C	-1.75899600	3.08278100	-1.21496800	C	-5.45689900	-0.90461100	0.53118000
C	-3.14536500	3.07649000	-1.38932000	H	-3.67158800	-0.90088700	1.74002100
C	-4.02882000	3.01529500	-0.30703900	C	-6.05154800	-1.28901200	-0.67388200
C	-3.49084900	2.99159500	0.98298400	H	-5.71922100	-2.28313700	-2.56027700
C	-2.11168800	2.99636800	1.21159400	H	-6.04676200	-0.39041500	1.28690700
C	-1.25253500	3.02300800	0.09753900	H	-7.09848800	-1.07520200	-0.86867900
H	-3.54489300	3.10857600	-2.40006700	B	-0.70453700	-2.12842300	-0.52894600
H	-4.16158500	2.95165800	1.83788800	C	1.10769200	-3.04291500	-1.69857700
Cu	0.30486300	0.23988000	-0.42302000	O	0.09719300	-3.29096500	-0.72443000
H	2.74413600	3.76502700	1.78931200	C	0.44743500	-1.93893700	-2.61023900
H	0.80349000	4.97752500	-0.16359400	O	-0.33904800	-1.18505200	-1.64208300
C	6.94919900	-0.96077800	-0.11190200	C	2.38173500	-2.55413100	-0.98623200
H	6.86442400	-1.88396800	0.46876300	H	2.66201200	-3.29680700	-0.23435100
H	7.16355700	-1.23057100	-1.15000600	H	3.22158400	-2.42515800	-1.67681500
H	7.82060100	-0.41455800	0.27050700	H	2.21922800	-1.60523500	-0.46447300
C	-5.51871400	2.93058300	-0.52844500	C	1.40836200	-4.35697300	-2.42646100
H	-6.07479500	3.38596500	0.29663900	H	0.49679000	-4.81085900	-2.81911000
H	-5.81581500	3.42679400	-1.45723000	H	2.11358700	-4.20660300	-3.25177100
H	-5.82863000	1.88081900	-0.59825100	H	1.85644300	-5.06554900	-1.72369400
C	3.00665600	0.64635200	2.59775500	C	1.42160700	-1.00196800	-3.31768900
H	2.67558700	1.64321500	2.90549700	H	2.05957200	-1.56468900	-4.00782500
H	2.11000500	0.02372200	2.50315500	H	0.87023000	-0.25848200	-3.90301500
H	3.60903000	0.22695900	3.40748300	H	2.06566500	-0.47549300	-2.60993900
C	3.69707800	2.31597400	-2.16485800	C	-0.54755500	-2.52227600	-3.62252500
H	2.65384600	2.12581100	-2.43494000	H	-1.22807600	-3.22657900	-3.13865200
H	3.78558200	3.38870700	-1.95384300	H	-1.14109900	-1.70897000	-4.04970000
H	4.31825100	2.10418200	-3.03862500	H	-0.03465100	-3.04124600	-4.43803500
C	-1.58058400	2.97757500	2.62556300	C	-0.71451400	-1.93980300	2.28459700
H	-1.32603500	3.98728900	2.97417800	C	-0.66308700	-3.32265900	2.53765900
				C	-0.35251200	-1.07045000	3.32878200
				C	-0.25701900	-3.80734200	3.77976300

H	-0.95028400	-4.00693300	1.74655700
C	0.05766600	-1.55595800	4.57170200
H	-0.41199000	0.00415900	3.16582600
C	0.11058800	-2.93112700	4.80528600
H	-0.22930600	-4.88094900	3.95024300
H	0.32218700	-0.85768000	5.36269900
H	0.42485300	-3.31422100	5.77225600
H	-1.42505700	-0.34703600	1.01596200
H	3.06867600	4.26006400	0.12098000
H	0.54913000	4.68215800	1.56433100

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Cu	0.69423900	0.29773700	0.28456900
N	-1.96197600	-0.68158400	-0.51316500
N	2.68494500	2.42397500	0.09952700
N	3.61821300	0.46150800	-0.08490000
O	-4.34346600	-0.90963600	-1.25710300
O	-3.92221400	-0.10468000	0.85659100
B	-3.37016300	-0.57026100	-0.32684000
C	2.44094600	1.09769400	0.07308700
C	4.10523600	2.75892700	-0.14975700
C	4.77997500	1.38029900	-0.06441500
C	3.80159400	-0.96371200	-0.10186400
C	4.01245400	-1.60105600	-1.33896100
C	4.22415600	-2.98277800	-1.34458700
H	4.38320900	-3.48423800	-2.29646200
C	4.22517700	-3.73537700	-0.16538800
C	4.00763000	-3.06983500	1.04394300
H	3.99467600	-3.63919500	1.97033000
C	3.79810400	-1.68773600	1.10405900
C	3.53647300	-1.02520700	2.43574700
C	3.96586600	-0.83282000	-2.63850300
C	1.67602300	3.44468200	0.16565400
C	0.95472200	3.78823500	-0.99174000
C	1.16810400	3.06673400	-2.30108500
C	-0.00292900	4.80351800	-0.89489400
H	-0.57098700	5.07109800	-1.78276100
C	-0.25199400	5.47573800	0.30497700
C	0.48149900	5.10435400	1.43690300
H	0.29076800	5.60511500	2.38332900
C	1.44712600	4.09532400	1.39204800
C	2.19542400	3.69823900	2.64243600
C	-1.10189800	-0.42339700	0.67516700

H	-1.57252300	0.40714000	1.21373500
C	-1.37259700	-1.04743700	-1.74451300
C	-0.16536400	-1.77335700	-1.78243000
H	0.29211100	-2.09560200	-0.85422500
C	0.42702500	-2.11841400	-2.99876200
H	1.34908200	-2.69391500	-2.98812500
C	-0.16075400	-1.75232900	-4.21006400
H	0.29932700	-2.02573200	-5.15542700
C	-1.35978800	-1.03562000	-4.18259300
H	-1.83565400	-0.73644100	-5.11334400
C	-1.95686400	-0.68346200	-2.97379000
H	-2.88652600	-0.12869100	-2.97338200
C	-5.61875600	-0.46464300	-0.73403800
C	-6.69109400	-1.46618000	-1.15964300
H	-6.78495700	-1.46299400	-2.24971400
H	-7.66530000	-1.20099400	-0.73470100
H	-6.43795300	-2.48084000	-0.84769800
C	-5.90712200	0.91099300	-1.35283500
H	-5.14777100	1.64118600	-1.05857600
H	-6.88928800	1.29296200	-1.05733500
H	-5.88803200	0.82083400	-2.44282100
C	-5.33761500	-0.39719400	0.81728100
C	-6.08194400	0.70698800	1.56695600
H	-5.79333700	0.69004800	2.62201100
H	-7.16569600	0.55831100	1.51000400
H	-5.84266000	1.69508900	1.16944900
C	-5.53929900	-1.74394900	1.52697900
H	-5.01223700	-2.54776200	1.00570400
H	-6.59803700	-2.01092300	1.60385300
H	-5.12436000	-1.67510700	2.53608700
C	-1.00845300	-1.57350200	1.63773300
C	-0.60689600	-1.33275000	2.97037000
H	-0.40381700	-0.30784900	3.27796500
C	-0.47741800	-2.36513900	3.89429100
H	-0.17415000	-2.13833200	4.91417300
C	-0.74776400	-3.68750200	3.52281500
H	-0.64865300	-4.49537600	4.24248200
C	-1.15882600	-3.94499700	2.21556900
H	-1.38700600	-4.96359000	1.90937700
C	-1.29132800	-2.90672500	1.28871600
H	-1.62911500	-3.13024700	0.28143800
H	0.76520400	2.04828800	-2.25996600
H	3.26955200	3.90607100	2.56541500
H	2.46059700	-0.89147400	2.59850400

H	4.67661400	0.00074800	-2.65853800	C	1.89054900	1.95687000	-4.02984000
H	4.47876700	3.46514600	0.59624400	H	2.49686400	1.23023700	-4.58221400
H	5.34474600	1.24478500	0.86607500	C	4.44366100	1.31969000	0.32399300
C	4.47808500	-5.22421000	-0.19445600	H	5.17887500	0.61680700	-0.08423400
H	5.53832900	-5.44892800	-0.02235900	C	1.46621400	-2.90269700	-1.85536400
H	3.90624500	-5.74048200	0.58228100	C	1.65854400	-3.78354800	-0.77632100
H	4.20514500	-5.65707400	-1.16112000	C	2.73068500	-3.54076200	0.25854600
C	-1.27022400	6.58911600	0.37520900	H	3.73263300	-3.49047200	-0.18335700
H	-1.77091400	6.61138400	1.34787000	C	0.80168700	-4.88063500	-0.66040000
H	-0.79632600	7.56836100	0.23127000	H	0.93417400	-5.56005300	0.17800800
H	-2.03591400	6.48013300	-0.39810800	C	-0.23123200	-5.11316800	-1.57379900
H	1.81796900	4.24767900	3.50836100	C	-0.38510100	-4.22372300	-2.64043500
H	2.08812500	2.62792700	2.84586300	H	-1.18116700	-4.39078900	-3.36221000
H	3.91834200	-1.64279800	3.25298300	C	0.44942300	-3.11375200	-2.80327000
H	4.00340000	-0.03854800	2.50855200	C	0.23007700	-2.15885200	-3.95260500
H	4.20474500	-1.48783000	-3.48014800	H	1.15076100	-1.96514200	-4.51412000
H	2.96755600	-0.41729200	-2.81145200	C	-1.15980600	0.98664700	-0.07311100
H	0.66515600	3.59205800	-3.11679400	H	-1.40556700	1.64039400	-0.91675800
H	2.22915800	2.98277600	-2.55863400	C	-2.19335800	-1.16138200	0.72169800
H	4.21347600	3.22059400	-1.13881200	C	-1.05007500	-1.45898400	1.49151500
H	5.45380600	1.17960100	-0.90103000	H	-0.28381300	-0.70519400	1.61960900
L₁-17				C	-0.89355800	-2.70260100	2.10620000
Cu	0.47221700	0.13164900	-0.78554200	H	-0.00053100	-2.88314300	2.69900100
N	-2.34670600	0.10361600	0.10814300	C	-1.87000800	-3.68987300	1.97892600
N	2.35285200	-1.78224100	-2.01300700	H	-1.75430900	-4.65277600	2.46839700
N	3.11326800	0.26202400	-2.03038300	C	-3.00412600	-3.40931900	1.21231200
O	-4.85524200	0.09825200	-0.04919200	H	-3.77982000	-4.16245800	1.09323700
O	-3.69786300	1.85051500	-0.98074700	C	-3.16574100	-2.17472100	0.58772000
B	-3.60383300	0.65022200	-0.28981800	H	-4.05517600	-1.98471800	0.00280400
C	2.07983100	-0.51557000	-1.64848100	C	-5.82873600	0.87173700	-0.79249600
C	3.63551500	-1.92200500	-2.73923100	C	-7.12171800	0.92833700	0.01964300
H	4.28666900	-2.64255600	-2.23576600	H	-7.54036000	-0.07793200	0.11454300
C	4.19562200	-0.48729600	-2.70785400	H	-7.86732100	1.55971000	-0.47556400
H	5.12854600	-0.41082200	-2.13983500	H	-6.94790300	1.31511100	1.02530900
C	3.18916600	1.68665200	-1.85931000	C	-6.07267900	0.13685700	-2.11891700
C	3.85928300	2.21490400	-0.74145400	H	-5.15713200	0.08235700	-2.71491200
C	3.95218700	3.60564100	-0.62424200	H	-6.84857300	0.62418700	-2.71737600
H	4.46737500	4.02282200	0.23784900	H	-6.39773100	-0.88506800	-1.90366300
C	3.39896000	4.46880900	-1.57512200	C	-5.08723300	2.25100300	-0.97539900
C	2.74203100	3.90811600	-2.67513700	C	-5.38577300	2.98270900	-2.28326400
H	2.30744400	4.56298000	-3.42682800	H	-4.79901700	3.90490500	-2.32733500
C	2.62592600	2.52450600	-2.83938600	H	-6.44528300	3.25256200	-2.34925900
				H	-5.12439100	2.37648600	-3.15253800
				C	-5.27739600	3.20212600	0.21514300

H	-5.06424800	2.69748700	1.16139600
H	-6.29315500	3.60783900	0.25557900
H	-4.57530500	4.03426700	0.11564800
C	-0.88940600	1.89271000	1.09892200
C	0.03837100	2.94887700	0.96350400
H	0.54490700	3.08417800	0.00985100
C	0.31708400	3.81626200	2.01481500
H	1.03444200	4.62076600	1.86890900
C	-0.31921800	3.66284500	3.25284200
H	-0.10179200	4.33979300	4.07442400
C	-1.24391500	2.63103400	3.40642200
H	-1.75768900	2.49859800	4.35591600
C	-1.52618200	1.76059300	2.34731600
H	-2.26210200	0.97473600	2.48448900
H	2.73787900	-4.34487600	0.99833800
H	2.56389000	-2.59920300	0.79200600
H	-0.50884600	-2.55938200	-4.65128800
H	-0.13709800	-1.19053500	-3.59383000
H	1.60748800	2.75190400	-4.72423900
H	0.97634700	1.44001400	-3.71753500
H	4.94728400	1.91307600	1.09089900
H	3.67099100	0.72430100	0.82108200
C	-1.18286000	-6.26848300	-1.38076000
H	-1.95795000	-6.00195800	-0.65214500
H	-1.68406100	-6.53861400	-2.31473000
H	-0.66765700	-7.15613200	-1.00004600
C	3.48344000	5.96730200	-1.40447200
H	2.62592700	6.34676400	-0.83514200
H	4.38805000	6.25872600	-0.86250500
H	3.48457600	6.48123400	-2.37036800
H	3.45460400	-2.28530800	-3.75673100
H	4.37569900	-0.07785500	-3.70713000
C	-0.31806500	-0.83895500	5.50749100
H	-0.73447900	-1.33501300	6.37918500
H	-0.97633900	-0.70519900	4.65363100
Br	2.96330300	-0.84987500	3.44954000
C	0.94957700	-0.41956500	5.48623400
H	1.59805200	-0.58127000	6.34547400
C	1.54853600	0.29406300	4.32983500
H	0.83249700	0.52216100	3.54366800
H	2.09996000	1.19043900	4.61010400

L₁- TS18

Cu	0.95520500	0.49559500	0.68604500
N	-1.53104500	-1.30576900	0.59672500
N	2.39812500	0.11226000	-2.02919700
N	1.34663900	2.01631800	-1.95863800
O	-3.31345700	-2.78300900	-0.32858400
O	-3.23565300	-0.59583300	-1.04313500
B	-2.66412200	-1.56267400	-0.22470400
C	1.59741300	0.88586100	-1.26312000
C	2.67409300	0.68582600	-3.36866700
H	3.74906400	0.70941100	-3.56537300
C	2.05505200	2.08435300	-3.25949300
H	2.80869500	2.87928200	-3.23628200
C	0.49921000	3.11112700	-1.57004200
C	1.04942500	4.20068900	-0.86521600
C	0.21013400	5.27286600	-0.54549800
H	0.62564100	6.11257600	0.00662100
C	-1.13517600	5.30298300	-0.92670900
C	-1.63542200	4.22713000	-1.66351900
H	-2.67400000	4.23986000	-1.98678500
C	-0.84252600	3.12389900	-1.99927300
C	-1.45613400	1.99506600	-2.79545200
H	-0.70921100	1.40907600	-3.33509800
C	2.50697300	4.23999700	-0.47521500
H	3.16071600	4.18848100	-1.35415200
C	2.79312000	-1.24356200	-1.76114900
C	4.10986600	-1.51357800	-1.34695200
C	5.11549600	-0.41071900	-1.12289300
H	5.33540500	0.13495200	-2.04852300
C	4.47728700	-2.84988100	-1.14743700
H	5.49028800	-3.06736300	-0.81701800
C	3.58745200	-3.90517700	-1.36193200
C	2.29606200	-3.60168300	-1.80589200
H	1.59146700	-4.40915500	-1.99007000
C	1.87956100	-2.28514800	-2.01829300
C	0.47869500	-2.00192800	-2.50569900
H	0.47734200	-1.36143800	-3.39490600
C	-1.07245700	0.09869500	0.71930000
H	-1.18633800	0.55362800	-0.26643000
C	-0.93145300	-2.36451000	1.34692300
C	0.45326300	-2.58750100	1.30919600
H	1.08069600	-1.94267900	0.70282400
C	1.03107000	-3.63042900	2.03211400

H	2.10622900	-3.77911200	1.97963700	C	3.99831700	-5.33763600	-1.11461300
C	0.23716000	-4.48581700	2.80030500	H	3.50711800	-5.73842800	-0.21979800
H	0.68749800	-5.29944300	3.36183100	H	3.71634100	-5.98525800	-1.95178900
C	-1.14277000	-4.28346700	2.83160800	H	5.07838600	-5.42537100	-0.96779500
H	-1.77744400	-4.93973500	3.42115400	C	-2.02812600	6.45983100	-0.54484000
C	-1.72163100	-3.23290200	2.11762700	H	-2.64411400	6.20806400	0.32723600
H	-2.79589800	-3.08920400	2.14176100	H	-1.44534600	7.34960900	-0.29014000
C	-4.25527900	-2.68444900	-1.42482900	H	-2.71326300	6.72210700	-1.35739000
C	-5.48916800	-3.51545200	-1.07659600	H	2.20199600	0.07140500	-4.14446400
H	-5.21140600	-4.57098600	-1.00347800	H	1.35126000	2.30899300	-4.06630000
H	-6.25760200	-3.42055100	-1.85130600	C	0.42569500	0.02558700	3.53530300
H	-5.91857200	-3.21343400	-0.11978100	H	-0.32275800	-0.74054300	3.39640500
C	-3.56516700	-3.26303000	-2.66846500	H	0.09419500	1.05397300	3.45001300
H	-2.68536600	-2.67366500	-2.94189600	Br	3.12131800	1.14298100	1.65858600
H	-4.23982300	-3.29954400	-3.52946500	C	1.68341700	-0.27772900	4.00018900
H	-3.23469000	-4.28139500	-2.44575200	H	1.97912200	-1.32160500	4.07566000
C	-4.49825000	-1.12863100	-1.51726900	C	2.66037100	0.70843400	4.15698100
C	-4.75734100	-0.59550900	-2.92513000	H	2.37520500	1.74997600	4.24415300
H	-4.88828500	0.49001300	-2.88847100	H	3.66456800	0.45811700	4.48069500
H	-5.67046500	-1.03043900	-3.34549700				
H	-3.92604700	-0.81332300	-3.59833100	L1-19			
C	-5.58543300	-0.62766700	-0.55602100				
H	-5.41594900	-0.99664300	0.45914600	Cu	0.91414700	0.70410200	0.91482000
H	-6.58557000	-0.93436200	-0.87734500	N	-1.05432500	-1.64623800	0.58879100
H	-5.55164800	0.46456700	-0.52265800	N	2.25366200	0.81077700	-1.86886700
C	-1.87034900	0.91863800	1.68514200	N	0.70623400	2.34285900	-1.75723200
C	-1.76178800	2.32655400	1.65463800	O	-2.46664400	-3.46642900	-0.34738400
H	-1.10027300	2.79016600	0.92798400	O	-3.01521000	-1.29474500	-0.87771500
C	-2.47810100	3.13062400	2.53518600	B	-2.14854900	-2.13030900	-0.18878900
H	-2.36903900	4.21131300	2.48065500	C	1.22905100	1.27249600	-1.11554100
C	-3.33488800	2.56062200	3.48483400	C	2.46482800	1.57832800	-3.11863400
H	-3.89327700	3.18865400	4.17321500	H	3.49824000	1.92784600	-3.18364100
C	-3.45712400	1.17339700	3.52960200	C	1.45875300	2.72466300	-2.97567300
H	-4.11762800	0.70904900	4.25813600	H	1.94622700	3.69313200	-2.82467900
C	-2.73766400	0.36453200	2.64459400	C	-0.50051300	3.06585000	-1.45065500
H	-2.85348500	-0.71248500	2.69701200	C	-0.43564400	4.31995000	-0.80676300
H	6.05918600	-0.82307700	-0.75638500	C	-1.63556400	4.99332000	-0.55177500
H	4.75080300	0.31250900	-0.38830500	H	-1.59175800	5.95013200	-0.03670400
H	-0.03041400	-2.93358500	-2.76498700	C	-2.87635100	4.48852700	-0.95184000
H	-0.11904500	-1.49662100	-1.74095500	C	-2.89608500	3.28793900	-1.66424100
H	-2.16896900	2.39122400	-3.52557700	H	-3.84471400	2.89820400	-2.02689800
H	-2.00618600	1.30082000	-2.14976300	C	-1.72756300	2.56825300	-1.93726400
H	2.73623400	5.17161000	0.04864400	C	-1.82643600	1.30795000	-2.76546600
H	2.7775900	3.40601900	0.17872600	H	-0.87982700	1.05234000	-3.24512600

C	0.87364600	4.97894800	-0.45094400	H	-5.46392800	-0.91905200	-0.09769900
H	1.31639900	5.45641400	-1.33571800	C	-1.84756900	0.39263700	1.81674900
C	2.97812200	-0.42143900	-1.70865900	C	-2.13210000	1.77294400	1.78592600
C	4.31841200	-0.39896800	-1.27930200	H	-1.69802700	2.38945100	1.00510400
C	5.02941800	0.88608500	-0.93538200	C	-2.95710600	2.35873300	2.74102300
H	5.31297700	1.43494900	-1.84347800	H	-3.15824400	3.42558700	2.69146100
C	5.00973200	-1.61623700	-1.21221700	C	-3.52569700	1.58350200	3.75733700
H	6.04085000	-1.60697500	-0.86697700	H	-4.17038700	2.04111500	4.50234300
C	4.42513900	-2.82809800	-1.58441300	C	-3.25534600	0.21666200	3.80144700
C	3.10533300	-2.80799900	-2.04897300	H	-3.68950000	-0.39933800	4.58463400
H	2.63435600	-3.73771900	-2.35955700	C	-2.42493900	-0.37219800	2.84492900
C	2.36887000	-1.62393700	-2.12606600	H	-2.22903600	-1.43714400	2.89276700
C	0.95088500	-1.65237700	-2.64484300	H	5.95158000	0.67755700	-0.38656400
H	0.80139900	-0.93952300	-3.46339900	H	4.40496000	1.54065000	-0.32251100
C	-0.94977600	-0.19153500	0.77246400	H	0.70243700	-2.64828500	-3.02029000
H	-1.16280300	0.28642400	-0.18052400	H	0.23029900	-1.40102100	-1.86070900
C	-0.20749200	-2.60024400	1.24959200	H	-2.57945600	1.43651500	-3.54974400
C	1.17613900	-2.60296200	1.03842300	H	-2.13729600	0.44944700	-2.16139100
H	1.62190500	-1.84559700	0.40492500	H	0.71631900	5.76634100	0.29110100
C	1.98452400	-3.57596700	1.62731700	H	1.59676300	4.26941900	-0.04418800
H	3.05502300	-3.55620400	1.44360900	C	5.18757500	-4.12877000	-1.49006100
C	1.42450300	-4.56874500	2.43335500	H	4.79499600	-4.75905100	-0.68299500
H	2.05450000	-5.32687700	2.88949800	H	5.10536900	-4.70758800	-2.41638200
C	0.04517000	-4.57723600	2.64341400	H	6.24893100	-3.95748900	-1.29089200
H	-0.40787500	-5.34366200	3.26614200	C	-4.15715400	5.21807300	-0.62337000
C	-0.76349200	-3.60176500	2.05984400	H	-4.60139900	4.83027700	0.30179900
H	-1.83692700	-3.62753600	2.21087000	H	-3.98393500	6.28854600	-0.47935900
C	-3.49518400	-3.54859200	-1.36719700	H	-4.90270300	5.09636200	-1.41534300
C	-4.43577900	-4.69789900	-1.01039400	H	2.26648700	0.93936700	-3.98732400
H	-3.88957200	-5.64465000	-1.05182000	H	0.77897800	2.81203500	-3.82860600
H	-5.26907300	-4.75670300	-1.71871100	C	0.89728800	0.14448800	2.90348500
H	-4.84087100	-4.58725900	-0.00302600	H	0.12470100	-0.61025900	2.98801500
C	-2.78756600	-3.83805000	-2.69826200	H	0.57346100	1.10144800	3.31283300
H	-2.11765100	-3.01899300	-2.97522100	Br	2.61662200	2.38783000	1.41978100
H	-3.50042400	-3.99472600	-3.51359900	C	2.18707900	-0.33732800	3.40716000
H	-2.18632100	-4.74453100	-2.58715400	H	2.43797100	-1.36876200	3.16844000
C	-4.13913000	-2.11066200	-1.30647200	C	3.02935900	0.36442400	4.18448800
C	-4.65736500	-1.57477500	-2.63918700	H	2.83296800	1.39878000	4.44794200
H	-5.05462700	-0.56506500	-2.50021500	H	3.94059400	-0.08104600	4.57414100
H	-5.46702900	-2.20533300	-3.02141900				
H	-3.86832500	-1.52799100	-3.39188300	L_I- TS20			
C	-5.22303600	-1.97740800	-0.22795800	Cu	1.04077100	0.37253600	0.74889000
H	-4.87434900	-2.36118500	0.73466800	N	-1.54057300	-1.55048800	0.29244600
H	-6.13771300	-2.51011700	-0.50514800				

N	3.05956200	0.76386200	-1.52929500	H	-0.91282900	-6.03253500	1.12977500
N	1.29092600	2.00287800	-1.78773300	C	-1.24469600	-3.93810300	0.78717800
O	-3.52072600	-2.74052900	-0.61429400	H	-2.19952700	-3.92585300	1.30043400
O	-3.64274200	-0.45019100	-0.42808500	C	-4.74551600	-2.34938500	-1.28778500
B	-2.87346600	-1.57968000	-0.23370600	C	-5.82631100	-3.37588000	-0.95428100
C	1.83025400	1.02519500	-1.02323600	H	-5.54987900	-4.34903100	-1.37041000
C	3.44880100	1.66582800	-2.63881100	H	-6.78911500	-3.08374300	-1.38667100
H	4.24374100	2.34403000	-2.30843500	H	-5.94961800	-3.49307100	0.12371600
C	2.13791600	2.39667400	-2.93639000	C	-4.45215700	-2.36330700	-2.79427600
H	2.25252800	3.48212500	-2.98048700	H	-3.68415600	-1.62932900	-3.05407600
C	-0.03846500	2.54167400	-1.70528000	H	-5.34818100	-2.15379500	-3.38649400
C	-0.22796800	3.83030500	-1.16653800	H	-4.07966600	-3.35328600	-3.07127200
C	-1.52623400	4.35081000	-1.15367100	C	-4.99452300	-0.90148000	-0.71111900
H	-1.68380700	5.34015500	-0.73059900	C	-5.64619100	0.07847800	-1.68401200
C	-2.61799200	3.64541800	-1.66853000	H	-5.72279400	1.06352900	-1.21513000
C	-2.38552900	2.38929100	-2.23339400	H	-6.65700100	-0.25060000	-1.94754400
H	-3.21624900	1.83378600	-2.65866600	H	-5.06704400	0.18390200	-2.60302300
C	-1.10805700	1.82133400	-2.26965300	C	-5.75809400	-0.90039500	0.62041800
C	-0.90798100	0.46307900	-2.90232800	H	-5.30917900	-1.59215300	1.33792500
H	0.00599900	0.41582900	-3.50204300	H	-6.80941100	-1.17191500	0.48393800
C	0.91632100	4.64209100	-0.61325700	H	-5.71155200	0.10168700	1.05440900
H	1.68360100	4.84285300	-1.37077000	C	-1.88171700	0.21980600	2.00731500
C	4.01810300	-0.19857400	-1.06296800	C	-2.00066900	1.60541900	2.21614500
C	4.94095500	0.15780400	-0.06211000	H	-1.48436000	2.29097800	1.55337500
C	4.92773700	1.52249700	0.58108900	C	-2.75677500	2.10328600	3.27450000
H	5.10743000	2.31413000	-0.15644600	H	-2.83213500	3.17734300	3.41838100
C	5.89836300	-0.79177100	0.31584200	C	-3.40921800	1.23148300	4.14977300
H	6.61505900	-0.52625300	1.08972300	H	-3.99855000	1.62206400	4.97466000
C	5.96678100	-2.05792000	-0.27234000	C	-3.29652900	-0.14707500	3.95659800
C	5.05909300	-2.36248900	-1.29181600	H	-3.79806900	-0.83504500	4.63209000
H	5.11665400	-3.33034700	-1.78529700	C	-2.53963800	-0.64750000	2.89815200
C	4.08916400	-1.44679300	-1.71173500	H	-2.46729200	-1.72072100	2.75080600
C	3.18514200	-1.78560900	-2.87484300	H	5.71607000	1.59647000	1.33483000
H	3.47270100	-1.23019200	-3.77665400	H	3.97062400	1.74592600	1.06590500
C	-1.06584800	-0.28394900	0.86809000	H	3.24931900	-2.84876400	-3.12015700
H	-0.99454700	0.49240100	0.09943800	H	2.13872600	-1.54479700	-2.67348500
C	-0.76023300	-2.75100200	0.21629100	H	-1.74986200	0.21979900	-3.55602800
C	0.46354900	-2.78238300	-0.46272600	H	-0.83934300	-0.32784100	-2.14790700
H	0.84537600	-1.86623200	-0.89932900	H	0.55545600	5.60852100	-0.25172900
C	1.19576900	-3.96804600	-0.55238800	H	1.39220400	4.11902800	0.22315100
H	2.15064500	-3.96731900	-1.06943100	C	6.98715900	-3.07356200	0.18497700
C	0.70721400	-5.14525700	0.01546600	H	6.57360400	-3.72453900	0.96539700
H	1.27501300	-6.06801700	-0.06039700	H	7.30738300	-3.71920000	-0.63861200
C	-0.51977500	-5.12433200	0.68142300	H	7.87462900	-2.58916300	0.60265900

C	-4.01322000	4.21956100	-1.60040000
H	-4.51453100	3.91688900	-0.67263400
H	-3.99877500	5.31347000	-1.62003200
H	-4.63190000	3.87210800	-2.43353500
H	3.82481900	1.09192000	-3.49012500
H	1.67070600	2.06734500	-3.87282700
C	0.61897000	-0.93846400	2.31814900
H	-0.09324700	-1.75200900	2.36414000
H	0.45829800	-0.18456300	3.08290200
Br	1.56347500	2.39046700	2.22590400
C	2.00189500	-1.41186800	2.15296300
H	2.13487200	-2.32899800	1.58548900
C	3.08020000	-0.81303100	2.69895000
H	2.99075300	0.12318200	3.24054700
H	4.06780600	-1.25079700	2.59513300

L₁-21

Cu	-0.00003500	1.16279300	-0.00030100
Br	-0.00067800	3.40453600	-0.00093700
C	0.00012600	-0.73945500	0.00067400
N	-1.09166400	-1.52719100	0.00099300
N	1.09201400	-1.52703900	0.00139200
C	-0.77081100	-2.97208800	0.00230900
C	0.77132100	-2.97200100	0.00197500
H	-1.19447200	-3.45650000	0.88797700
H	1.19543100	-3.45693800	0.88712300
C	2.45030300	-1.05660200	0.00054100
C	3.10289400	-0.84305200	-1.22652200
C	3.10441300	-0.84311200	1.22679300
C	4.43260200	-0.41295000	-1.20117300
C	4.43409800	-0.41302000	1.19981600
C	5.11474900	-0.18945500	-0.00109400
H	4.94493000	-0.24101400	-2.14481800
H	4.94760000	-0.24111600	2.14282700
C	-2.44999700	-1.05688300	0.00050000
C	-3.10358400	-0.84554700	-1.22633900
C	-3.10315200	-0.84129100	1.22697200
C	-4.43337000	-0.41549700	-1.20065600
C	-4.43282100	-0.41134500	1.20033100
C	-5.11451200	-0.18994000	-0.00046800
H	-4.94647800	-0.24525400	-2.14417400
H	-4.94556800	-0.23783600	2.14346900
C	2.39026500	-1.03884200	2.54283800

H	1.54746600	-0.34594400	2.64016900
H	1.98886600	-2.05303700	2.65014100
H	3.06917400	-0.86085200	3.38023500
C	2.38712600	-1.03869200	-2.54170200
H	1.98428600	-2.05241800	-2.64794600
H	1.54512100	-0.34474700	-2.63857200
H	3.06537500	-0.86206400	-3.37992100
C	6.53857900	0.31378800	-0.00198800
H	7.08337800	-0.02531500	-0.88808400
H	6.56484500	1.41037100	-0.00265500
H	7.08412900	-0.02427500	0.88403800
C	-2.38786400	-1.03458900	2.54275900
H	-1.98393000	-2.04772300	2.65040500
H	-1.54668100	-0.33958200	2.63921900
H	-3.06674200	-0.85769700	3.38041500
C	-2.38892700	-1.04351800	-2.54177800
H	-1.98840300	-2.05821700	-2.64764000
H	-3.06725000	-0.86597700	-3.37974300
H	-1.54546100	-0.35150400	-2.63955400
C	-6.53838800	0.31317000	-0.00067600
H	-7.07969900	-0.01497300	-0.89295300
H	-7.08733600	-0.03588600	0.87902800
H	-6.56478700	1.40967200	0.01239200
H	1.19506300	-3.45752500	-0.88304200
H	-1.19485800	-3.45826200	-0.88218800

1b-product

B	-1.08554100	-0.04314500	0.06457100
C	-2.84295500	1.40739500	0.17845600
O	-1.53717500	1.08431900	0.72615800
C	-3.32289100	0.00979800	-0.37628300
O	-2.06455700	-0.63991700	-0.70467200
C	-3.70134300	1.99583500	1.29601800
H	-3.27204000	2.94614000	1.62577200
H	-4.72042600	2.18925600	0.94530600
H	-3.74896900	1.33091400	2.16001000
C	-2.61972400	2.45165500	-0.92335000
H	-2.01206700	2.04589400	-1.73680800
H	-3.56565100	2.80951300	-1.34060200
H	-2.08521500	3.30508600	-0.49808100
C	-4.01152300	-0.85575200	0.68734700
H	-5.00100400	-0.46802000	0.94703100
H	-4.13304400	-1.86949800	0.29578400

H	-3.41187900	-0.91301900	1.60024000	N	1.09180000	-1.54520700	-1.25518000
C	-4.17641200	0.06927800	-1.64095200	N	-1.09480500	-1.54376100	-1.25224200
H	-3.64807800	0.55975700	-2.46005300	C	3.14096400	-2.33348900	-0.16529100
H	-4.42708400	-0.94564100	-1.96213300	C	2.44490800	-1.30687500	-0.82976200
H	-5.11227200	0.60646500	-1.45518500	C	3.04383800	-0.06384500	-1.10458500
N	0.26598700	-0.49346500	0.17215900	C	4.36623200	0.12844300	-0.68696700
C	1.19889400	0.36610200	0.94070900	C	5.08628900	-0.86323400	-0.01528700
C	1.96006000	1.38987700	0.08366500	C	4.45782300	-2.08893600	0.23170600
C	2.85980100	2.28149300	0.68914900	H	4.84217700	1.08393300	-0.89390000
C	1.72460900	1.53060600	-1.28959400	H	5.00440900	-2.87421800	0.74872800
C	3.51610400	3.26140700	-0.05421500	C	-3.13706200	-2.33008900	-0.14712600
H	3.04469600	2.22468100	1.75788700	C	-4.45056700	-2.08451600	0.25864900
C	2.38219700	2.50930200	-2.03820800	C	-5.08396200	-0.86208900	0.00509700
H	1.02437800	0.86249600	-1.77889500	C	-4.36765100	0.12860300	-0.67105700
C	3.28354600	3.37807300	-1.42559800	C	-3.04781500	-0.06482700	-1.09770500
H	4.20772700	3.93723100	0.44105700	C	-2.44688400	-1.30636000	-0.82308700
H	2.18480300	2.59030100	-3.10353400	H	-4.99011400	-2.86514600	0.79000400
H	3.79524500	4.13982400	-2.00645000	H	-4.84313400	1.08537100	-0.87263400
C	0.71379200	-1.70700400	-0.42983100	Cu	0.00334400	-0.45566900	1.19785600
C	-0.10910900	-2.84685800	-0.40332800	H	1.19016300	-1.45276400	-3.37516600
C	1.97349600	-1.81397700	-1.04377000	H	-1.20212900	-1.45767900	-3.37214900
C	0.30605300	-4.04082400	-0.98791000	C	6.49909800	-0.61083300	0.45522500
H	-1.08212700	-2.78588100	0.06819800	H	7.00370700	0.12978100	-0.17192200
C	2.38961800	-3.01964000	-1.61004300	H	6.50646900	-0.22734700	1.48296700
H	2.62699400	-0.95173900	-1.09241500	H	7.09493600	-1.52854200	0.44652400
C	1.56034800	-4.13977600	-1.59210000	C	-6.51494900	-0.63299500	0.43070200
H	-0.35343800	-4.90369600	-0.95664300	H	-7.21643100	-1.07020500	-0.29088900
H	3.36938600	-3.07341900	-2.07646600	H	-6.72130500	-1.09335700	1.40189400
H	1.88561300	-5.07440600	-2.03867800	H	-6.74362400	0.43363800	0.50527800
C	1.32823100	-1.15566100	4.16699600	C	2.30054600	1.04742600	-1.80623000
H	1.88028200	-0.35252000	4.65068000	H	1.74496700	0.68612800	-2.67793700
H	0.76100400	-1.81417000	4.81826800	H	1.57671100	1.55431700	-1.15236400
C	1.35156500	-1.32598400	2.84498600	H	3.00346700	1.80778500	-2.15670800
H	0.78729800	-2.14565800	2.40363300	C	2.48592000	-3.66140600	0.13481400
C	2.11787600	-0.45578500	1.88563200	H	2.14553400	-4.16910600	-0.77513000
H	2.73636900	0.24450100	2.45363100	H	3.18489900	-4.32955900	0.64363900
H	2.80431100	-1.07045900	1.29322100	H	1.60920000	-3.53789200	0.78003700
H	0.55146600	0.95346600	1.59870000	C	-2.30790100	1.04687700	-1.80216600
L₁-22				H	-3.01298400	1.80468700	-2.15384000
C	-0.00037200	-1.24342900	-0.53590900	H	-1.58468600	1.55688100	-1.14994000
C	-0.77545300	-2.09296600	-2.59000200	H	-1.75216700	0.68484900	-2.67343700
C	0.76812600	-2.09138500	-2.59317100	C	-2.47561500	-3.65278500	0.16183500
				H	-2.13192800	-4.16400500	-0.74484600
				H	-1.59997500	-3.52108700	0.80698500

H	-3.17167800	-4.32135800	0.67410300	C	6.50791600	-0.75326200	0.85496300
O	-0.00502100	3.19233400	-0.06893900	H	7.20258200	-0.58257800	0.02731900
C	-0.00484400	4.39561500	-0.76382000	H	6.54396100	0.13337300	1.49989300
C	-0.00546900	4.14323200	-2.29105200	H	6.87936700	-1.59768900	1.44346000
H	-0.89196600	3.56865200	-2.57993500	C	-6.55593600	-0.29561500	-0.02927500
H	-0.00522600	5.07866400	-2.86428000	H	-7.17554700	-1.19592800	0.03245800
H	0.88032000	3.56783400	-2.58047600	H	-6.65005300	0.22818200	0.92994500
C	-1.26402700	5.21647700	-0.39804000	H	-6.97736200	0.35534700	-0.80050100
H	-1.26993800	5.43037400	0.67770800	C	2.93946800	-0.06147400	-2.64685600
H	-1.31982300	6.17157900	-0.93587300	H	2.95650800	-0.81345400	-3.44678700
H	-2.16436000	4.63682900	-0.63012700	H	1.92876200	0.35142600	-2.60259400
C	1.25518800	5.21561100	-0.39897000	H	3.61858700	0.74071300	-2.94522800
H	2.15493300	4.63533700	-0.63177600	C	1.94426200	-2.79052200	1.54513200
H	1.31124200	6.17070100	-0.93679700	H	1.39405400	-3.53103900	0.95484700
H	1.26207200	5.42947900	0.67678200	H	2.50025200	-3.32390200	2.32024000
Li	-0.00241500	2.47094900	1.45127900	H	1.19972700	-2.15814800	2.04176100
Br	0.00815100	0.71364800	3.16170500	C	-2.18455900	0.82283400	-2.29476200
H	-1.19860200	-3.09641800	-2.70056900	H	-2.84576900	1.43715800	-2.91238900
H	1.19290000	-3.09352500	-2.70860500	H	-1.56798900	1.49880900	-1.68289100
L₁- TS23							
C	0.01837600	-1.06216400	-0.46636300	H	-1.50943000	0.28011300	-2.96444600
C	-0.69133400	-2.50515200	-2.19057200	C	-2.54906200	-3.27734500	0.70373500
C	0.82849200	-2.65569400	-2.00407700	H	-2.16598000	-4.00699100	-0.01944200
N	1.12949000	-1.61174700	-0.99654400	H	-1.70838700	-2.98098000	1.33993000
N	-1.05321500	-1.58586500	-1.08903700	H	-3.28107600	-3.79065600	1.33205200
C	2.88175800	-1.96821000	0.69216800	O	-0.32789000	2.85569500	-0.29906800
C	2.46959400	-1.39600500	-0.52721700	C	0.58041600	3.64602100	-1.00370600
C	3.36028900	-0.65042800	-1.32151500	C	0.43746300	3.40841400	-2.52456900
C	4.66678200	-0.46631400	-0.85763300	H	-0.58010700	3.65220900	-2.84867300
C	5.10380500	-1.00118600	0.35703900	H	1.13910400	4.01679900	-3.10863500
C	4.19794200	-1.75335400	1.11154100	H	0.62097400	2.35468800	-2.76111000
H	5.35717200	0.11817700	-1.46123600	C	0.30887900	5.14274000	-0.71592300
H	4.52285200	-2.18925300	2.05346400	H	0.43206500	5.34685900	0.35596800
C	-3.17307600	-2.07723700	0.03169600	H	0.98600600	5.81139800	-1.26252000
C	-4.51228700	-1.75717600	0.26319400	H	-0.72062300	5.39387700	-0.99538300
C	-5.11323700	-0.63549600	-0.32037800	C	2.02534600	3.30911800	-0.56974100
C	-4.33875000	0.17053100	-1.15755900	H	2.23070700	2.24814300	-0.74565000
C	-2.99117000	-0.10612000	-1.42338100	H	2.77670600	3.90230800	-1.10700800
C	-2.42317600	-1.24025300	-0.81739300	H	2.14674600	3.49533700	0.50370300
H	-5.09846400	-2.39650300	0.91935000	Li	-0.94521700	2.86610400	1.28783000
H	-4.79049700	1.04336200	-1.62318900	Br	-0.66668800	1.20536400	2.99482800
Cu	-0.13274000	0.21591600	0.94846200	H	-0.95605200	-2.05603500	-3.15488100
				H	-1.22953100	-3.45239600	-2.09912500
				H	1.38838100	-2.48158600	-2.92593600
				H	1.11153500	-3.64091400	-1.61430700

L₁-TS13₂

Cu	0.31111600	0.49890200	0.08192400	C	1.12856800	-2.40151000	3.72463100
N	-0.37595500	-1.31381600	0.48908200	H	0.82208500	-2.50716100	4.76204400
N	2.32174500	2.53350600	-0.30846200	C	2.44051700	-2.70429400	3.34646800
N	0.29346400	3.33698100	-0.45844900	H	3.15955400	-3.04891000	4.08386300
O	-2.37925800	-2.76494200	0.95128800	C	2.80569000	-2.57761700	2.00535000
O	-2.75817200	-0.58970100	0.27338600	H	3.81605200	-2.82468800	1.69086700
B	-1.81350300	-1.57771400	0.53021500	C	1.88422000	-2.15255000	1.04797200
C	1.01273500	2.21905400	-0.22605000	H	2.16019400	-2.07678300	0.00287900
C	2.55414400	3.94082800	-0.70089500	C	-3.78099400	-2.70381900	0.58147600
H	3.24386600	4.42923100	-0.00714200	C	-4.58230600	-3.50967300	1.60190100
C	1.13573600	4.53671400	-0.65712400	H	-4.28925500	-4.56186200	1.54479900
H	0.99827800	5.23700400	0.17491700	H	-5.65622500	-3.44573000	1.39605200
C	-1.13760400	3.44144300	-0.38296600	H	-4.40047700	-3.16553900	2.62177200
C	-1.75220300	3.65731700	0.86305300	C	-3.90602700	-3.33765800	-0.81082600
C	-3.14244200	3.80593000	0.89658100	H	-3.31078500	-2.79172500	-1.54730300
H	-3.62748800	3.97021200	1.85592800	H	-4.94625100	-3.37509900	-1.14946400
C	-3.92098900	3.74880200	-0.26321700	H	-3.51679700	-4.35794500	-0.76825700
C	-3.27646200	3.52002200	-1.48355600	C	-4.05940500	-1.14501200	0.58725600
H	-3.86720000	3.45569500	-2.39433700	C	-5.05842800	-0.66351200	-0.46411200
C	-1.89037600	3.36337200	-1.56852100	H	-5.14830600	0.42567100	-0.40844600
C	-1.23008700	3.08776600	-2.89841600	H	-6.04985200	-1.09684800	-0.29309200
H	-0.48817700	3.85190000	-3.15788400	H	-4.73306700	-0.92343000	-1.47277000
C	-0.94819200	3.70034000	2.14051100	C	-4.44937700	-0.60264000	1.96982100
H	-0.17104700	4.47282900	2.11471600	H	-3.74582500	-0.93693400	2.73755400
C	3.41563600	1.60601400	-0.20828900	H	-5.45679600	-0.91454400	2.26319500
C	4.13474000	1.53583800	0.99904600	H	-4.42079200	0.49045300	1.93858400
C	3.73353300	2.35691600	2.20153100	C	-0.00969500	-2.91221700	-1.55071300
H	3.87519900	3.43170400	2.03338900	C	0.06959500	-3.00956500	-2.97110200
C	5.22409800	0.66376500	1.07120900	H	-0.06959400	-2.10597600	-3.56277200
H	5.77825600	0.59444300	2.00420600	C	0.31975300	-4.21285000	-3.61324900
C	5.60980300	-0.12782300	-0.01552800	H	0.36766800	-4.23357200	-4.70041400
C	4.86730700	-0.03843600	-1.19649600	C	0.51594300	-5.39300400	-2.88206400
H	5.14391700	-0.65625600	-2.04748800	H	0.71876500	-6.33369900	-3.38542900
C	3.76951200	0.81975900	-1.32007000	C	0.43740300	-5.32460700	-1.48994000
C	2.97615200	0.84974900	-2.60438200	H	0.57158500	-6.22706600	-0.89661900
H	2.70607300	1.86746100	-2.90365000	C	0.18068300	-4.12361300	-0.83024800
C	-0.28737500	-1.63138000	-0.96907900	H	0.09227800	-4.12741700	0.24901800
H	-0.67450400	-0.84052700	-1.60212600	H	4.33248100	2.08093600	3.07268300
C	0.57474500	-1.82725000	1.43447900	H	2.67946100	2.20486700	2.45367500
C	0.20012000	-1.97028100	2.78056900	H	3.54608600	0.39729300	-3.41975300
H	-0.82080400	-1.75059900	3.07716400	H	2.04382400	0.28272700	-2.49381100
				H	-1.97210100	3.06206400	-3.70006600
				H	-0.70928500	2.12447900	-2.88942500
				H	-1.59440000	3.90949200	2.99649200

H	-0.44616200	2.74341600	2.32079100	C	1.96938000	5.02202300	0.42856700
C	6.80995100	-1.04042400	0.07682700	C	1.91333400	4.70470200	-0.93114600
H	6.69226300	-1.92056200	-0.56188000	H	2.75349700	4.95915900	-1.57300000
H	7.72389800	-0.52468400	-0.24399200	C	0.81066200	4.05228600	-1.49132300
H	6.97327000	-1.38342200	1.10267300	C	0.79896100	3.69491800	-2.95898900
C	-5.41666700	3.95351800	-0.20614200	H	-0.05325300	4.13855900	-3.48733500
H	-5.68127800	4.99476400	-0.42940500	C	0.99235300	-1.04620100	-0.37995100
H	-5.93460500	3.32487800	-0.93689600	H	1.21632400	-1.28389500	-1.42608800
H	-5.81527600	3.72093900	0.78536700	C	2.30208100	0.26308200	1.32121400
H	2.99755400	3.98080900	-1.70276400	C	1.16935500	0.40598300	2.14655800
H	0.86185800	5.05407700	-1.58110300	H	0.27995800	-0.17715200	1.94464400
L₁-17₂				C	1.18109500	1.26750000	3.24458200
Cu	-0.33454800	0.38990500	-0.66667400	H	0.28955000	1.33377300	3.86263500
N	2.28985100	-0.62043400	0.21605000	C	2.31724000	2.01283100	3.55707600
N	-1.41177400	3.06389600	-1.21177700	H	2.32996100	2.67213300	4.42053800
N	-2.81133900	1.50180100	-1.81022700	C	3.44430000	1.88381300	2.74079200
O	4.75274700	-1.11097700	0.16912700	H	4.34441000	2.45306800	2.96234200
O	3.41806000	-2.01657100	-1.46835900	C	3.44032500	1.03338700	1.63760600
B	3.46261800	-1.21870400	-0.33284100	H	4.32662900	0.94931800	1.02330000
C	-1.60902000	1.73286800	-1.23944200	C	5.65114900	-1.71543200	-0.79281800
C	-2.56065600	3.83839600	-1.73150800	C	6.79003500	-2.39034500	-0.02984500
H	-3.04259300	4.39084200	-0.91685900	H	7.37542700	-1.63391900	0.50129000
C	-3.46249500	2.73517300	-2.30998000	H	7.46191000	-2.91855000	-0.71504900
H	-4.49607400	2.80255900	-1.96097600	H	6.41365800	-3.10095800	0.70817500
C	-3.34166300	0.20723800	-2.13633200	C	6.20370100	-0.58221800	-1.66970600
C	-4.37921500	-0.32323900	-1.34818600	H	5.40172000	-0.08521000	-2.22309300
C	-4.91117300	-1.56715200	-1.70407700	H	6.94632700	-0.94643700	-2.38643400
H	-5.71389800	-1.98469000	-1.10059800	H	6.68362800	0.16162600	-1.02727900
C	-4.44131500	-2.28602800	-2.80713100	C	4.69211500	-2.69200000	-1.57595300
C	-3.41625100	-1.72396200	-3.57455900	C	5.01965200	-2.87746800	-3.05691300
H	-3.04440900	-2.26290600	-4.44303400	H	4.28179400	-3.54363000	-3.51365500
C	-2.85445300	-0.48160500	-3.26341300	H	6.00905200	-3.32910800	-3.18656600
C	-1.74041200	0.07966000	-4.11488500	H	4.99484000	-1.92854600	-3.59597100
H	-1.91994500	1.12283400	-4.39570000	C	4.53737500	-4.05951800	-0.89487900
C	-4.90291600	0.40771500	-0.13486200	H	4.29492000	-3.94643100	0.16528500
H	-5.30528800	1.39534600	-0.38780100	H	5.44496100	-4.66460700	-0.98444300
C	-0.26287900	3.71883000	-0.64793000	H	3.71286800	-4.59845600	-1.36931800
C	-0.24767800	4.03498200	0.72244400	C	0.42938700	-2.30683600	0.21877600
C	-1.39000900	3.65428100	1.63292300	C	-0.61844700	-2.98541100	-0.44225400
H	-2.35139200	4.04259100	1.27763900	H	-1.01267400	-2.56872500	-1.36730500
C	0.87669600	4.68664800	1.23425200	C	-1.15155900	-4.17083100	0.05423400
H	0.90771800	4.91772600	2.29573400	H	-1.95149400	-4.66817500	-0.48983700
				C	-0.66157100	-4.72913400	1.24161500
				H	-1.07461100	-5.65633000	1.62870600

C	0.37117600	-4.07377100	1.91198000	C	-2.67758500	2.24186500	-3.02511200
H	0.77695300	-4.49461400	2.82959500	H	-3.63708600	2.76440200	-2.96829700
C	0.90801800	-2.88247300	1.41075200	C	-3.47569800	0.18615100	-1.78524100
H	1.72153400	-2.40069300	1.94309900	C	-4.68083000	0.38952000	-1.08730100
H	-1.22504300	4.04854200	2.63845800	C	-5.58513300	-0.67673100	-1.00498100
H	-1.48752100	2.56667100	1.71377600	H	-6.51815700	-0.52854600	-0.46598100
H	1.71018400	4.04785800	-3.44838300	C	-5.32743600	-1.91663200	-1.59705500
H	0.73747500	2.61078400	-3.10252000	C	-4.13188600	-2.07475400	-2.30632900
H	-1.62762600	-0.50138000	-5.03358800	H	-3.92214500	-3.02517600	-2.79197000
H	-0.78500300	0.05233800	-3.57807200	C	-3.19789300	-1.04013900	-2.42017100
H	-5.70994000	-0.15999800	0.33560600	C	-1.93281000	-1.24073100	-3.22120100
H	-4.11993000	0.56163200	0.61494600	H	-1.88387200	-0.55676300	-4.07691100
C	3.19259400	5.67198500	1.02822500	C	-5.00233400	1.71291800	-0.43501700
H	3.82126200	6.13373000	0.26152600	H	-5.02432400	2.53166000	-1.16342600
H	2.92164300	6.44237200	1.75749900	C	0.47146800	3.04167500	-1.18755500
H	3.79981800	4.92562800	1.55419200	C	0.48080000	4.08024700	-0.23732000
C	-5.00884400	-3.64315600	-3.14966800	C	-0.79706500	4.63408900	0.34394200
H	-5.02995400	-3.80741300	-4.23143600	H	-1.45839800	5.04095300	-0.43044700
H	-4.40129300	-4.44507900	-2.71225300	C	1.71713700	4.58871300	0.16983300
H	-6.02711800	-3.76005400	-2.76753800	H	1.73522400	5.38231900	0.91305800
H	-2.23215900	4.56185100	-2.48282000	C	2.92397200	4.10582900	-0.34509700
H	-3.47604600	2.73264800	-3.40665800	C	2.87496700	3.09829900	-1.31145200
C	-2.81067800	-1.91747300	2.67089400	H	3.80291700	2.72283900	-1.73699700
Br	-2.75124000	0.01950300	3.23215300	C	1.66383600	2.55009400	-1.74693000
C	-3.50347100	-2.72986300	3.70397600	C	1.66389600	1.44595700	-2.77783200
C	-2.90992100	-3.72089400	4.37249200	H	0.84961800	1.54948900	-3.50125800
H	-3.45159700	-4.31734400	5.10052700	C	0.50237700	-1.20512000	0.23958600
H	-1.86713000	-3.97317000	4.20164200	H	0.42493800	-1.25413900	-0.84828200
H	-4.54963000	-2.49152700	3.88792600	C	2.14770400	0.02623700	1.70385700
H	-3.33879900	-1.88235700	1.71880700	C	1.23377100	0.08432000	2.77050300
H	-1.77317800	-2.20477600	2.51440800	H	0.31516000	-0.48578900	2.72292100
L₁-TS18₂				C	1.49204800	0.86801700	3.89661400
Cu	-0.90623400	0.31847800	0.46918900	H	0.75551400	0.89537000	4.69467000
N	1.88216100	-0.76009200	0.55241500	C	2.67142300	1.60210700	4.00073000
N	-0.78348700	2.51973600	-1.65457300	H	2.87341900	2.20598100	4.88063300
N	-2.54303800	1.26872800	-1.91547400	C	3.58871700	1.54580800	2.94815100
O	4.26999800	-1.27240400	-0.03372000	H	4.51706600	2.10960400	3.00507100
O	2.61177500	-1.96043000	-1.46892000	C	3.33249200	0.78180300	1.81267700
B	2.90681000	-1.30141000	-0.28211200	H	4.05441200	0.76079600	1.00775400
C	-1.42973100	1.44305000	-1.16780200	C	4.94784100	-1.79664800	-1.20172100
C	-1.47651800	3.17184700	-2.79103800	C	6.16438000	-2.59350200	-0.73289900
H	-1.77645500	4.18960900	-2.52017700	H	6.87257200	-1.92356600	-0.23658100
				H	6.67708700	-3.06067800	-1.58053700
				H	5.88411000	-3.37145400	-0.02088000

C	5.40175400	-0.59370000	-2.04123800
H	4.54574700	-0.00540000	-2.38332600
H	5.98152400	-0.90330200	-2.91617500
H	6.03227000	0.05170800	-1.42298400
C	3.81301900	-2.64767300	-1.89474700
C	3.85007100	-2.66044800	-3.42210600
H	3.00751300	-3.24480800	-3.80348600
H	4.77371600	-3.12204600	-3.78716900
H	3.77593500	-1.65315500	-3.83611400
C	3.72191900	-4.08363200	-1.35882500
H	3.68095300	-4.09582600	-0.26628900
H	4.56959500	-4.69431900	-1.68462300
H	2.80157000	-4.54135200	-1.73131100
C	0.15494500	-2.54209700	0.78279800
C	-0.92691400	-3.26974700	0.22919400
H	-1.47601900	-2.84070200	-0.60616700
C	-1.29080900	-4.52458800	0.71318800
H	-2.12313800	-5.05376300	0.25534000
C	-0.59032300	-5.10705900	1.77302700
H	-0.87130400	-6.08584500	2.15058600
C	0.48923000	-4.41280100	2.32732800
H	1.05805900	-4.85692800	3.14093200
C	0.85502600	-3.15488200	1.84678600
H	1.70384500	-2.64146800	2.28516200
H	-0.57805000	5.44241100	1.04621700
H	-1.35642700	3.86075600	0.88048100
H	2.60557600	1.44406100	-3.33439700
H	1.55655200	0.46212600	-2.30885600
H	-1.88050200	-2.26017900	-3.61149900
H	-1.03832300	-1.06294200	-2.61778800
H	-5.98393100	1.67510000	0.04463400
H	-4.25838500	1.97056200	0.32576100
C	4.24416300	4.63977400	0.15554400
H	5.04061800	4.50278500	-0.58198300
H	4.18219300	5.70538900	0.39756000
H	4.54606000	4.11434500	1.06977800
C	-6.30460700	-3.06066100	-1.46252000
H	-6.32390000	-3.67976000	-2.36482900
H	-6.03138900	-3.71598200	-0.62612000
H	-7.32029600	-2.70016800	-1.27565300
H	-0.81025400	3.23679700	-3.65706400
H	-2.63246300	1.72551600	-3.99084600
C	-2.69562500	-0.98626100	2.01442600
Br	-2.20924200	1.61904500	2.21931700

C	-2.77635000	-1.21396200	3.42575600
C	-1.97545000	-2.09023600	4.07381300
H	-2.08917700	-2.26638600	5.13929700
H	-1.20339500	-2.65071300	3.55569000
H	-3.53369700	-0.66334300	3.97802500
H	-3.56561200	-0.62610800	1.48287500
H	-1.99226600	-1.58317900	1.44693100

L₁-19₂

Cu	-1.12481100	0.57887800	0.82104200
N	1.30399600	-0.95353600	0.63155000
N	-0.10162100	2.54819300	-1.55187300
N	-2.00241500	1.52605500	-1.85179300
O	3.43978800	-2.12292800	0.05644600
O	1.63646900	-2.39230400	-1.34408100
B	2.12834000	-1.78373100	-0.19987000
C	-0.89748400	1.57208600	-1.06852600
C	-0.69383800	3.27958900	-2.70036000
H	-0.85517100	4.32773800	-2.43173600
C	-2.00669700	2.52491300	-2.94456200
H	-2.88528400	3.17162700	-2.87046600
C	-3.05111200	0.54360300	-1.79320900
C	-4.28894300	0.87578500	-1.20178300
C	-5.29474000	-0.09533000	-1.18277200
H	-6.24529300	0.15102500	-0.71530600
C	-5.12177000	-1.35998900	-1.75457300
C	-3.90723100	-1.63411100	-2.38726800
H	-3.76722000	-2.59521400	-2.87758800
C	-2.86310100	-0.70093200	-2.42755500
C	-1.59410100	-1.05186200	-3.17162100
H	-1.10081400	-0.16943500	-3.58434900
C	-4.55833700	2.24623600	-0.62938000
H	-4.65553900	2.99498600	-1.42608900
C	1.27247600	2.82372000	-1.22279500
C	1.61111700	3.96136300	-0.46629700
C	0.57158500	4.92322600	0.05155200
H	0.21322000	5.58252500	-0.75097700
C	2.96809700	4.22182000	-0.24189000
H	3.23572200	5.08886300	0.35746600
C	3.98047400	3.41828200	-0.76999300
C	3.60986100	2.33438000	-1.57117900
H	4.38281300	1.72063700	-2.02860100
C	2.26912300	2.02434300	-1.81666600

C	-1.42428600	4.97995700	-0.57188000	C	-3.73026100	-2.07374400	-1.89805500
H	-1.45398700	5.91268000	-0.01355200	C	-4.05694500	-1.41074200	-3.23393400
C	-2.60757500	4.47106600	-1.11500400	H	-4.53851400	-0.44482100	-3.05648800
C	-2.53483000	3.29533900	-1.86596300	H	-4.74867000	-2.03063100	-3.81393800
H	-3.43663900	2.90070200	-2.32884700	H	-3.16056900	-1.23815900	-3.83150500
C	-1.32999300	2.60942200	-2.04937500	C	-4.98731200	-2.12802400	-1.01898800
C	-1.31186500	1.36202100	-2.90163900	H	-4.78240200	-2.61218000	-0.06048300
H	-0.34806700	1.21123600	-3.39351000	H	-5.80237600	-2.66545500	-1.51302900
C	1.06224500	4.97244000	-0.18104500	H	-5.31862700	-1.10716800	-0.81211000
H	1.69270300	5.36669500	-0.98878800	C	-2.28660400	0.23599700	1.60654700
C	3.40136300	-0.26797500	-1.31132400	C	-2.53377600	1.62388700	1.64488100
C	4.63530900	-0.19125000	-0.63959400	H	-1.82186300	2.30631500	1.18732100
C	5.18777900	1.11693900	-0.13137700	C	-3.67302600	2.13173700	2.25851600
H	5.48969500	1.77411400	-0.95699000	H	-3.83621800	3.20582200	2.28022400
C	5.35795900	-1.37792000	-0.45487300	C	-4.61012200	1.26685200	2.83854100
H	6.30697500	-1.32892100	0.07359900	H	-5.50548300	1.66422900	3.30810700
C	4.90304500	-2.61003200	-0.92857300	C	-4.38185600	-0.10652600	2.80594300
C	3.68125800	-2.64565400	-1.61089400	H	-5.09785500	-0.78899500	3.25610000
H	3.30821800	-3.59434200	-1.98989000	C	-3.22372300	-0.61777700	2.21139400
C	2.92096000	-1.49305800	-1.81863400	H	-3.05478800	-1.68824600	2.19138400
C	1.60986500	-1.57513500	-2.56389200	H	6.07565700	0.94271900	0.48209700
H	1.58621100	-0.89755800	-3.42533600	H	4.45143700	1.65487400	0.47444400
C	-1.07314000	-0.25662000	0.90598400	H	1.44106400	-2.58999700	-2.93224800
H	-0.95627700	0.35179800	0.00378800	H	0.76645500	-1.30487000	-1.92077300
C	-0.17833400	-2.64000900	1.15993200	H	-2.08186600	1.42636900	-3.67635700
C	1.21093200	-2.47201400	1.15663400	H	-1.53017500	0.46650200	-2.31103900
H	1.64503200	-1.60199300	0.67587500	H	0.80838700	5.81470800	0.46788300
C	2.04243200	-3.40976300	1.77028200	H	1.65777600	4.26326300	0.40132100
H	3.11631000	-3.24892000	1.76408100	C	5.70563200	-3.87373600	-0.72428700
C	1.50017900	-4.54906600	2.36755500	H	6.04400200	-4.28925400	-1.68091800
H	2.14716200	-5.28069900	2.84277100	H	6.59084700	-3.69048200	-0.10930200
C	0.11729600	-4.74195200	2.34062400	H	5.10766400	-4.64898100	-0.23227800
H	-0.31894200	-5.62710500	2.79539200	C	-3.93032000	5.16616900	-0.89490800
C	-0.71627000	-3.79428200	1.74747200	H	-3.79122500	6.20671100	-0.58835500
H	-1.79003400	-3.94383400	1.73770700	H	-4.54393300	5.15756200	-1.80168900
C	-2.98181400	-3.45849700	-2.00163100	H	-4.50940100	4.66447600	-0.10971800
C	-3.88268300	-4.69031200	-1.93476500	H	3.01064100	1.13986800	-3.66700400
H	-3.27029500	-5.59527400	-1.98366400	H	1.41015800	2.92104600	-3.68641600
H	-4.58179800	-4.70898400	-2.77743400	C	0.27398200	0.06451100	2.88797500
H	-4.45463900	-4.72114300	-1.00588700	Br	2.42271300	2.38729500	2.07147900
C	-2.04834100	-3.55394400	-3.21643300	C	-0.35201300	-0.94785500	3.72237600
H	-1.39933000	-2.67661500	-3.28783000	C	-1.35898000	-0.68729800	4.57649100
H	-2.60791700	-3.64918100	-4.15191800	H	-1.74660300	-1.45355300	5.24156600
H	-1.41289600	-4.43662000	-3.10386600	H	-1.79999900	0.30136600	4.65689900

H 0.06918300 -1.94795000 3.69766900
H 1.35432400 -0.07039900 2.82667600
H -0.01171400 1.08539700 3.12620200

(E)-2b

C 2.25196900 0.17670800 0.35965400
Br -1.60841200 -0.22909200 0.03171900
C 1.19649000 0.33677200 -0.44596500
H 1.22298600 -0.05237800 -1.46257500
C -0.04654700 1.03675300 -0.04060200
H 0.01208000 1.46667500 0.95816400
H -0.37373600 1.78807800 -0.75874900
H 2.19453900 0.56298500 1.37841600
C 3.53313000 -0.50128400 -0.02147100
H 3.50891200 -0.86022300 -1.05431300
H 4.38810500 0.17804100 0.08527500
H 3.73128100 -1.35864600 0.63390500

L₁-17₃

Cu 0.19450400 0.40251400 -0.74618200
N -2.37135400 -0.91824400 -0.02300800
N 2.67351900 0.06293200 -2.36658800
N 2.09184600 2.14334400 -2.06774100
O -4.77977800 -1.63240300 -0.12529900
O -4.29556100 0.61333200 -0.09200100
B -3.77650400 -0.67352400 -0.08268800
C 1.76493500 0.86613800 -1.78198900
C 3.66827700 0.80032400 -3.18098900
H 4.68603100 0.53790000 -2.87981500
C 3.31730700 2.26979100 -2.88790700
H 4.10208700 2.78681000 -2.32536400
C 1.35664000 3.30343100 -1.64439000
C 1.73174700 3.97039000 -0.46409000
C 1.01952400 5.11842400 -0.10088800
H 1.30145700 5.63949000 0.81113100
C -0.04066200 5.60836000 -0.87004100
C -0.38206100 4.92209700 -2.03965600
H -1.20252400 5.28874600 -2.65209800
C 0.29967400 3.77140400 -2.44649200
C -0.11464900 3.04332100 -3.70273700
H -0.50647600 2.04728200 -3.46851100

C 2.84995600 3.45906100 0.41151900
H 3.80247400 3.39845300 -0.12730600
C 2.64464200 -1.37374900 -2.38866100
C 3.51428700 -2.08796400 -1.54663600
C 4.40769000 -1.38517800 -0.55283600
H 5.12249000 -0.71263300 -1.04170500
C 3.51985900 -3.48443100 -1.63611100
H 4.18879400 -4.04604100 -0.98819300
C 2.68949300 -4.17269700 -2.52403700
C 1.83547900 -3.42873300 -3.34447400
H 1.17735900 -3.94715700 -4.03775600
C 1.79466400 -2.03370600 -3.29610200
C 0.83927000 -1.27070300 -4.18226000
H 1.33303700 -0.45419500 -4.72065400
C -1.51308200 0.27076600 0.23904400
H -2.03426200 1.11702400 -0.22238100
C -1.78915200 -2.20351700 -0.10992500
C -0.51030900 -2.45896500 0.42541400
H 0.02784900 -1.66271800 0.92474500
C 0.06682200 -3.72721800 0.33825700
H 1.05952900 -3.88212200 0.75318300
C -0.61055700 -4.78256200 -0.27176800
H -0.16706500 -5.77318500 -0.32207500
C -1.87648800 -4.53894300 -0.81021100
H -2.42296700 -5.34135200 -1.30010500
C -2.45612900 -3.27481300 -0.74098800
H -3.43822000 -3.11352200 -1.16448900
C -6.03322700 -0.94765100 -0.36939500
C -7.13832000 -1.67964700 0.39014800
H -7.25733400 -2.68871600 -0.01552500
H -8.09588400 -1.15801600 0.28665600
H -6.90240800 -1.77062000 1.45172800
C -6.29757400 -1.01486800 -1.88061500
H -5.51529800 -0.49479200 -2.44084900
H -7.26462400 -0.57601400 -2.14528000
H -6.29959400 -2.06281200 -2.19391700
C -5.71910600 0.51153000 0.13955400
C -6.41692900 1.63358600 -0.62789800
H -6.11221000 2.60075300 -0.21747300
H -7.50541800 1.55456800 -0.53486400
H -6.15422700 1.62092900 -1.68732300
C -5.94313400 0.68799100 1.64875400
H -5.44567000 -0.10241500 2.21745600
H -7.00673600 0.68954800 1.90708700

H	-5.51021700	1.64281600	1.95898900			
C	-1.37322800	0.60859900	1.69848000	Cu	-0.97441500	-0.10584300 -0.53674700
C	-0.86110300	1.86920600	2.07662200	N	1.99543100	-1.24053400 -0.26712400
H	-0.57289900	2.57393100	1.29897500	N	-3.38080100	0.48708300 1.36996300
C	-0.72504900	2.23311700	3.41289300	N	-1.57244400	1.37339500 2.18940200
H	-0.33521800	3.21724600	3.66330800	O	4.36508900	-2.03574400 -0.45388900
C	-1.09566300	1.34761500	4.43332200	O	4.00807700	0.22362700 -0.32769300
H	-0.99573200	1.63232000	5.47707300	B	3.42737800	-1.02508900 -0.36705900
C	-1.60969500	0.09971800	4.08124900	C	-2.04693900	0.61822000 1.16730000
H	-1.91698900	-0.59884500	4.85644100	C	-3.86141400	1.10977500 2.62674000
C	-1.74632900	-0.26505900	2.73737100	H	-4.71364200	1.76516000 2.43411200
H	-2.16108900	-1.23682600	2.48914500	C	-2.62380600	1.86433900 3.11135300
H	4.98599900	-2.11067900	0.02443300	H	-2.72659400	2.95072600 3.01673000
H	3.83140600	-0.78240300	0.15606200	C	-0.21251900	1.75685200 2.46228000
H	0.38628600	-1.93530500	-4.92215000	C	0.29775800	2.96040500 1.92753200
H	0.03071400	-0.82492300	-3.59180600	C	1.61816300	3.30568000 2.22690600
H	0.72301400	2.90486700	-4.39544300	H	2.02213800	4.22320700 1.80547500
H	-0.89550900	3.59679500	-4.23028800	C	2.42620000	2.52067000 3.05743900
H	2.99961400	4.11967800	1.26870300	C	1.86361800	1.38255600 3.63523500
H	2.63589800	2.45810000	0.79925100	H	2.45800600	0.78118800 4.31958400
C	2.68390800	-5.68131500	-2.58008800	C	0.54393600	0.99345300 3.37144600
H	1.79267600	-6.08099100	-2.08176000	C	-0.03637600	-0.17551300 4.13465300
H	2.66708400	-6.04426500	-3.61311400	H	-0.92600700	-0.58707000 3.65557600
H	3.56157700	-6.10594200	-2.08479400	C	-0.55569100	3.88904200 1.10221600
C	-0.81557200	6.82890900	-0.43307600	H	-1.37678300	4.30324800 1.70102700
H	-0.18524000	7.52392300	0.12974100	C	-4.32504700	-0.29825500 0.62355100
H	-1.23436100	7.36560700	-1.28958700	C	-5.25340800	0.35273600 -0.21403700
H	-1.65313500	6.54891600	0.21763600	C	-5.23220500	1.84715100 -0.41949200
H	3.55141100	0.53887700	-4.23889800	H	-5.45274400	2.39044400 0.50739600
H	3.11450300	2.84980000	-3.79350400	C	-6.20822800	-0.43096100 -0.87224200
C	1.49230200	-2.22687400	4.13381500	H	-6.92375400	0.06373100 -1.52525700
Br	3.99930300	0.56591000	3.00330900	C	-6.27413200	-1.81895900 -0.71407900
C	2.57894700	-1.51806100	4.46549700	C	-5.35901100	-2.42664600 0.14996100
H	3.46881400	-2.02195900	4.84126400	H	-5.40560300	-3.50203100 0.30618400
C	2.63764000	-0.04013100	4.37949500	C	-4.38609200	-1.68863300 0.83372900
H	1.70081600	0.41630300	4.06418900	C	-3.42350300	-2.39314400 1.75789200
H	3.00912200	0.43325100	5.28803600	H	-3.33861500	-1.88627800 2.72519600
H	0.61750200	-1.69696000	3.75661600	C	1.14764500	-0.08378100 -0.56598100
C	1.36675300	-3.71556900	4.25489100	H	1.07378200	0.61295700 0.27880700
H	0.57133000	-3.98491900	4.96177400	C	1.54824700	-2.34410200 0.51377600
H	1.08469700	-4.15908400	3.29235100	C	0.53746000	-2.20235300 1.47509800
H	2.29784600	-4.17881800	4.59531500	H	0.08630700	-1.23198700 1.62911100
				C	0.12232100	-3.29483100 2.24208900
				H	-0.65290200	-3.15301700 2.99003500

L₁-TS18₃

C	0.42306800	-0.52050400	-3.93842000	H	5.12259100	0.36428200	2.46417100
H	-0.54584000	-0.06443800	-3.73330100	H	6.74765300	-0.20044900	2.01598000
C	-0.96938000	-3.98142100	-0.44663500	H	5.34512100	-1.28237600	1.88209200
H	-1.90610700	-4.17049300	-0.98356100	C	1.64743200	-0.48260400	1.68184600
C	-4.33514400	0.19630900	-0.65916300	C	1.64647200	-1.88801300	1.75312000
C	-5.22066000	-0.47839800	0.20378000	H	1.28538900	-2.45706700	0.90585500
C	-5.01449300	-1.92340600	0.58068400	C	2.12085100	-2.55268800	2.87979900
H	-4.94945200	-2.57735100	-0.29650400	H	2.10964500	-3.63857900	2.90417900
C	-6.29948600	0.23999800	0.73221200	C	2.59046800	-1.83268900	3.97950000
H	-6.98893900	-0.27390100	1.39798700	H	2.94887300	-2.35172200	4.86388400
C	-6.51595800	1.58832800	0.43193300	C	2.58667200	-0.43606600	3.93440600
C	-5.61781100	2.22442400	-0.43120400	H	2.94210000	0.13735300	4.78645700
H	-5.77374000	3.27000900	-0.68766400	C	2.12757400	0.23062400	2.80108700
C	-4.53104500	1.54774500	-0.99476700	H	2.13989500	1.31441400	2.78608700
C	-3.59576600	2.26965600	-1.93316400	H	-5.84349900	-2.28007100	1.19747800
H	-3.44745400	1.71974500	-2.86933500	H	-4.08212500	-2.04117400	1.14805700
C	1.14989600	0.19530900	0.46482800	H	-3.98766300	3.25856200	-2.18539700
H	0.94197000	-0.49540000	-0.35899100	H	-2.60682200	2.40498500	-1.48535200
C	1.45093900	2.31444000	-0.84548400	H	0.41739900	-0.87585300	-4.97608000
C	0.37215500	2.04469200	-1.70024000	H	1.17870400	0.26697200	-3.86898100
H	-0.11856500	1.08283800	-1.65786900	H	-0.60691800	-4.94248100	-0.07208500
C	-0.07183200	3.00599800	-2.61341900	H	-1.21419400	-3.34970400	0.41655900
H	-0.89655000	2.76170300	-3.27699200	C	-7.67591900	2.34281200	1.03867900
C	0.53515100	4.25688900	-2.68965500	H	-7.39217400	2.80550300	1.99220600
H	0.18686200	4.99938800	-3.40137500	H	-8.02112600	3.14514900	0.37948700
C	1.59794900	4.53840200	-1.82733700	H	-8.52258200	1.67976700	1.24000500
H	2.07731500	5.51337800	-1.85384300	C	3.67354700	-4.04373000	-2.41722700
C	2.05030000	3.58932000	-0.91568400	H	3.63237800	-5.11929000	-2.22044500
H	2.86400400	3.83188300	-0.24620600	H	4.12521600	-3.89386700	-3.40253900
C	5.60546900	1.73904200	0.08278400	H	4.35079100	-3.60147700	-1.67617400
C	6.59181200	2.43328500	1.01868900	H	-4.04705900	-0.52794400	-3.33154100
H	6.60955000	3.50598600	0.80506700	H	-2.18749200	-1.88134400	-3.98129900
H	7.60463400	2.04316700	0.87369100	C	-0.87570200	1.70357700	2.02324000
H	6.31432300	2.30159200	2.06571900	Br	-1.71878900	-1.73761900	2.38063500
C	5.90257000	2.11518600	-1.37464600	C	-2.29538800	1.95436800	1.80965300
H	5.19781400	1.63605400	-2.05984800	H	-2.53546600	2.74071600	1.09313100
H	6.91827300	1.83188400	-1.66622300	C	-3.31238700	1.33138800	2.44795400
H	5.80112300	3.19761400	-1.49048700	H	-3.12663300	0.52383900	3.14715000
C	5.43993400	0.18442200	0.30949600	H	-4.34174500	1.60659600	2.24737900
C	6.24519800	-0.69679900	-0.64409700	H	-0.64144500	1.06817000	2.87741600
H	6.04025900	-1.74911400	-0.42694600	C	-0.01174900	2.93606300	1.90116100
H	7.31989500	-0.53022800	-0.51565000	H	-0.11869100	3.53235800	2.81981900
H	5.98424500	-0.50996000	-1.68732700	H	1.04729700	2.71480400	1.77844900
C	5.68501300	-0.25097700	1.75892400	H	-0.32147100	3.56578400	1.06266200

L₁-TS20₃

Cu	-1.08490100	-0.36171500	0.76006000	C	-1.20879100	3.88347100	-0.38997000
N	1.61720200	1.54982500	0.41844200	H	-2.20007200	3.83733600	-0.83073000
N	-3.06401000	-0.70784200	-1.57998800	C	-0.69910700	5.09959000	0.06312100
N	-1.28579600	-1.93279000	-1.83040000	H	-1.28535300	6.00955400	-0.02578200
O	3.55463000	2.76687300	-0.54739600	C	0.57577300	5.13159000	0.63308300
O	3.67496200	0.47333900	-0.49091700	H	0.98852800	6.06937000	0.99475400
B	2.92234600	1.58970200	-0.18640500	C	1.32239800	3.96232900	0.76148800
C	-1.84075500	-0.96941700	-1.05608800	H	2.30575100	3.99264700	1.21470700
C	-3.43159500	-1.59782000	-2.70662800	C	4.72371200	2.41127100	-1.32876500
H	-4.21755000	-2.29390100	-2.39253300	C	5.83093300	3.41906000	-1.02534500
C	-2.10893700	-2.30219300	-3.00436800	H	5.53027900	4.41142800	-1.37371600
H	-2.20886500	-3.38672000	-3.08399200	H	6.75854600	3.14660700	-1.53969200
C	0.04289800	-2.47312500	-1.74749100	H	6.03254300	3.48481900	0.04511500
C	0.22537500	-3.78710700	-1.27057300	C	4.32125000	2.50185300	-2.80703000
C	1.52443300	-4.30521600	-1.25923800	H	3.53064900	1.78519700	-3.04622000
H	1.67709700	-5.31295800	-0.88004900	H	5.17078400	2.31824500	-3.47185500
C	2.62329200	-3.57439600	-1.71912700	H	3.93730900	3.50585100	-3.00718800
C	2.39716000	-2.29529900	-2.23247100	C	5.00650900	0.93718700	-0.84514900
H	3.23322900	-1.71929500	-2.61611700	C	5.58763400	0.00849500	-1.90865300
C	1.11939700	-1.72872700	-2.26554200	H	5.69664500	-0.99869600	-1.49666400
C	0.92128800	-0.35254900	-2.85921800	H	6.57810300	0.35407800	-2.22322600
H	0.05437300	-0.31270900	-3.52648800	H	4.94826500	-0.05206100	-2.79101800
C	-0.92660900	-4.63372900	-0.78991500	C	5.86383200	0.87042000	0.42591900
H	-0.55932600	-5.58813700	-0.40379400	H	5.48498300	1.54573900	1.19731400
C	-4.04634500	0.23495800	-1.12552800	H	6.90794900	1.12677800	0.22172400
C	-5.02498900	-0.16444500	-0.19719800	H	5.82444300	-0.14532600	0.82697300
C	-5.04163600	-1.55384300	0.39234200	C	1.97973000	-0.42698000	1.89581500
H	-5.29640800	-2.30431700	-0.36660500	C	1.84314700	-1.81953100	2.07284600
C	-6.01184100	0.76469400	0.15785400	H	1.07824300	-2.35395100	1.52082200
H	-6.77063800	0.46630300	0.87773300	C	2.64485800	-2.51004900	2.97613500
C	-6.05400000	2.05192000	-0.38438300	H	2.50655700	-3.58057000	3.09830400
C	-5.08838800	2.40010300	-1.33543100	C	3.61578100	-1.83731000	3.72402000
H	-5.12470000	3.38502300	-1.79610700	H	4.24149200	-2.37899000	4.42783900
C	-4.08883700	1.50626400	-1.73126800	C	3.77455400	-0.46167300	3.55292100
C	-3.12334300	1.88800200	-2.82981000	H	4.53024200	0.07534600	4.12027700
H	-3.31530800	1.31251100	-3.74414600	C	2.96852900	0.23410800	2.65190900
C	1.11157700	0.26226400	0.91000900	H	3.12134500	1.29939800	2.51621200
H	0.90298500	-0.42485400	0.08417100	H	-5.79691100	-1.62571200	1.17944600
C	0.81545000	2.73277200	0.30723000	H	-4.07502900	-1.83974400	0.82126400
C	-0.45299900	2.71276200	-0.28359400	H	-3.22690300	2.94528000	-3.08652800
H	-0.85766900	1.76973800	-0.63602200	H	-2.08241100	1.70659000	-2.55288400
				H	1.80069400	-0.05847500	-3.43765500
				H	0.76594300	0.40846700	-2.08789600
				H	-1.47353700	-4.12913800	0.01254000

H	-1.63256400	-4.86194500	-1.59830100	H	-2.74411800	-1.11570300	-5.02272300
C	-7.10811800	3.04459800	0.04597300	C	-2.50131500	0.43669200	-3.56242300
H	-7.43680800	3.66836800	-0.79132100	C	-1.26619500	1.00011600	-4.22408300
H	-7.98632600	2.54138100	0.46041800	H	-1.32718800	2.08566900	-4.35578700
H	-6.72229600	3.71982700	0.81987800	C	-4.74656900	1.05914300	-0.50568600
C	4.01936800	-4.14524500	-1.64496800	H	-5.04063500	2.10710000	-0.63562900
H	4.49562500	-3.88197300	-0.69238100	C	0.23862000	3.86453600	-0.11751400
H	4.01143900	-5.23726300	-1.71422200	C	0.15364900	4.01561800	1.27810700
H	4.65565100	-3.75791400	-2.44677600	C	-1.10876000	3.67443900	2.03198600
H	-3.81091700	-1.01486800	-3.55021100	H	-1.98210600	4.21233800	1.64610200
H	-1.63025700	-1.93729500	-3.92178900	C	1.28884800	4.45761300	1.96140000
C	-0.67652400	0.78014000	2.62475200	H	1.24029200	4.56204400	3.04219500
H	-0.65889000	-0.19544800	3.10750500	C	2.48783100	4.74150400	1.29980000
Br	-1.70068400	-2.51974700	2.08676200	C	2.53259700	4.58816000	-0.08847500
C	-2.00638100	1.27753100	2.25928800	H	3.45708800	4.80372500	-0.61906600
H	-2.03587200	2.28661700	1.85372100	C	1.42309600	4.14979500	-0.81789200
C	-3.17178400	0.62982000	2.48116500	C	1.51734900	3.95672800	-2.31261100
H	-3.19263000	-0.37591400	2.88639900	H	0.74608700	4.51715300	-2.85344500
H	-4.11616900	1.11184900	2.25206700	C	0.97704700	-0.99428900	-0.55048300
C	0.17176800	1.81184500	3.32344200	H	1.24760400	-1.08960400	-1.60808900
H	1.19936200	1.48824100	3.47977200	C	2.29675800	-0.11968700	1.40425800
H	0.16040000	2.78196000	2.82496700	C	1.12836100	0.04254900	2.17482000
H	-0.26821400	1.94960200	4.32237900	H	0.19426400	-0.38743700	1.83628200
L_I-17₄				C	1.15612000	0.72725700	3.39071200
Cu	-0.17290300	0.60765200	-0.67265700	H	0.23309400	0.81689100	3.95757500
N	2.26662400	-0.81938000	0.17443500	C	2.34400400	1.26828200	3.88074100
N	-0.91917200	3.43720900	-0.85499600	H	2.36642900	1.78856000	4.83426700
N	-2.40432500	2.15653100	-1.80953900	C	3.50825400	1.11602900	3.12278200
O	4.65322800	-1.60515800	0.18618700	H	4.44922200	1.52695500	3.48201000
O	3.35260400	-2.05807800	-1.65385500	C	3.48960800	0.44367400	1.90295100
B	3.40160900	-1.46556600	-0.39888700	H	4.40517900	0.33752200	1.33672500
C	-1.24740200	2.15795100	-1.11228500	C	5.54664400	-2.15771800	-0.81084400
C	-1.91318100	4.41264700	-1.35529100	C	6.53510100	-3.08877000	-0.11059900
H	-2.40149400	4.92114000	-0.51648200	H	7.16644000	-2.51084100	0.57091400
C	-2.88054800	3.51753000	-2.14961400	H	7.18718100	-3.58491700	-0.83756100
H	-3.92458100	3.65201300	-1.85472200	H	6.02058900	-3.85190200	0.47595500
C	-3.02574600	0.99456200	-2.38143400	C	6.29529400	-0.97901100	-1.45025600
C	-4.17953500	0.46579300	-1.77342500	H	5.60338200	-0.30165200	-1.95908400
C	-4.78918600	-0.64525500	-2.36443800	H	7.04567300	-1.31535100	-2.17268600
H	-5.68086100	-1.05993500	-1.89958800	H	6.80547100	-0.41486100	-0.66424300
C	-4.28534000	-1.23633800	-3.52748700	C	4.54331400	-2.86456700	-1.80136600
C	-3.14486900	-0.67749200	-4.11162600	C	4.96045700	-2.85016500	-3.27128600
				H	4.18729200	-3.33429500	-3.87514600
				H	5.89718400	-3.39837200	-3.41865000

H	5.08869700	-1.83197900	-3.64350000
C	4.17703600	-4.29262500	-1.37155400
H	3.86945900	-4.32155500	-0.32271700
H	5.01067700	-4.98772100	-1.51208000
H	3.33313600	-4.63670200	-1.97558400
C	0.24530900	-2.25977400	-0.19522900
C	-0.80221100	-2.71607200	-1.02598100
H	-1.06990800	-2.12981600	-1.90309200
C	-1.49139500	-3.89407800	-0.75588300
H	-2.28568100	-4.21609600	-1.42571900
C	-1.16488300	-4.66868700	0.36431000
H	-1.69965000	-5.59068000	0.57441800
C	-0.13441700	-4.23586900	1.19871400
H	0.14674400	-4.82765000	2.06741300
C	0.55926000	-3.05144400	0.92567400
H	1.36602500	-2.74486000	1.58331000
H	-1.00415700	3.92883400	3.08953600
H	-1.33220000	2.60431400	1.96636000
H	2.49035700	4.28789800	-2.68412800
H	1.39556100	2.90126900	-2.58053600
H	-1.11674000	0.55020300	-5.20889600
H	-0.37214800	0.80032500	-3.62219600
H	-5.63752200	0.50940600	-0.19100200
H	-4.02377700	1.02689900	0.31614400
C	3.71193200	5.16000500	2.07747400
H	4.46367700	5.61994600	1.42969600
H	3.46117500	5.87341300	2.86928700
H	4.17271700	4.28864100	2.55791400
C	-4.94294200	-2.45902100	-4.12234900
H	-4.55219800	-3.37667900	-3.66538200
H	-6.02503500	-2.45158400	-3.95991000
H	-4.76039000	-2.52869000	-5.19866000
H	-1.42847900	5.17346400	-1.97416000
H	-2.81201600	3.67825900	-3.23212400
C	-3.13526000	-1.82889100	2.04794900
Br	-2.86849400	0.00315800	2.87715300
C	-3.93706300	-2.69332300	2.94533800
C	-3.45301700	-3.80024500	3.52098400
H	-2.41392300	-4.07037300	3.33317700
H	-4.97151100	-2.39736500	3.11682500
H	-3.62949500	-1.59218500	1.10681600
H	-2.12991900	-2.20076100	1.86252300
C	-4.23734300	-4.72169200	4.40583900
H	-5.26690100	-4.37680300	4.54012800

H	-4.26734100	-5.73749200	3.99156300
H	-3.77172000	-4.80297500	5.39629900

L₁-TS18₄

Cu	0.86754300	-0.36463900	0.37335300
N	-1.88462900	0.82438700	0.41941400
N	0.62701400	-2.79305800	-1.47074100
N	2.37088200	-1.59309500	-1.96822900
O	-4.26518600	1.38952000	-0.14910700
O	-2.62426200	1.85969800	-1.68826300
B	-2.90999100	1.33140700	-0.43555300
C	1.29982700	-1.67220100	-1.14556500
C	1.24724200	-3.56780500	-2.57157500
H	1.54008300	-4.56242100	-2.22020700
C	2.45288200	-2.69482600	-2.95566200
H	3.40642100	-3.22456300	-2.86633400
C	3.31997600	-0.51786400	-2.00561200
C	4.54775600	-0.65375800	-1.33065900
C	5.46890500	0.39748800	-1.41577400
H	6.42050200	0.30021700	-0.89794800
C	5.20496100	1.55853100	-2.14836600
C	3.98455000	1.64979900	-2.82600600
H	3.76839100	2.53655800	-3.41762200
C	3.03313300	0.62575800	-2.77574700
C	1.73744000	0.75125800	-3.54223400
H	1.62878700	-0.04557900	-4.28735100
C	4.87273400	-1.88853100	-0.52458800
H	4.81598800	-2.79914900	-1.13149800
C	-0.60732500	-3.24352900	-0.88877800
C	-0.57857600	-4.19567600	0.14783200
C	0.72163100	-4.71500200	0.71067600
H	1.33803100	-5.20007300	-0.05569400
C	-1.79781600	-4.64610000	0.66141300
H	-1.78624100	-5.37238600	1.47076800
C	-3.02434400	-4.18614700	0.17268500
C	-3.01474000	-3.26338000	-0.87587200
H	-3.95932900	-2.90643900	-1.28013300
C	-1.82201100	-2.77803600	-1.42199100
C	-1.86276400	-1.76676100	-2.54300100
H	-1.10318100	-1.95969600	-3.30660600
C	-0.49697800	1.18153100	0.03219800
H	-0.44748500	1.11635400	-1.05663300
C	-2.14771100	0.16607200	1.64864100

C	-1.20428800	0.17047800	2.69117500	H	0.86905500	0.69046400	-2.88008600
H	-0.26350900	0.68939200	2.56059700	H	5.88624100	-1.82599700	-0.11939400
C	-1.45940400	-0.49011500	3.89426500	H	4.17481400	-2.01093100	0.31090200
H	-0.69959000	-0.47665100	4.67070200	C	-4.32261700	-4.65231800	0.78605200
C	-2.66431100	-1.15816100	4.10093800	H	-5.15504800	-4.56728900	0.08103500
H	-2.86322600	-1.66627700	5.04008900	H	-4.26063000	-5.69361900	1.11744700
C	-3.61083200	-1.16253000	3.07309300	H	-4.57096900	-4.04426300	1.66459500
H	-4.55951300	-1.67656500	3.20960600	C	6.20306500	2.69151800	-2.19561600
C	-3.35900500	-0.52240100	1.86252300	H	5.99236800	3.43544700	-1.41718500
H	-4.10431800	-0.54654800	1.07933000	H	7.22409200	2.33300300	-2.03530400
C	-4.95436200	1.82973000	-1.34483000	H	6.17239400	3.21234000	-3.15754100
C	-6.12418200	2.71820800	-0.92481400	H	0.53495200	-3.69770300	-3.39292900
H	-6.84505200	2.12815500	-0.35132700	H	2.38274800	-2.29887600	-3.97502600
H	-6.64043300	3.12613000	-1.80045700	C	2.79345200	1.07289500	1.70635800
H	-5.79265300	3.54621900	-0.29617700	Br	2.17810000	-1.52708900	2.21640600
C	-5.47769000	0.57259300	-2.05431000	C	2.91671500	1.45160800	3.06971200
H	-4.65372500	-0.07866500	-2.35895500	C	2.13569500	2.40871000	3.63940000
H	-6.06990500	0.82085300	-2.94045200	H	1.36805700	2.88659000	3.03366700
H	-6.11410900	0.01428700	-1.36182700	H	3.67746600	0.95565200	3.66880900
C	-3.80660700	2.56078100	-2.14321100	H	3.61559200	0.58125800	1.20637400
C	-3.89037700	2.43757700	-3.66384500	H	2.08912500	1.60815400	1.08162100
H	-3.03675400	2.94805700	-4.11939600	C	2.25572900	2.86236300	5.05494700
H	-4.80491400	2.90482600	-4.04443100	H	3.05414300	2.34215600	5.59108900
H	-3.87044100	1.39502600	-3.98678900	H	2.44336000	3.94296500	5.10425500
C	-3.63602000	4.03382900	-1.74391000	H	1.31088700	2.69389400	5.58922400
H	-3.56188600	4.14373300	-0.65862800				
H	-4.46434900	4.65231100	-2.10337000	L₁-19₄			
H	-2.70723200	4.41156800	-2.17986700				
C	-0.09642600	2.55566000	0.42355000	Cu	1.17890500	-0.45006000	0.67384300
C	0.98463100	3.19178500	-0.23489000	N	-1.33825400	0.92329800	0.51148400
H	1.49383900	2.66331500	-1.03803900	N	0.01667400	-2.72227700	-1.33885200
C	1.39828600	4.47738900	0.10649000	N	1.91701500	-1.79676500	-1.86559700
H	2.22867200	4.93156300	-0.42897800	O	-3.59493800	1.86678000	-0.02241800
C	0.74892900	5.18688400	1.12128900	O	-1.90615300	2.13050400	-1.56070500
H	1.06739700	6.19103900	1.38571700	B	-2.27775300	1.60100600	-0.33448800
C	-0.33056100	4.58573300	1.77490200	C	0.84845700	-1.70416700	-1.03652900
H	-0.86188000	5.12812700	2.55376600	C	0.55799400	-3.63900500	-2.37420100
C	-0.74484300	3.29596200	1.43876600	H	0.75293500	-4.62204800	-1.93432400
H	-1.59214700	2.85711800	1.95465300	C	1.84296400	-2.92907600	-2.81638100
H	0.53056400	-5.45353800	1.49347400	H	2.72796700	-3.56471000	-2.73012000
H	1.31439400	-3.90341200	1.14582700	C	2.97166100	-0.82875600	-2.00261400
H	-2.84001500	-1.78073800	-3.03402200	C	4.24767900	-1.10303400	-1.46734500
H	-1.69465300	-0.75127700	-2.16959000	C	5.25434700	-0.14546900	-1.63288600
H	1.69275000	1.70614600	-4.07188900	H	6.23583200	-0.34627000	-1.20964900

C	5.04224400	1.04760300	-2.32967400	H	-2.14996100	3.36573700	-3.94178500
C	3.78511000	1.25908600	-2.90200900	H	-3.89145500	3.65993300	-3.82583500
H	3.61175900	2.15826100	-3.48944200	H	-3.26609800	1.99810500	-3.84249300
C	2.74111700	0.33680600	-2.76234700	C	-2.49141700	4.45521200	-1.51677000
C	1.42422000	0.60708900	-3.45518700	H	-2.36775400	4.50603000	-0.43186200
H	0.94649000	-0.31105300	-3.80496500	H	-3.19808900	5.23078900	-1.82731100
C	4.55629200	-2.39958500	-0.75891900	H	-1.51999000	4.67043500	-1.96977700
H	4.61777600	-3.23393000	-1.46969200	C	0.47369900	2.62571100	0.63328000
C	-1.34789100	-2.91950000	-0.92435600	C	1.48869200	3.29369500	-0.08417000
C	-1.67179900	-3.90045700	0.03109900	H	1.98184100	2.77820100	-0.90511300
C	-0.62219900	-4.75466000	0.69617700	C	1.86246100	4.59773200	0.23027800
H	-0.26413400	-5.53771700	0.01400300	H	2.64434000	5.08643200	-0.34518100
C	-3.02444200	-4.11296400	0.32352900	C	1.22744400	5.28202800	1.27159700
H	-3.27956400	-4.85912000	1.07240100	H	1.51346700	6.30131300	1.51469200
C	-4.04745500	-3.41621400	-0.32246400	C	0.21365700	4.64188200	1.98558000
C	-3.69215600	-2.48902400	-1.30669400	H	-0.29583600	5.16291900	2.79199000
H	-4.47363200	-1.96351900	-1.85101300	C	-0.15726100	3.33154500	1.67527400
C	-2.35623500	-2.22956600	-1.62649300	H	-0.95593700	2.85864400	2.23571200
C	-2.02377100	-1.25607300	-2.73242400	H	-1.03971100	-5.25902500	1.57160200
H	-1.30004200	-1.67377900	-3.44056100	H	0.24047600	-4.16766100	1.01895200
C	0.06944100	1.25028700	0.22402400	H	-2.92423400	-1.00194300	-3.29846800
H	0.22265700	1.15002400	-0.84771900	H	-1.59867300	-0.32476300	-2.34801500
C	-1.73846400	0.26665300	1.71049100	H	1.58190900	1.25616800	-4.32139200
C	-0.91718300	0.24292200	2.84782900	H	0.70169600	1.11135500	-2.80430200
H	0.04331100	0.74062600	2.83960000	H	5.52387300	-2.33686600	-0.25412000
C	-1.32740800	-0.41748700	4.00783200	H	3.79701700	-2.64891000	-0.01239100
H	-0.66420000	-0.42643200	4.86813900	C	-5.49555100	-3.65262100	0.03552200
C	-2.56484500	-1.05399600	4.06732500	H	-6.15756200	-3.44578800	-0.81100600
H	-2.88224800	-1.56407900	4.97201500	H	-5.66603500	-4.68456100	0.35701300
C	-3.38625500	-1.03212200	2.93749200	H	-5.80840100	-3.00036400	0.86058500
H	-4.35134900	-1.53189000	2.95679200	C	6.14004700	2.07658600	-2.46058100
C	-2.97970900	-0.39201300	1.77040400	H	6.12955200	2.77263700	-1.61262300
H	-3.62046400	-0.40555900	0.89880300	H	7.12834000	1.60755400	-2.48177600
C	-4.20421600	2.52480000	-1.16275600	H	6.02544300	2.67146600	-3.37169300
C	-5.14461100	3.61020600	-0.63964200	H	-0.16541400	-3.76510300	-3.18526200
H	-5.95783300	3.14782600	-0.07285500	H	1.79401800	-2.55347800	-3.84559100
H	-5.58629000	4.17570300	-1.46700200	C	2.61501400	0.66539000	1.62490000
H	-4.62697700	4.30578200	0.02281900	Br	1.95847000	-2.42625800	1.92930200
C	-5.00835600	1.46264400	-1.92323000	C	2.51824700	0.80591700	3.06773100
H	-4.35941700	0.66924900	-2.30160000	C	2.38235500	1.98582600	3.71294900
H	-5.55666700	1.89514500	-2.76572500	H	2.33361100	2.90410100	3.13001900
H	-5.73149600	1.01069500	-1.23853700	H	2.57129800	-0.11458400	3.64658000
C	-2.94736800	3.05905300	-1.96227900	H	3.36079400	-0.06163500	1.30253900
C	-3.07805200	3.01163400	-3.48351100	H	2.66809400	1.60121700	1.07833500

C	2.31551100	2.13587300	5.20241500	H	0.18374700	1.11209200	-1.00069100
H	2.36965700	1.16815600	5.71015300	C	-1.54078800	0.56515100	1.82300900
H	3.13436900	2.76470700	5.57708500	C	-0.89688300	1.09138200	2.94991400
H	1.38362900	2.63092800	5.50690600	H	-0.13088000	1.84638500	2.83399100
L₁-TS20₄				C	-1.21532400	0.62440900	4.22540800
Cu	1.01360700	-0.50071600	0.53887300	H	-0.69386500	1.03606700	5.08494200
N	-1.28515100	1.03396200	0.49402100	C	-2.18522200	-0.36052700	4.40150800
N	0.22030000	-2.93070100	-1.23594600	H	-2.42970000	-0.72033100	5.39657100
N	2.16806300	-2.06741100	-1.67039400	C	-2.82120800	-0.89509200	3.27946500
O	-3.68760000	1.53253200	0.05743000	H	-3.56309400	-1.68055400	3.39426000
O	-2.21511300	1.66830900	-1.70578500	C	-2.49686400	-0.44740900	2.00171400
B	-2.38543000	1.37659300	-0.36285800	H	-2.97524400	-0.88786000	1.13420000
C	1.03696100	-1.89768500	-0.94478600	C	-4.49882600	1.84866000	-1.10230500
C	0.80963100	-3.91013100	-2.18162900	C	-5.52702600	2.90141700	-0.68821900
H	0.92289800	-4.88341700	-1.69335500	H	-6.19960700	2.47799400	0.06311800
C	2.15588400	-3.26508300	-2.53878200	H	-6.13142300	3.21706600	-1.54532900
H	3.00951800	-3.91219600	-2.31630800	H	-5.04957000	3.78111300	-0.25363400
C	3.28425000	-1.16541000	-1.70003900	C	-5.21488700	0.55825200	-1.51929700
C	4.40586700	-1.42004800	-0.88829200	H	-4.49908800	-0.21687100	-1.80140800
C	5.48305000	-0.52811600	-0.95795600	H	-5.89869400	0.72627300	-2.35692600
H	6.35139600	-0.71272500	-0.32992200	H	-5.79442600	0.18683200	-0.66962500
C	5.47482200	0.58573100	-1.80239100	C	-3.42256300	2.34284300	-2.15374200
C	4.35416400	0.79261100	-2.61426800	C	-3.69615600	1.93795700	-3.60125200
H	4.33744600	1.64150500	-3.29445400	H	-2.88034300	2.28979500	-4.23951200
C	3.25475200	-0.07068700	-2.58542700	H	-4.62547900	2.39073600	-3.96246800
C	2.07443700	0.16976000	-3.49823000	H	-3.76996300	0.85502300	-3.71442900
H	1.94435200	-0.64885500	-4.21621400	C	-3.14275200	3.85013400	-2.07842500
C	4.45368600	-2.59943600	0.05208600	H	-2.92003500	4.16585100	-1.05610200
H	4.25585100	-3.54465100	-0.46563100	H	-3.98828900	4.43646800	-2.45072300
C	-1.11562900	-3.16501800	-0.76064400	H	-2.26713400	4.07814000	-2.69210800
C	-1.32365400	-3.98791500	0.36245300	C	0.17980100	2.97848500	-0.00622700
C	-0.17617100	-4.56247900	1.15285400	C	0.96780900	3.58774000	-1.00442200
H	0.52010600	-5.11920400	0.51499100	H	1.45887600	2.96225700	-1.74617500
C	-2.64340200	-4.26520500	0.73771200	C	1.11075700	4.97064600	-1.07355200
H	-2.81298000	-4.88947400	1.61175800	H	1.71839000	5.41057000	-1.85979300
C	-3.73995000	-3.77983600	0.02079700	C	0.46099600	5.79228000	-0.14667800
C	-3.49468700	-2.98574000	-1.10418600	H	0.56725300	6.87185400	-0.20097500
H	-4.33468800	-2.61607000	-1.68749400	C	-0.33559200	5.20910400	0.83844200
C	-2.19552700	-2.66621300	-1.51314200	H	-0.85494600	5.83476900	1.55930900
C	-1.97893600	-1.80045000	-2.73274200	C	-0.47492200	3.82078400	0.91041200
H	-1.17311100	-2.17564000	-3.37072000	H	-1.11771900	3.38990800	1.66913900
C	0.02076300	1.49658300	0.00499500	H	-0.54628500	-5.25121200	1.91681300
				H	0.39934500	-3.77367300	1.65147100
				H	-2.88885900	-1.76017600	-3.33871900

H	-1.72070900	-0.77244700	-2.45646800			
H	2.21174900	1.08930000	-4.07331900	Cu	-0.12029500	0.02931700 -0.92471700
H	1.13601500	0.25300500	-2.94180900	N	2.41603500	-0.43167900 0.48605000
H	5.44019700	-2.67714600	0.51643000	N	-1.34532200	2.41559900 -2.10245700
H	3.70755800	-2.49956300	0.85017700	N	-2.58886600	0.65040900 -2.40618100
C	-5.15148000	-4.14091200	0.42131500	O	4.89073100	-0.51897600 0.91599400
H	-5.85761200	-3.34633700	0.16194200	O	4.00131700	-1.89544000 -0.69557200
H	-5.48641000	-5.05306300	-0.08873100	B	3.73676000	-0.91864000 0.25433600
H	-5.22706000	-4.32447000	1.49707100	C	-1.44871100	1.09903200 -1.84257800
C	6.63693100	1.55046900	-1.82527200	C	-2.48658200	2.95617200 -2.87469100
H	6.49402300	2.35585400	-1.09412100	H	-3.03367000	3.69455900 -2.27896100
H	7.57730900	1.05001400	-1.57620000	C	-3.31855800	1.69289100 -3.16393000
H	6.75015700	2.01928100	-2.80756200	H	-4.35179800	1.77459400 -2.81438600
H	0.15463900	-4.04297000	-3.04837200	C	-3.03516700	-0.71463000 -2.40909000
H	2.22135900	-2.97183600	-3.59287800	C	-4.01163400	-1.11708800 -1.48014900
C	2.19033700	1.26828700	0.89670800	C	-4.46738200	-2.43846700 -1.53191800
Br	1.71760900	-1.69226900	2.59381800	H	-5.22646000	-2.75702300 -0.82106700
C	2.28484400	1.85036400	2.22569000	C	-3.97558800	-3.35622200 -2.46569300
C	2.45255800	3.16781100	2.46484800	C	-3.00721900	-2.92033200 -3.37517000
H	2.50023000	3.85791200	1.62345900	H	-2.61651400	-3.61802200 -4.11225900
H	2.24551700	1.14616200	3.05442600	C	-2.52476100	-1.60758800 -3.36901000
H	2.78186500	0.34944000	0.80258200	C	-1.46797300	-1.17842400 -4.35859000
H	2.39485400	1.93726100	0.07115400	H	-1.76381600	-0.28243000 -4.91548300
C	2.61266800	3.76920200	3.82835900	C	-4.54467700	-0.16570300 -0.43613400
H	3.58066100	4.27832800	3.92683700	H	-4.99768500	0.72722700 -0.88154700
H	1.84376900	4.53077900	4.01415300	C	-0.27810400	3.26632700 -1.65083800
H	2.54446700	3.01219800	4.61507700	C	-0.39956500	3.92628600 -0.41438600
				C	-1.60576900	3.72580800 0.47066100
(Z)-2b				H	-2.54090800	3.98733000 -0.03818500
				C	0.64709500	4.75603300 -0.00682800
C	2.33906600	0.44088200	-0.39725200	H	0.57328400	5.25459000 0.95607200
Br	-1.50821200	-0.15929300	-0.12708500	C	1.79268100	4.94076200 -0.78772900
C	1.15871900	0.98081000	-0.06318800	C	1.87224400	4.28074800 -2.01671800
H	0.88768400	1.94289200	-0.49220300	H	2.75492500	4.41501300 -2.63769200
C	0.15457700	0.39656900	0.86034300	C	0.85167400	3.43754400 -2.46830600
H	0.48465100	-0.50564700	1.36863500	C	0.98489300	2.71451200 -3.78767500
H	-0.22048400	1.11877500	1.58454100	H	0.14433200	2.92238500 -4.45988400
H	2.97041500	1.01743300	-1.07267600	C	1.31862000	-1.13681200 -0.23536000
C	2.91567100	-0.87370000	0.03899200	H	1.75737000	-1.46925700 -1.18315000
H	3.13845700	-1.49841100	-0.83453400	C	2.10659900	0.60745100 1.39402900
H	3.86596600	-0.72462900	0.56662500	C	0.82478200	0.70610300 1.97288500
H	2.25253900	-1.44254100	0.69422600	H	0.07676600	-0.04341700 1.74424500
				C	0.51009000	1.74002100 2.85760500
L₁-17₅				H	-0.49239600	1.78764600 3.27570700

C	1.46152900	2.69908800	3.20372000	H	3.48193600	5.29160400	0.50190100
H	1.21809000	3.49665100	3.90004000	H	3.63189100	6.04416300	-1.09194300
C	2.73693700	2.60670800	2.64053000	H	2.55829800	6.74745200	0.12981700
H	3.49768800	3.34170200	2.89394700	C	-4.45774500	-4.78753700	-2.47282300
C	3.05688600	1.58813900	1.74588100	H	-4.38184600	-5.23162200	-3.46973400
H	4.05083700	1.54024700	1.32202400	H	-3.85822200	-5.40626500	-1.79361400
C	6.01810400	-1.12154000	0.23343200	H	-5.49915000	-4.86181200	-2.14534000
C	7.08589300	-1.45891400	1.27263000	H	-2.13347400	3.45180700	-3.78422500
H	7.46503300	-0.53720800	1.72403000	H	-3.34277500	1.43691500	-4.22927800
H	7.93023500	-1.98256900	0.81152600	C	-2.56299700	-2.08399700	3.05381400
H	6.68187400	-2.08241100	2.07176900	H	-1.62983700	-2.56018200	2.75898200
C	6.55607000	-0.08083200	-0.75932100	Br	-3.84473200	1.59603400	3.25623800
H	5.80178600	0.17272100	-1.50961300	C	-2.47090800	-0.93519700	3.74226700
H	7.45353400	-0.43665300	-1.27486900	H	-1.48017600	-0.53708700	3.94945800
H	6.81295500	0.83148000	-0.21332000	C	-3.60289400	-0.14236900	4.27525900
C	5.35152200	-2.36271500	-0.47422200	H	-4.57183400	-0.62913200	4.19850800
C	5.95759500	-2.74821900	-1.82293100	H	-3.43782000	0.20730300	5.29340200
H	5.40640700	-3.59525800	-2.24179000	C	-3.80294200	-2.81612600	2.63406800
H	7.00523100	-3.04804500	-1.71191200	H	-3.80009100	-2.95552400	1.54634600
H	5.90298200	-1.92555000	-2.53833100	H	-3.82107700	-3.82147700	3.07365100
C	5.25952400	-3.59801300	0.43378400	H	-4.73054200	-2.30850800	2.91118200
H	4.82571100	-3.34372200	1.40470700				
H	6.23954400	-4.05722900	0.59759700				
H	4.60538900	-4.33498100	-0.03981500	L₁-TS18₅			
C	0.83638100	-2.38194900	0.45919800	Cu	0.90468900	-0.45738500	0.60685600
C	0.03107000	-3.30480300	-0.24269000	N	-1.90612700	0.69422300	0.57994300
H	-0.24449900	-3.08404600	-1.27213100	N	1.13289800	-2.12877500	-1.99496700
C	-0.41212000	-4.48515500	0.34545500	N	2.67655200	-0.59710100	-1.93901700
H	-1.02234200	-5.17575900	-0.23263800	O	-4.24599100	1.28420900	-0.04140700
C	-0.07095500	-4.79255200	1.66849200	O	-2.52324000	2.26125100	-1.21931400
H	-0.41220700	-5.71607800	2.12809000	B	-2.87255100	1.39465400	-0.19347300
C	0.72184500	-3.89293500	2.38094700	C	1.59497400	-1.07527500	-1.28536300
H	1.00540300	-4.11383100	3.40766200	C	1.88360600	-2.38021900	-3.24845100
C	1.16724400	-2.70666400	1.78770700	H	2.22097100	-3.41897600	-3.29485400
H	1.79401600	-2.02844000	2.35774400	C	3.04110900	-1.38053200	-3.14461900
H	-1.53166300	4.34613300	1.36661400	H	4.00918100	-1.87107900	-2.99708200
H	-1.69143600	2.68506900	0.79752000	C	3.44783200	0.57132000	-1.61460000
H	1.90191400	3.01481900	-4.30079300	C	4.63394700	0.44876000	-0.86584800
H	1.01974900	1.62918700	-3.64233400	C	5.38617600	1.60483900	-0.62850500
H	-1.27134300	-1.97244500	-5.08338000	H	6.29882200	1.51919000	-0.04320600
H	-0.52607800	-0.94350100	-3.85013200	C	5.00884300	2.85488700	-1.12724900
H	-5.31065700	-0.65170100	0.17282000	C	3.84730000	2.93296600	-1.90141900
H	-3.75439600	0.17952700	0.23786300	H	3.54665000	3.89181400	-2.31731200
C	2.92607400	5.80580700	-0.29123400	C	3.05598900	1.80888400	-2.16127000

C	1.81510900	1.93930400	-3.01326000	H	-3.77883800	4.12047900	0.24632800
H	1.83664700	1.26066900	-3.87351300	H	-4.58744300	4.92402200	-1.11691500
C	5.11437600	-0.88436400	-0.34713300	H	-2.81506900	4.83844000	-1.04618600
H	5.36681300	-1.56714500	-1.16786900	C	-0.14602100	2.38550400	1.06002200
C	-0.08295500	-2.85882800	-1.76191700	C	1.00933200	3.08742200	0.65329200
C	-0.02033300	-4.15039500	-1.20209600	H	1.65162500	2.65136500	-0.10517800
C	1.29156500	-4.78897600	-0.81590800	C	1.34547600	4.32314900	1.19900200
H	1.90963400	-5.00607100	-1.69628500	H	2.23950600	4.83441800	0.84980700
C	-1.21880200	-4.84812600	-1.01943400	C	0.54346800	4.90708800	2.18550000
H	-1.18037600	-5.84049500	-0.57596500	H	0.80470700	5.87091800	2.61294100
C	-2.45589800	-4.31339000	-1.39241900	C	-0.60100100	4.22955700	2.60495200
C	-2.47488500	-3.05250400	-1.99306100	H	-1.24234600	4.66691500	3.36659800
H	-3.42412200	-2.62905200	-2.31308900	C	-0.94284400	2.99331900	2.05053300
C	-1.30622900	-2.30994800	-2.19177000	H	-1.84938500	2.49610800	2.37834300
C	-1.38963400	-0.94913700	-2.84057400	H	1.11657300	-5.73792300	-0.30214200
H	-0.52239700	-0.73217300	-3.46989500	H	1.86929700	-4.14181500	-0.15069400
C	-0.48159500	1.07385600	0.42133600	H	-2.28401800	-0.88130400	-3.46646800
H	-0.29250900	1.18448700	-0.65011600	H	-1.45201400	-0.15456600	-2.09084000
C	-2.32759100	-0.29911100	1.51671200	H	1.71874500	2.95784900	-3.39717000
C	-1.84153100	-1.61230600	1.44113400	H	0.90670600	1.71011600	-2.44759600
H	-1.13115300	-1.87390800	0.66438800	H	6.01663000	-0.75592100	0.25661100
C	-2.28169400	-2.59004800	2.33321600	H	4.35742600	-1.37817700	0.26896000
H	-1.88757000	-3.59882800	2.24889600	C	-3.73837300	-5.06666400	-1.13228900
C	-3.22795500	-2.27933700	3.31345700	H	-4.17026800	-4.77168500	-0.16802300
H	-3.57447800	-3.04186000	4.00545100	H	-4.48922600	-4.85946100	-1.90098000
C	-3.72857400	-0.97826300	3.38752500	H	-3.57113600	-6.14743400	-1.10047900
H	-4.46889800	-0.72043800	4.14025900	C	5.82681200	4.08852100	-0.82639300
C	-3.28191600	0.00299300	2.50051800	H	5.70922100	4.84754500	-1.60549300
H	-3.68804500	1.00740500	2.55261500	H	5.51713200	4.54350500	0.12265000
C	-4.86310600	1.97215000	-1.15730900	H	6.89162100	3.85175500	-0.73921300
C	-6.14856200	2.63468500	-0.66362000	H	1.23699300	-2.19554300	-4.11450800
H	-6.85991200	1.86564100	-0.34839100	H	3.12341800	-0.72510300	-4.01681900
H	-6.61699100	3.22385500	-1.45934900	C	0.72238600	0.40101200	3.51099400
H	-5.96004400	3.28837700	0.18972100	H	-0.15110500	0.99981600	3.28567800
C	-5.19401700	0.91029400	-2.21562300	Br	2.23475000	-2.19783500	1.71860300
H	-4.28541700	0.42873800	-2.58714000	C	0.51362900	-0.86899600	4.03991100
H	-5.73484200	1.33586200	-3.06662600	H	-0.50476800	-1.24520300	4.05229300
H	-5.82168100	0.14065200	-1.75769900	C	1.53395700	-1.73949700	4.37135900
C	-3.72502200	2.96991100	-1.60879000	H	2.56128900	-1.41528800	4.46840100
C	-3.66124300	3.24564300	-3.11020800	H	1.31629700	-2.74978100	4.69990200
H	-2.82671200	3.92022200	-3.32313500	C	2.03794300	1.10756100	3.47545300
H	-4.58131800	3.72624000	-3.45958800	H	2.04872400	1.86961200	2.69293900
H	-3.50756100	2.32881300	-3.68231700	H	2.20001200	1.63298900	4.42990300
C	-3.73881900	4.29423300	-0.83225100	H	2.87473300	0.42281100	3.31974700

L₁-19₅

Cu	-0.80193200	0.87859700	0.88383000	C	3.32678200	2.16946200	1.81358400
N	1.64574600	-0.94844700	0.59605000	H	3.25220400	3.24121200	1.65289900
N	-0.67219400	2.18559700	-1.97326100	C	4.30517400	1.64840700	2.66182400
N	-2.31361900	0.75343200	-1.86515300	H	4.99812900	2.30981900	3.17379900
O	3.56899000	-2.32113700	-0.19496000	C	4.38350900	0.26676600	2.84209500
O	1.46531400	-2.85935500	-0.95766700	H	5.13972800	-0.15648500	3.49751800
B	2.22206400	-2.01148600	-0.16126500	C	3.49225800	-0.58258900	2.18647000
C	-1.22278200	1.21389300	-1.20854400	H	3.57381000	-1.65599300	2.31470000
C	-1.42440200	2.46119600	-3.22011300	C	3.76056700	-3.34395500	-1.20532300
H	-1.75063300	3.50471600	-3.24301300	C	4.85004000	-4.29899500	-0.71982600
C	-2.59671600	1.47864900	-3.12685800	H	5.80012100	-3.76243000	-0.64308200
H	-3.56457900	1.98427200	-3.05965500	H	4.98528800	-5.12813400	-1.42244500
C	-3.11749700	-0.40582700	-1.57292500	H	4.61523100	-4.70925900	0.26377900
C	-4.38733000	-0.25498500	-0.97274600	C	4.21805500	-2.63630900	-2.48795300
C	-5.15963900	-1.40087400	-0.76104400	H	3.44854200	-1.95544900	-2.86108000
H	-6.13040100	-1.28886300	-0.28345600	H	4.46267100	-3.35077100	-3.27994600
C	-4.73867800	-2.67233900	-1.16497000	H	5.11258500	-2.04787500	-2.26600500
C	-3.51165600	-2.77705700	-1.82073200	C	2.31871300	-3.97684200	-1.32097500
H	-3.17819000	-3.74915300	-2.17705600	C	1.93125800	-4.45495100	-2.71863600
C	-2.69035600	-1.66415100	-2.04435400	H	0.91273800	-4.85374300	-2.70203800
C	-1.39372800	-1.86222100	-2.79493600	H	2.59985800	-5.25409300	-3.05565500
H	-1.04945200	-0.94575900	-3.27728700	H	1.96421800	-3.64264100	-3.44694500
C	-4.95614100	1.09683200	-0.62083800	C	2.05831200	-5.08684700	-0.29310900
H	-5.34829600	1.59619100	-1.51726600	H	2.32045100	-4.76155100	0.71729700
C	0.62032900	2.79892600	-1.82086500	H	2.62176500	-5.99558200	-0.52542400
C	0.72907200	4.13920300	-1.40387200	H	0.99229400	-5.32915900	-0.29718500
C	-0.47905500	4.98783100	-1.09618300	C	-0.35901200	-1.99190100	1.64201500
H	-0.93135200	5.37113500	-2.02095500	C	-1.63942700	-2.53594800	1.41715100
C	2.00986100	4.70290200	-1.32343400	H	-2.22261600	-2.18817400	0.57108100
H	2.10084600	5.73180300	-0.98302800	C	-2.16541100	-3.51648200	2.25452000
C	3.16075400	3.99632400	-1.67697100	H	-3.15234800	-3.92257700	2.04893600
C	3.01050800	2.68811400	-2.14900100	C	-1.43093400	-3.98018600	3.34989000
H	3.89040200	2.12674800	-2.45418000	H	-1.84102800	-4.74453500	4.00380600
C	1.75896700	2.07545600	-2.23588300	C	-0.16153400	-3.45320500	3.58802500
C	1.64830300	0.67046000	-2.77604200	H	0.42393500	-3.80557500	4.43328100
H	0.91949100	0.60338800	-3.59150800	C	0.36953600	-2.47499800	2.74500700
C	0.17363600	-0.95180900	0.70992400	H	1.36361300	-2.08935400	2.94022100
H	-0.23677600	-1.13385400	-0.27969400	H	-0.19475600	5.85640900	-0.49611000
C	2.50559700	-0.06640400	1.33114000	H	-1.23846000	4.42732500	-0.54781500
C	2.43788900	1.32054100	1.15162700	H	2.61352200	0.33862700	-3.16683200
H	1.69753700	1.73733500	0.47927400	H	1.33732700	-0.03843200	-2.00395800
				H	-1.52268500	-2.62484400	-3.56953900
				H	-0.58780000	-2.20617300	-2.13708600
				H	-5.79168500	0.99025800	0.07619000

H	-4.21148400	1.75292900	-0.16597600	H	3.23068200	-1.93658000	-2.66718600
C	4.53214400	4.61394100	-1.54261100	C	1.11859600	-1.70551900	-2.37654600
H	5.03902400	4.24358900	-0.64301200	C	1.10127700	-0.32678400	-2.99379600
H	5.16978400	4.36394700	-2.39684500	H	0.15781000	-0.10753500	-3.50011300
H	4.47684100	5.70350500	-1.46625200	C	-1.26322000	-4.31375900	-0.85619400
C	-5.59434500	-3.88945700	-0.90423800	H	-2.05652800	-4.31868500	-1.61214600
H	-5.28783600	-4.73536600	-1.52594300	C	-4.17623200	0.28761700	-1.06013300
H	-5.52146200	-4.20705400	0.14320500	C	-5.09732200	-0.34024300	-0.19742800
H	-6.65131900	-3.68538300	-1.10401100	C	-4.95765400	-1.78748900	0.20029300
H	-0.78439800	2.28553900	-4.09181300	H	-4.87467600	-2.44495600	-0.67260900
H	-2.63708700	0.77451200	-3.96441600	C	-6.16386600	0.42225800	0.29215600
C	-0.51381000	0.76564800	2.98326900	H	-6.87746600	-0.05359900	0.96080900
H	0.24916400	-0.00495100	3.02085000	C	-6.34085000	1.76659600	-0.05085800
Br	-2.28738200	2.78688100	1.21135400	C	-5.42570200	2.34764200	-0.93393100
C	0.03598400	2.03769600	3.47781500	H	-5.55746700	3.38489200	-1.23391600
H	1.05652300	2.25447900	3.17577400	C	-4.35074500	1.62409600	-1.46141600
C	-0.57313300	2.89673900	4.31210800	C	-3.43644700	2.26610400	-2.47672000
H	-1.58911500	2.74973500	4.66223400	H	-3.68212700	1.94089600	-3.49616400
H	-0.05897100	3.78473500	4.66823900	C	1.13042200	0.24967400	0.81889900
C	-1.83154800	0.29612600	3.56886500	H	0.88567200	-0.45945100	0.02557300
H	-2.18338300	-0.62139800	3.09305400	C	1.10112400	2.72134400	0.08632600
H	-1.69361300	0.07219100	4.63709700	C	0.07212500	2.86282700	-0.85269900
H	-2.60846000	1.05667900	3.47464700	H	-0.26795200	1.98776600	-1.39583200
L₁-TS20₅				C	-0.50656300	4.11296400	-1.08610100
Cu	-1.15788300	-0.23310700	0.71407100	H	-1.29664200	4.20784600	-1.82433800
N	1.76669300	1.46406600	0.29072100	C	-0.06434800	5.23816000	-0.38995400
N	-3.11841000	-0.48495400	-1.65154200	H	-0.51368000	6.20915500	-0.57669500
N	-1.31158700	-1.64299100	-2.00076100	C	0.96535700	5.10534800	0.54363700
O	3.86671700	2.51757300	-0.48346900	H	1.32146000	5.97342600	1.09116500
O	3.82576200	0.22124100	-0.36061200	C	1.54375100	3.85889800	0.77799500
B	3.12627500	1.39380300	-0.16333300	H	2.35524300	3.75749900	1.49060100
C	-1.90155700	-0.78706600	-1.13194600	C	5.08014000	2.06310000	-1.13505200
C	-3.42473400	-1.19093100	-2.91872500	C	6.21792400	3.00387200	-0.74227900
H	-4.27229800	-1.86967400	-2.77542300	H	6.01399700	4.00649500	-1.12925100
C	-2.11549500	-1.92677700	-3.21213900	H	7.16974800	2.66529200	-1.16501600
H	-2.24785600	-3.00427700	-3.34230500	H	6.32371400	3.07655300	0.34143300
C	-0.04468100	-2.31053400	-1.86780200	C	4.83307400	2.14107100	-2.64824900
C	-0.01607000	-3.62048700	-1.34378100	H	4.02146800	1.47378400	-2.95185200
C	1.21746100	-4.27528600	-1.27799200	H	5.72856900	1.88211800	-3.22142400
H	1.24980600	-5.28060300	-0.86452600	H	4.54264900	3.16331200	-2.90559100
C	2.40092600	-3.68206600	-1.72885900	C	5.21242100	0.58461800	-0.59762400
C	2.32687600	-2.40580100	-2.28922400	C	5.81635500	-0.41119500	-1.58542300
				H	5.82429700	-1.41012400	-1.14018600
				H	6.84963700	-0.14051100	-1.82721100

H	5.24500800	-0.45818100	-2.51419900	H	0.38857800	0.03389100	3.81389900
C	5.94459000	0.49254500	0.74809400	H	-0.58364800	1.38750000	4.38757400
H	5.53679200	1.20178400	1.47285000				
H	7.01605800	0.68524400	0.63635300	L₁-17₆			
H	5.81129800	-0.51203500	1.15737300				
C	1.89833800	-0.41697200	1.89084100	Cu	-0.36986100	0.48341000	-0.81761400
C	1.82872600	-1.81641100	2.03286700	N	2.31769200	-0.38994100	0.03917700
H	1.19073900	-2.38819300	1.36877200	N	-1.78222300	3.06082900	-0.94024900
C	2.55560500	-2.46991100	3.02474700	N	-2.86172300	1.48644800	-1.99491300
H	2.48234500	-3.54999300	3.11504900	O	4.82201100	-0.61279200	-0.02006600
C	3.36973800	-1.74745100	3.90091800	O	3.60696500	-1.34714400	-1.82622600
H	3.93648300	-2.26034600	4.67290100	B	3.55451100	-0.76207500	-0.56805900
C	3.44369500	-0.35754700	3.77811000	C	-1.76731300	1.75189300	-1.25232200
H	4.06770900	0.21720500	4.45748300	C	-2.95732600	3.78277800	-1.47857800
C	2.71525900	0.29914100	2.78849500	H	-3.56663800	4.18310900	-0.66159200
H	2.77900700	1.37950600	2.70337500	C	-3.68360600	2.68518700	-2.27867200
H	-5.82971300	-2.11060300	0.77487000	H	-4.71637700	2.53342000	-1.95106300
H	-4.06265700	-1.95224300	0.81304900	C	-3.17555700	0.21739000	-2.59117000
H	-3.53686600	3.35431400	-2.45467200	C	-4.10365700	-0.62872200	-1.95820700
H	-2.39040800	2.00897100	-2.29999200	C	-4.41871500	-1.84324000	-2.57659900
H	1.90923300	-0.22383100	-3.72387200	H	-5.12953600	-2.50733400	-2.09049500
H	1.24924000	0.44664600	-2.23326800	C	-3.84155400	-2.22942400	-3.78987200
H	-1.04460400	-5.35404000	-0.60132400	C	-2.92044300	-1.36435100	-4.38956800
H	-1.65469300	-3.81634100	0.03867500	H	-2.45533200	-1.65023000	-5.33020500
C	-7.48264900	2.57004800	0.52643800	C	-2.57637900	-0.13729800	-3.81422500
H	-7.20948300	3.00502900	1.49586300	C	-1.56270700	0.75940000	-4.48432800
H	-7.76576000	3.39610100	-0.13270800	H	-1.93468800	1.78236300	-4.60780500
H	-8.36700600	1.94672100	0.69003900	C	-4.72540300	-0.26795100	-0.63065000
C	3.72441900	-4.39673600	-1.59657000	H	-5.22136300	0.70868900	-0.65717300
H	4.18664500	-4.17888500	-0.62574500	C	-0.78575600	3.73851200	-0.15681500
H	3.60403700	-5.48236400	-1.66337600	C	-0.96984200	3.86502900	1.23173600
H	4.42985200	-4.08345200	-2.37217900	C	-2.15958100	3.24997400	1.92817900
H	-3.69644300	-0.47363400	-3.69899400	H	-3.11156000	3.60012700	1.51280700
H	-1.60044600	-1.54271300	-4.10036800	C	0.00365800	4.54710800	1.96511000
C	-0.55792800	1.22142400	2.27451300	H	-0.12088100	4.63754500	3.04123200
H	0.22562400	1.95722200	2.15092700	C	1.14130100	5.09058700	1.36001300
Br	-1.77666700	-2.24041400	2.12520300	C	1.28511500	4.95576700	-0.02331200
C	-1.82910800	1.70425100	1.72228500	H	2.16303500	5.37301000	-0.51092600
H	-1.75522400	2.49371900	0.97900300	C	0.33726400	4.28429600	-0.80182700
C	-3.06337400	1.26990500	2.07594500	C	0.54463200	4.12663000	-2.28946500
H	-3.21151100	0.47258800	2.79526800	H	-0.31898600	4.47364300	-2.86796600
H	-3.94786900	1.71207500	1.63235400	C	1.08211200	-0.84666900	-0.65940900
C	-0.53830400	0.58128600	3.63988000	H	1.35897800	-0.93051800	-1.71588800
H	-1.36459200	-0.10741300	3.80143000	C	2.21339700	0.30256900	1.26796300

C	-5.06799900	-1.86083300	-2.11613900	H	3.21453700	-3.43354200	-3.60232400
C	-3.81400300	-2.03969200	-2.71208600	H	4.97925200	-3.37311600	-3.47221300
H	-3.57003500	-2.99900100	-3.16320000	H	4.04210200	-1.87160000	-3.62029500
C	-2.86319800	-1.01590500	-2.75336200	C	3.72672700	-4.23444700	-1.09787400
C	-1.53091300	-1.24015800	-3.42926900	H	3.61316200	-4.21755100	-0.01060700
H	-1.38647900	-0.55668000	-4.27424900	H	4.56630000	-4.88842000	-1.35327200
C	-4.79635600	1.76842800	-0.94125700	H	2.81350800	-4.66229600	-1.52022200
H	-4.71863100	2.59182800	-1.66031800	C	0.10697400	-2.51085400	0.77141500
C	0.71131500	3.06437100	-1.23193100	C	-0.94265700	-3.22218800	0.14295400
C	0.63948300	4.11548900	-0.29856600	H	-1.40410900	-2.80177600	-0.74810300
C	-0.68380200	4.67250900	0.16548100	C	-1.38206000	-4.45535900	0.62044900
H	-1.28472800	5.05424000	-0.66857000	H	-2.18790700	-4.97233800	0.10459200
C	1.83696800	4.63231700	0.20367100	C	-0.78867800	-5.03322400	1.74600100
H	1.79226100	5.43692900	0.93386400	H	-1.12886700	-5.99491500	2.11901900
C	3.08315200	4.14554200	-0.20208600	C	0.26142700	-4.35682100	2.37279500
C	3.11657000	3.12263800	-1.15300800	H	0.74895200	-4.79782600	3.23925200
H	4.07733500	2.74275900	-1.49327000	C	0.70385800	-3.12183900	1.89712900
C	1.94710700	2.56538300	-1.68006600	H	1.52849700	-2.62306900	2.39526900
C	2.03454800	1.44345800	-2.68794100	H	-0.52693900	5.49969600	0.86255200
H	1.29090600	1.53884900	-3.48476100	H	-1.27841900	3.90690700	0.67455300
C	0.53709900	-1.19352400	0.23080700	H	3.02341500	1.42707100	-3.15525400
H	0.53274200	-1.26747900	-0.85869000	H	1.87672100	0.46867300	-2.21405700
C	2.14673300	0.01578300	1.75968500	H	-1.46052800	-2.26027000	-3.81491900
C	1.18776300	0.12945900	2.78121700	H	-0.69580000	-1.08062100	-2.74138300
H	0.25721300	-0.41611200	2.70507600	H	-5.82454900	1.75418300	-0.56968700
C	1.41775900	0.93604700	3.89713700	H	-4.13038400	2.00248200	-0.10392200
H	0.64778200	1.00579500	4.66055200	C	4.35687500	4.69137500	0.39654300
C	2.61248100	1.63910600	4.03675400	H	5.20696100	4.56638700	-0.28093500
H	2.79249100	2.26020700	4.90944400	H	4.26528200	5.75510300	0.63715200
C	3.57384500	1.52896100	3.02874900	H	4.59733100	4.16501100	1.32831900
H	4.51514100	2.06721200	3.11361300	C	-6.08297200	-2.97982600	-2.10871700
C	3.34602700	0.74230600	1.90267700	H	-5.62979400	-3.92766800	-1.80000400
H	4.10273100	0.67973800	1.13250700	H	-6.91173800	-2.76441500	-1.42873100
C	5.03749300	-1.99777300	-0.91109000	H	-6.50739600	-3.13655900	-3.10797600
C	6.18889400	-2.83196400	-0.35123700	H	-0.32432000	3.21616000	-3.81300500
H	6.89395200	-2.17950500	0.17218000	H	-2.12074400	1.71396400	-4.29520500
H	6.73124300	-3.34138600	-1.15497400	Br	-2.25992500	1.68692100	1.96676100
H	5.83301400	-3.57968100	0.35944700	C	-3.14208100	-1.39617800	4.07120500
C	5.59035700	-0.83139600	-1.74286200	H	-2.77689800	-1.98023600	4.91505900
H	4.78039400	-0.22083900	-2.15146700	C	-2.46145000	-1.51451600	2.89704000
H	6.21346100	-1.18185400	-2.57144800	H	-1.57569600	-2.14090400	2.87497500
H	6.20353100	-0.19569800	-1.09764700	C	-2.84216400	-0.90067000	1.67327200
C	3.91507700	-2.81751100	-1.65844500	H	-3.81596300	-0.44820000	1.56142100
C	4.05145300	-2.87010400	-3.17932300	H	-2.38036500	-1.25220600	0.75827900

C	-4.34243600	-0.54793400	4.33546900	H	0.01622200	-1.25208600	-0.74265400
H	-4.22957300	-0.02875000	5.29431300	C	1.71635400	-0.00601500	1.84424200
H	-4.50368400	0.20448200	3.56149300	C	0.85591800	0.01040800	2.95171200
H	-5.24609400	-1.16799000	4.42548500	H	-0.03979200	-0.59477800	2.95932400
L₁-19₆							
Cu	-1.17665900	0.35018600	0.60516300	C	1.13644100	0.81296600	4.05924800
N	1.45547100	-0.80887900	0.69552100	H	0.44365700	0.81060300	4.89583800
N	-0.17538000	2.47787100	-1.66021200	C	2.28243700	1.60373000	4.09521500
N	-2.00772600	1.37530800	-2.07277700	H	2.49943800	2.22461100	4.95941700
O	3.81767000	-1.57973800	0.41173800	C	3.14154300	1.59313200	2.99371500
O	2.28809400	-2.12111400	-1.21806400	H	4.03410200	2.21350800	2.99365700
B	2.51235600	-1.46385300	-0.01866700	C	2.86084200	0.81041000	1.87757600
C	-0.93879000	1.44770800	-1.24268300	H	3.52396000	0.83555200	1.02246600
C	-0.75869800	3.22075600	-2.80646000	C	4.57398200	-2.25707600	-0.62365500
H	-0.99430300	4.24624400	-2.50623300	C	5.56413300	-3.20377000	0.05426800
C	-2.01243700	2.40225900	-3.13944500	H	6.27946100	-2.62283200	0.64338500
H	-2.92844000	2.99757800	-3.09682500	H	6.12564600	-3.78103300	-0.68800200
C	-2.99663900	0.33177900	-2.09074800	H	5.05987200	-3.89743000	0.72894500
C	-4.28753000	0.57506100	-1.58105100	C	5.33720700	-1.17945400	-1.40542000
C	-5.22598600	-0.46280200	-1.63612800	H	4.65130900	-0.47884600	-1.88820400
H	-6.21988800	-0.28473900	-1.23221400	H	5.98519500	-1.61618600	-2.17139500
C	-4.92975700	-1.70785600	-2.19625800	H	5.96154800	-0.61382700	-0.70827000
C	-3.65775500	-1.89565200	-2.74679100	C	3.44093900	-2.96699300	-1.46991100
H	-3.41996100	-2.84181900	-3.22790400	C	3.68872800	-3.01221000	-2.97686000
C	-2.68332700	-0.89258600	-2.71736000	H	2.83493300	-3.48220000	-3.47360400
C	-1.34964200	-1.12594700	-3.38923300	H	4.58070600	-3.60404200	-3.20765000
H	-1.12206800	-0.33995400	-4.11776500	H	3.81577000	-2.01314400	-3.39750700
C	-4.68502100	1.91658600	-1.01528500	C	3.08345900	-4.36840200	-0.95567900
H	-4.78075800	2.66879700	-1.80880200	H	2.87011300	-4.35693500	0.11629200
C	1.16060100	2.82685300	-1.25230100	H	3.88621100	-5.08676400	-1.14760200
C	1.37992100	3.93518700	-0.41182700	H	2.18107600	-4.71275100	-1.46781300
C	0.24602600	4.76724000	0.13094400	C	-0.22251500	-2.64767600	0.81519500
H	-0.18093800	5.40949000	-0.65109100	C	-1.17450600	-3.41938300	0.11808000
C	2.70183700	4.28865100	-0.11866900	H	-1.67145800	-2.99189300	-0.74924100
H	2.87648300	5.13466400	0.54187900	C	-1.47699800	-4.72291000	0.50731100
C	3.79439500	3.60542400	-0.65713900	H	-2.21400400	-5.29301400	-0.05230200
C	3.54086100	2.54474900	-1.53140800	C	-0.82970300	-5.30067200	1.60194500
H	4.37686300	2.02626600	-1.99523800	H	-1.06183000	-6.31772700	1.90435900
C	2.23888400	2.14176100	-1.84600600	C	0.12898100	-4.55775400	2.29482700
C	2.02023100	1.01524000	-2.82855100	H	0.64971500	-4.99745900	3.14146600
H	1.21824900	1.23944900	-3.53843000	C	0.42947900	-3.25098800	1.90894500
C	0.10315700	-1.27148600	0.34178900	H	1.18270800	-2.69227400	2.45418900
				H	0.60269900	5.42569500	0.92734500
				H	-0.55771600	4.14664600	0.53368900
				H	2.93139300	0.83270300	-3.40567900

H	1.75693100	0.07957500	-2.32647700	C	5.01678200	2.02813700	1.77682600
H	-1.35341000	-2.07996700	-3.92260400	H	5.23281200	2.34692600	2.79392100
H	-0.51827500	-1.14820000	-2.67937800	C	5.31026900	2.88751200	0.71346900
H	-5.65686100	1.84843500	-0.51931300	C	5.02623400	2.45543800	-0.58593400
H	-3.95464200	2.28525000	-0.28942500	H	5.24856400	3.10926800	-1.42609200
C	5.20849200	3.99911500	-0.30114900	C	4.46052000	1.20207000	-0.83855600
H	5.91190000	3.73250300	-1.09585800	C	4.15094800	0.77550000	-2.25424600
H	5.29147000	5.07507900	-0.11980400	H	4.66505100	-0.15363900	-2.52641800
H	5.54057800	3.49029500	0.61245700	C	4.10565200	-0.11243500	2.75599400
C	-5.95141300	-2.82008800	-2.20424000	H	4.45706200	-1.14089800	2.62093800
H	-5.87759800	-3.42755700	-1.29366000	C	1.09917100	-3.37777900	-0.61269100
H	-6.97140000	-2.42697400	-2.24969700	C	0.38316400	-3.87475700	0.49302300
H	-5.80674900	-3.49152500	-3.05603700	C	0.80381300	-3.57385200	1.90954400
H	-0.04189300	3.26417300	-3.63232300	H	1.87191600	-3.76325700	2.06325800
H	-1.96420100	1.92472800	-4.12498200	C	-0.73630700	-4.67740300	0.24336700
Br	-2.10055200	2.37093200	1.64642600	H	-1.29303400	-5.07017200	1.09112800
C	-2.92110200	-0.86016800	4.06832700	C	-1.14939200	-4.99993500	-1.05230800
H	-2.68053300	-1.41120900	4.97818600	C	-0.39253900	-4.52054300	-2.12584200
C	-2.37305800	-1.32085700	2.91883900	H	-0.68168900	-4.78188200	-3.14146300
H	-1.73720200	-2.19889600	2.99926600	C	0.73821600	-3.72093500	-1.93030300
C	-2.58260500	-0.80860600	1.57497000	C	1.56327300	-3.27547700	-3.11564700
H	-3.38384300	-0.08231900	1.47785000	H	1.85210800	-2.22422600	-3.04114200
H	-2.61643100	-1.58309100	0.81166500	C	-1.23377700	0.60345200	-1.13533500
C	-3.85891300	0.29368700	4.24743700	H	-1.02070300	-0.39989100	-0.77217900
H	-3.53221700	0.92179500	5.08489700	C	-3.14931200	2.21534100	-0.98328800
H	-3.91771900	0.93005100	3.36378700	C	-3.93468400	1.99751500	-2.12268500
H	-4.86681500	-0.06438300	4.50326400	H	-3.86676700	1.04878100	-2.64437400
L₁-TS20₆				C	-4.79367600	2.99544000	-2.58273100
Cu	0.89124300	0.05110300	0.28137500	H	-5.39283800	2.81908500	-3.47146200
N	-2.32133100	1.14730700	-0.46930400	C	-4.89316800	4.20755200	-1.89705700
N	2.28016500	-2.59066800	-0.40258700	H	-5.56480200	4.98306200	-2.25383600
N	3.63938300	-0.94489400	0.01474900	C	-4.13315200	4.41240300	-0.74422800
O	-3.88662900	0.96060000	1.43599300	H	-4.21521900	5.34649400	-0.19599700
O	-2.63224800	-0.89589900	0.91109100	C	-3.26582700	3.42075300	-0.28389400
B	-2.90572200	0.41735200	0.65491100	H	-2.67427700	3.56584200	0.61175800
C	2.33314900	-1.26402900	-0.13509700	C	-4.18186600	-0.00291200	2.48980900
C	3.60097300	-3.26091400	-0.36237500	C	-5.69285700	0.00624500	2.72197700
H	3.63758900	-3.96720500	0.47488900	H	-5.99467900	0.98804100	3.09754100
C	4.56572000	-2.08071800	-0.18414100	H	-5.97627100	-0.74220800	3.46938300
H	5.22559800	-2.19510300	0.68101900	H	-6.24963800	-0.18781700	1.80337400
C	4.16905600	0.36754900	0.25646700	C	-3.45395800	0.48139700	3.74916100
C	4.44559500	0.76615100	1.57751000	H	-2.37216200	0.51237500	3.59855800
				H	-3.67510200	-0.16032400	4.60775900
				H	-3.79849000	1.49327600	3.98257600

C -3.60588800 -1.35748300 1.89463600
 C -2.88537200 -2.24254600 2.90875800
 H -2.54187500 -3.15572400 2.41400600
 H -3.56113300 -2.53045800 3.72141100
 H -2.01287000 -1.73277800 3.31940000
 C -4.64253900 -2.17438700 1.11198600
 H -5.15600600 -1.56205700 0.36504800
 H -5.39309000 -2.61608600 1.77460200
 H -4.12716000 -2.98425900 0.58795900
 C -0.95417400 0.77622300 -2.57180900
 C -0.56849700 -0.37391200 -3.29021000
 H -0.51395100 -1.32459200 -2.76878800
 C -0.28145000 -0.31443400 -4.65182800
 H -0.00016100 -1.22036200 -5.18122900
 C -0.36135200 0.90081300 -5.33574500
 H -0.13749200 0.95021100 -6.39739800
 C -0.73150200 2.05224700 -4.63809000
 H -0.79264400 3.00556800 -5.15546900
 C -1.02474700 1.99625400 -3.27689900
 H -1.30740500 2.90632100 -2.76400300
 H 0.25015600 -4.20127300 2.61317900
 H 0.62112700 -2.52484400 2.17155700
 H 2.48642000 -3.86244800 -3.20457900
 H 1.00755000 -3.41446900 -4.04691500
 H 4.46114900 1.54549000 -2.96510800
 H 3.07871400 0.60115100 -2.39090300
 H 4.55890400 0.27970000 3.67030400
 H 3.01906500 -0.15369800 2.90287200
 C -2.38649400 -5.83427900 -1.28753800
 H -2.56139000 -6.53261900 -0.46353600
 H -3.27841300 -5.20069200 -1.37173300
 H -2.31127100 -6.41261800 -2.21343900
 C 5.89212100 4.25849400 0.96549400
 H 6.56639500 4.25502100 1.82749600
 H 6.44990800 4.62339800 0.09795900
 H 5.10002100 4.98766300 1.17576000
 H 3.78039600 -3.82203300 -1.28384500
 H 5.19395800 -1.90910400 -1.06603800
 Br 0.22917800 0.13332100 2.63978100
 C 0.22925700 3.90419300 1.04841300
 H -0.43594500 4.75422200 1.20409500
 C 0.08857600 3.22576600 -0.11530000
 H -0.66750300 3.61130100 -0.79560500
 C 0.82163000 2.06210700 -0.57458800

H 1.76217500 1.90850100 -0.02768600
 H 0.98193200 2.01168300 -1.64685000
 C 1.20261900 3.63532100 2.15569200
 H 1.55796300 4.57673300 2.59259400
 H 0.73578000 3.04749200 2.95567000
 H 2.07123300 3.06343300 1.82005600

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C 0.43510200 -0.71567100 0.39285400
 Br -3.27899400 0.16418000 -0.37361300
 C -0.61036200 0.04525300 0.75901800
 H -0.50212000 1.11775900 0.89991900
 C -1.96244900 -0.50571300 0.99927900
 H -2.00439100 -1.59085900 0.91985900
 H -2.40500800 -0.17394200 1.93798800
 C 1.81803100 -0.28462700 0.15709000
 C 2.77263500 -1.24995500 -0.20897800
 C 2.24224500 1.05234700 0.27873200
 C 4.10011700 -0.89886700 -0.44640200
 H 2.46354400 -2.28739500 -0.30824500
 C 3.56701800 1.40340900 0.04175500
 H 1.53179000 1.82375300 0.55856300
 C 4.50321400 0.43052600 -0.32169500
 H 4.81820000 -1.66312600 -0.72874500
 H 3.87298100 2.44092800 0.13986000
 H 5.53648300 0.70905800 -0.50576400
 H 0.26000000 -1.78269300 0.25311200

L₁-17₇

Cu 0.47594000 -0.64026700 -0.76298800
 N 2.38090300 1.55835400 -0.16036900
 N -1.67003900 -1.67345800 -2.57117100
 N -0.20890800 -3.17279700 -1.96276900
 O 4.45846900 2.96061900 -0.01473600
 O 4.47268300 0.86763600 0.93596000
 B 3.73132000 1.80376200 0.23015000
 C -0.56247100 -1.87689700 -1.83539400
 C -2.15722900 -2.89696600 -3.25065200
 H -3.15464900 -3.16100000 -2.88475000
 C -1.08924800 -3.93914300 -2.87243800
 H -1.50773100 -4.81109700 -2.36096500
 C 0.94031900 -3.78122500 -1.35140300

C	0.78585400	-4.46752900	-0.13285400	H	6.50110200	3.09061000	-1.63078600
C	1.91120100	-5.08129600	0.42584800	C	5.66602100	1.52872000	1.41536800
H	1.80267200	-5.61269300	1.36855000	C	6.80862700	0.51411500	1.43066600
C	3.16652900	-5.02643700	-0.18861900	H	6.58572500	-0.27585500	2.15392400
C	3.28126100	-4.33974300	-1.40096100	H	7.75049300	0.98807700	1.72719000
H	4.24910700	-4.28845600	-1.89428600	H	6.94456300	0.04644900	0.45375600
C	2.18586300	-3.71049200	-2.00061500	C	5.37199500	2.01169500	2.84308600
C	2.35600600	-2.95181300	-3.29506500	H	4.55232900	2.73529000	2.85398000
H	2.20167300	-1.87756500	-3.14305500	H	6.25065800	2.47043300	3.30738500
C	-0.54642100	-4.52585900	0.57506000	H	5.06725700	1.15423900	3.44905200
H	-1.32226300	-4.99379300	-0.04189400	C	1.23976100	0.49010100	1.80236800
C	-2.40108200	-0.44220300	-2.69664500	C	1.06328900	-0.65347800	2.61213900
C	-3.46583300	-0.18135500	-1.81342900	H	1.31020500	-1.62979700	2.19910300
C	-3.80193600	-1.12328900	-0.68286100	C	0.60776400	-0.55899100	3.92405200
H	-4.18134000	-2.08567600	-1.04835200	H	0.50772600	-1.46207100	4.52256900
C	-4.20521600	0.98960000	-2.00106800	C	0.30193700	0.68907700	4.48337000
H	-5.01624200	1.21217400	-1.31192500	H	-0.04563400	0.76582100	5.50982100
C	-3.92314400	1.88412900	-3.03992500	C	0.47342400	1.83231400	3.70204100
C	-2.85361300	1.59585600	-3.89153800	H	0.25823700	2.81277200	4.12094000
H	-2.60610300	2.29038800	-4.69048500	C	0.93754800	1.73644700	2.38591200
C	-2.07528300	0.44374600	-3.73693000	H	1.09044600	2.64208800	1.80729700
C	-0.89433000	0.19274200	-4.64318300	H	-4.57003000	-0.69362400	-0.03702000
H	-0.91459600	-0.80912900	-5.08598500	H	-2.93143000	-1.33941200	-0.05775200
C	1.74833100	0.33145000	0.39884900	H	-0.87134400	0.91989600	-5.45843300
H	2.54548800	-0.41919300	0.44300400	H	0.04619800	0.28304800	-4.08861200
C	1.63136300	2.44097800	-0.97064100	H	1.64194100	-3.27391600	-4.06106800
C	0.22678400	2.49551400	-0.87851700	H	3.36274500	-3.09320800	-3.69605300
H	-0.28435200	1.86178700	-0.16359000	H	-0.46806700	-5.10448300	1.49851100
C	-0.51506000	3.36456100	-1.68068600	H	-0.90806400	-3.52705100	0.83896900
H	-1.59617500	3.37669200	-1.57867600	C	-4.76320600	3.12502700	-3.23209200
C	0.11652500	4.20557200	-2.59628300	H	-4.95746600	3.62133900	-2.27593400
H	-0.46117900	4.88510000	-3.21661000	H	-4.27192900	3.84206900	-3.89575900
C	1.50902800	4.15649000	-2.69912100	H	-5.73692500	2.87958600	-3.67419200
H	2.02465700	4.79588400	-3.41169900	C	4.37234400	-5.66826200	0.45601600
C	2.25728900	3.28819300	-1.90809800	H	4.09624800	-6.56499400	1.01900600
H	3.33473900	3.26868600	-2.00449200	H	5.12202900	-5.95077400	-0.28900900
C	5.82883900	2.70929800	0.38153000	H	4.85464200	-4.97808700	1.15915000
C	6.40949600	4.00216700	0.95224900	H	-2.22761400	-2.72990100	-4.32999000
H	6.44742400	4.76466400	0.16864000	H	-0.52073800	-4.29702800	-3.73803900
H	7.42861300	3.84491700	1.32161800	C	-3.31089500	1.02852300	2.69082000
H	5.79719300	4.38962200	1.76823600	Br	-3.53803500	-2.86270500	2.90830100
C	6.59829400	2.29869200	-0.88256100	C	-3.96222100	-0.00108700	3.26207200
H	6.19245400	1.37696400	-1.30940400	H	-5.04901700	-0.04465500	3.27912700
H	7.66287400	2.14716300	-0.67907000	C	-3.25087900	-1.12204000	3.91335800

H	-2.17053700	-0.99062300	3.93277000
H	-3.63319300	-1.36570100	4.90418100
H	-2.22163400	1.01112400	2.70562600
C	-3.90057300	2.20778800	2.04409300
C	-3.03531200	3.17395200	1.49846000
C	-5.28861700	2.42347000	1.93649700
C	-3.53392000	4.31180700	0.86505400
H	-1.96173500	3.02469300	1.57382000
C	-5.78652700	3.55939600	1.30461900
H	-5.98418100	1.70122200	2.35323800
C	-4.91222800	4.51013300	0.76577400
H	-2.84333300	5.04070000	0.45116800
H	-6.86054900	3.70902600	1.23602900
H	-5.30462900	5.39942500	0.28066200

L₁-TS18₇

Cu	-0.91995300	-0.06130900	0.42471500
N	2.01283200	0.95923900	-0.13652600
N	-3.43095800	-1.21580600	-0.99998600
N	-1.68792000	-2.40979300	-1.52416200
O	4.32125400	1.91582200	0.11596000
O	4.10660900	-0.36396500	0.13073400
B	3.45388700	0.84576300	0.05718900
C	-2.08527700	-1.29983900	-0.85427600
C	-4.01002000	-2.28414400	-1.84867500
H	-4.82528900	-2.79328500	-1.33011100
C	-2.80608300	-3.19493400	-2.09608900
H	-2.89183500	-4.15465000	-1.57649200
C	-0.34424300	-2.84475600	-1.80052200
C	0.25645300	-3.84520600	-1.00785200
C	1.56959100	-4.22308200	-1.30813000
H	2.04676100	-4.97566900	-0.68475700
C	2.28117600	-3.67076500	-2.37734000
C	1.62052300	-2.75911600	-3.20304000
H	2.13418000	-2.35638100	-4.07307900
C	0.30589400	-2.35166400	-2.95026200
C	-0.39675700	-1.47649500	-3.96265800
H	-1.17979600	-0.86318200	-3.51544500
C	-0.48933000	-4.54741800	0.09902800
H	-1.23317600	-5.24076800	-0.31516000
C	-4.28841700	-0.13135000	-0.61101600
C	-5.21772500	-0.31686900	0.43142700
C	-5.32488300	-1.61793100	1.18788400

H	-5.82098800	-2.39015200	0.58561400
C	-6.06538100	0.74956200	0.75725800
H	-6.77514900	0.61623000	1.57047300
C	-6.03094900	1.96810500	0.07458600
C	-5.13106500	2.09960600	-0.98833300
H	-5.11101000	3.02593000	-1.55811300
C	-4.26357700	1.06551800	-1.35534600
C	-3.33501200	1.24827400	-2.53157900
H	-3.37479700	0.39407800	-3.21614300
C	1.20962400	-0.13379400	0.38286600
H	1.11241400	-0.97263900	-0.31792800
C	1.58423300	1.73335800	-1.25281400
C	0.62129200	1.25040800	-2.15274600
H	0.17832800	0.27857400	-1.98660700
C	0.25181700	2.00014000	-3.27295000
H	-0.48757100	1.59759300	-3.95966200
C	0.83026400	3.24167500	-3.52610600
H	0.54349800	3.81831000	-4.40067900
C	1.78363900	3.73065900	-2.63024000
H	2.23820400	4.70380300	-2.79628400
C	2.15429900	2.99637400	-1.50765300
H	2.88092200	3.39831600	-0.81571100
C	5.67171400	1.39460300	-0.02161400
C	6.60345600	2.24392100	0.83996000
H	6.62185700	3.26949600	0.45974100
H	7.62612900	1.85365600	0.80864800
H	6.27387700	2.27501300	1.87973500
C	6.05178400	1.53013700	-1.50245800
H	5.38791500	0.93857500	-2.13888600
H	7.08307300	1.21374800	-1.68565900
H	5.95484600	2.57783700	-1.79984800
C	5.49945900	-0.10486900	0.44773100
C	6.35721900	-1.12007800	-0.30673400
H	6.14668300	-2.12537800	0.06967400
H	7.42338900	-0.92031700	-0.15561900
H	6.14907600	-1.10862000	-1.37832200
C	5.66873600	-0.29831600	1.95927800
H	5.06481100	0.41493300	2.52375700
H	6.71526700	-0.19500300	2.26268700
H	5.32556200	-1.30070100	2.22780100
C	1.62750700	-0.57587400	1.73156900
C	1.59159900	-1.94109900	2.07832300
H	1.27355800	-2.66315100	1.33639500
C	1.97657300	-2.37442200	3.34357500

H	1.93578600	-3.43384200	3.57992900			
C	2.40222100	-1.45886300	4.30878400	L₁-19₇		
H	2.69551200	-1.79857000	5.29792100			
C	2.44671600	-0.10007300	3.98566900	Cu	1.03396400	-0.07289100 -0.62615700
H	2.77974900	0.62469800	4.72443600	N	-1.96504100	0.78147900 0.40126200
C	2.07023300	0.33509500	2.71665100	N	3.62418900	-0.92984700 0.78428400
H	2.13438000	1.38977600	2.47065800	N	2.12570800	-2.42778200 1.26691700
H	-5.92933100	-1.48512300	2.08941600	O	-4.05881100	1.85894500 -0.54145400
H	-4.34165800	-1.99725100	1.48564900	O	-4.23340900	-0.21960000 0.40411800
H	-3.60534100	2.14291000	-3.09892000	B	-3.41112400	0.81182800 0.05121800
H	-2.29400000	1.35918700	-2.21485400	C	2.30592400	-1.22051900 0.67228300
H	-0.86764500	-2.09637700	-4.73738700	C	4.42655900	-1.98186200 1.45149100
H	0.31116100	-0.81268900	-4.46416400	H	5.17214100	-2.38770200 0.76164800
H	0.19782500	-5.14397200	0.70518600	C	3.36234300	-3.01049000 1.84002600
H	-1.01484200	-3.85386700	0.76221400	H	3.55048700	-4.00015000 1.41394300
C	-6.93035400	3.11302400	0.47588800	C	0.89580800	-3.13118300 1.51069000
H	-6.41806100	3.79096300	1.16979000	C	0.50797500	-4.17578900 0.64231400
H	-7.23412700	3.70703100	-0.39168200	C	-0.66950500	-4.87232500 0.93420400
H	-7.83434700	2.75548400	0.97730800	H	-0.97698800	-5.67208000 0.26415900
C	3.72238100	-4.04438000	-2.62522400	C	-1.45431400	-4.57949600 2.05556000
H	3.92976200	-5.07319800	-2.31538400	C	-1.00408600	-3.59060700 2.93070100
H	3.98824700	-3.94498500	-3.68199900	H	-1.57192300	-3.37739000 3.83373900
H	4.39207400	-3.38934300	-2.05446700	C	0.17790400	-2.87635400 2.69544400
H	-4.41357700	-1.84702400	-2.77019800	C	0.68199000	-1.93567800 3.76536300
H	-2.62729600	-3.39359500	-3.15681600	H	1.41505800	-1.22343800 3.38467000
C	-0.93341900	1.66094800	1.65410000	C	1.33599200	-4.56278700 -0.55585100
Br	-1.89299400	-2.19790200	2.49936700	H	2.34195200	-4.88381400 -0.25946300
C	-2.28398300	1.23721300	1.88331400	C	4.29903600	0.27850600 0.40029300
H	-3.07181900	1.58386600	1.22183000	C	5.08742700	0.29719600 -0.76589400
C	-2.62221900	0.42629800	2.94345200	C	5.16146600	-0.88733800 -1.69641300
H	-1.91434000	0.21563400	3.73261000	H	5.69264500	-1.73123500 -1.23843200
H	-3.65268400	0.14845100	3.12437000	C	5.80589900	1.46401100 -1.05458400
H	-0.22897400	1.36830900	2.42969900	H	6.41563300	1.48713800 -1.95497500
C	-0.63824200	2.96821300	1.03781100	C	5.76325800	2.59202600 -0.23078000
C	0.43773100	3.72639300	1.53764700	C	4.98626800	2.53047300 0.93091800
C	-1.44794800	3.55185600	0.04306800	H	4.95598900	3.38807200 1.59938800
C	0.69265300	5.01417400	1.07098500	C	4.25886100	1.38516300 1.27048400
H	1.05788400	3.30838100	2.32421400	C	3.45863700	1.35281700 2.55081700
C	-1.18730200	4.83372500	-0.42928500	H	3.68686400	0.46551400 3.15200400
H	-2.28866900	2.99708200	-0.35943800	C	-1.18494700	-0.22762400 -0.17837700
C	-0.11710100	5.57409500	0.08259100	H	-0.77067500	-0.95237100 0.52664500
H	1.52298100	5.58099800	1.48304900	C	-1.62982300	1.36719800 1.64796800
H	-1.82257600	5.26097300	-1.20021800	C	-0.51270800	0.95777400 2.39408100
H	0.07960700	6.57706500	-0.28514700	H	0.16174400	0.21190500 1.99654600

C	-0.25247600	1.52948500	3.64041100	H	1.45367800	-3.72764600	-1.25708300
H	0.61669000	1.19641300	4.20062400	C	6.52085900	3.84806900	-0.59145100
C	-1.08641200	2.51129100	4.17392200	H	5.89397200	4.53193500	-1.17706600
H	-0.87757300	2.94508700	5.14706800	H	6.84583400	4.39077900	0.30156200
C	-2.18703900	2.93407400	3.42668600	H	7.40594200	3.62242400	-1.19359700
H	-2.83994500	3.71407700	3.80856800	C	-2.74875900	-5.31502900	2.30826800
C	-2.45406600	2.37900400	2.17946900	H	-2.68576700	-6.35904100	1.98580500
H	-3.27931900	2.76014900	1.59177000	H	-3.01765600	-5.30115400	3.36854000
C	-5.49374300	1.59066600	-0.49436200	H	-3.57590000	-4.85356500	1.75478600
C	-6.08323000	1.96724900	-1.85296200	H	4.95614000	-1.56226300	2.31326900
H	-5.95144400	3.03959900	-2.02300300	H	3.25470100	-3.12415800	2.92459100
H	-7.15521100	1.74815800	-1.88757900	C	0.73300600	1.80730000	-1.51133600
H	-5.59108800	1.43232700	-2.66665000	Br	1.57690300	-1.60773000	-2.68250600
C	-6.07391300	2.50080100	0.59524500	C	2.14959900	1.95750200	-1.86692600
H	-5.64893600	2.27752600	1.57704600	H	2.79213100	2.45399100	-1.14405400
H	-7.16160500	2.40392200	0.65969700	C	2.68914900	1.57744600	-3.04231300
H	-5.83738900	3.54052800	0.35210400	H	2.10876400	1.05791100	-3.79569500
C	-5.55857100	0.03968700	-0.14065700	H	3.73951000	1.75111800	-3.25241400
C	-6.58496000	-0.33385800	0.92943200	H	0.11516600	1.49645200	-2.35276200
H	-6.51707000	-1.40561000	1.13519900	C	0.14916100	2.92494900	-0.73741000
H	-7.60229100	-0.11981800	0.58613800	C	-1.08625400	3.48043700	-1.12098900
H	-6.41215000	0.19890600	1.86594200	C	0.82759300	3.54142600	0.33763300
C	-5.72730700	-0.87497200	-1.35872700	C	-1.61830400	4.59569900	-0.47362400
H	-4.97461900	-0.67648600	-2.12327100	H	-1.61912500	3.05794800	-1.96620900
H	-6.72168300	-0.76693800	-1.80258100	C	0.29953500	4.65163700	0.98431500
H	-5.60630100	-1.91293300	-1.03753700	H	1.77878100	3.13758000	0.66905500
C	-1.69198800	-0.79979500	-1.43675200	C	-0.93030400	5.18781400	0.58400200
C	-1.68971200	-2.19616700	-1.61706300	H	-2.57178200	4.99984400	-0.80231500
H	-1.30718200	-2.83111200	-0.82663500	H	0.84402800	5.10141600	1.81019300
C	-2.18401000	-2.76688500	-2.78538400	H	-1.33990000	6.05737500	1.09020000
H	-2.17427100	-3.84693200	-2.89907700				
C	-2.66869500	-1.95965500	-3.81601400				
H	-3.03616400	-2.40614400	-4.73542400				
C	-2.66347200	-0.57081300	-3.66129100				
H	-3.02078200	0.06852600	-4.46398500				
C	-2.18913200	0.00360700	-2.48455200				
H	-2.18611600	1.08130400	-2.38176900				
H	5.70634000	-0.62252600	-2.60646800				
H	4.16190600	-1.23344300	-1.98436600				
H	3.67323000	2.23421600	3.16101500				
H	2.38319600	1.33889000	2.35044700				
H	1.16051400	-2.50592000	4.57232600				
H	-0.13916700	-1.36972100	4.21120000				
H	0.87067100	-5.39840900	-1.08570200				
				L₁-TS20₇			
				Cu	-0.79428600	-0.61630300	0.62908800
				N	1.48002500	1.64904900	0.21802100
				N	-2.55746600	-1.35184200	-1.85840800
				N	-0.66517200	-2.42135200	-1.85256500
				O	3.23626300	3.13128700	-0.70713400
				O	3.72735700	0.89144800	-0.56716200
				B	2.79217500	1.87762900	-0.32800800
				C	-1.35208800	-1.42124600	-1.24428300
				C	-2.78555300	-2.43737400	-2.84155200
				H	-3.50912600	-3.15539300	-2.43885900
				C	-1.38790200	-3.03603200	-2.98919300

H	-1.38151200	-4.12506500	-2.91265400	H	3.44087000	2.08527200	-3.16900000
C	0.70828100	-2.78111200	-1.64441300	H	4.98570900	2.86101200	-3.57616600
C	1.02430400	-4.02669800	-1.06479500	H	3.56545800	3.84930500	-3.18254300
C	2.37508200	-4.34838200	-0.89196300	C	4.97513200	1.55576200	-0.90852300
H	2.62524300	-5.29909400	-0.42646600	C	5.72352400	0.70028700	-1.92837200
C	3.40333600	-3.49205500	-1.29330300	H	6.00255200	-0.25427400	-1.47309800
C	3.05486100	-2.29776700	-1.92899700	H	6.64252300	1.19990900	-2.25252900
H	3.83693700	-1.63144100	-2.27949700	H	5.11416400	0.49313800	-2.80999300
C	1.72129000	-1.92942800	-2.12822100	C	5.79927300	1.66836000	0.38106600
C	1.39890800	-0.65511500	-2.87555800	H	5.30255900	2.30485000	1.11770900
H	1.11208500	0.15973400	-2.20374100	H	6.79625200	2.07516600	0.18586500
C	-0.03579300	-5.02667900	-0.67346100	H	5.90620700	0.67390200	0.82122200
H	-0.34447100	-5.62885700	-1.53914600	C	2.13186000	-0.16260400	1.77079900
C	-3.60852700	-0.39304500	-1.66029700	C	2.30307500	-1.54803900	1.94699500
C	-4.63731100	-0.65085200	-0.73554500	H	1.69437900	-2.23903200	1.37305800
C	-4.66602800	-1.91266800	0.09091800	C	3.23102500	-2.04180200	2.85993900
H	-4.92362400	-2.77983100	-0.53146100	H	3.34350800	-3.11590500	2.97831300
C	-5.67775500	0.27946100	-0.63505800	C	4.01418500	-1.16622000	3.61736900
H	-6.46891500	0.09554600	0.08747700	H	4.74282100	-1.55318200	4.32434600
C	-5.73363300	1.42582400	-1.43122000	C	3.84601200	0.21045300	3.46160700
C	-4.72459800	1.62139700	-2.37866000	H	4.44107700	0.90261900	4.05157700
H	-4.76947100	2.48796500	-3.03487600	C	2.90966300	0.70596800	2.55459900
C	-3.66143900	0.72372100	-2.51790600	H	2.78567600	1.77842400	2.44380600
C	-2.63532600	0.93587200	-3.60795900	H	-5.42711500	-1.84039700	0.87190300
H	-2.72388600	0.17573300	-4.39429000	H	-3.70582500	-2.13020600	0.56711100
C	1.15705700	0.32276100	0.75935500	H	-2.77384400	1.90981700	-4.08443200
H	1.11561600	-0.42440600	-0.04340600	H	-1.61007800	0.88701700	-3.23321500
C	0.51152500	2.67364000	-0.05069900	H	0.57309700	-0.79560400	-3.57976800
C	-0.60696800	2.43980300	-0.85819400	H	2.27076500	-0.31895200	-3.44245800
H	-0.79654500	1.43703300	-1.22407400	H	0.35245100	-5.72049500	0.07661100
C	-1.48808700	3.47864000	-1.16364200	H	-0.91213000	-4.53659300	-0.24706200
H	-2.36442000	3.27185800	-1.76870800	C	-6.84545100	2.43275500	-1.25899800
C	-1.25538400	4.76834800	-0.68569400	H	-6.98831400	3.03431300	-2.16153400
H	-1.93810100	5.57616300	-0.93304300	H	-7.79579800	1.94491500	-1.02055600
C	-0.14136000	5.00864800	0.12166700	H	-6.61946700	3.12211200	-0.43599600
H	0.04904000	6.00585600	0.50872700	C	4.84971200	-3.83681800	-1.03122300
C	0.73017200	3.96887400	0.44435700	H	5.50553200	-3.44239300	-1.81382600
H	1.59884300	4.15582600	1.06533700	H	5.18167800	-3.40621700	-0.07833600
C	4.46966900	2.94933500	-1.44809300	H	5.00174300	-4.91876400	-0.97265800
C	5.38759200	4.13432300	-1.15422700	H	-3.18605600	-2.03628700	-3.77602100
H	4.92906300	5.05393400	-1.52908300	H	-0.90197200	-2.75618000	-3.93291000
H	6.35540300	4.01209100	-1.65191000	C	-0.53048400	0.74772500	2.28617000
H	5.55889900	4.25602800	-0.08334100	H	0.04315200	1.66715600	2.23080000
C	4.09950600	2.92718800	-2.93770600	Br	-1.35697300	-2.79478800	1.80475400

C	-0.21023600	-0.00142300	3.53136300
H	-0.61512900	-1.00420500	3.62265700
C	0.47457400	0.53316600	4.54879900
H	0.89019000	1.53606600	4.50519200
H	0.63022000	-0.01886400	5.47109400
C	-2.00180000	1.11072600	2.20702800
C	-3.02902500	0.22989900	2.60951800
C	-2.35481100	2.44847800	1.93832200
C	-4.34048500	0.67889600	2.74775300
H	-2.79380600	-0.80693000	2.81956100
C	-3.66890100	2.89041600	2.07146900
H	-1.58365300	3.15805500	1.66491300
C	-4.67081700	2.00889700	2.48086300
H	-5.10628500	-0.01745700	3.07851400
H	-3.90302200	3.93262100	1.87207500
H	-5.69349100	2.35630900	2.60070100

L₁-17_g

Cu	-1.11260000	0.87895200	0.43959900
N	-1.69762600	-1.98571300	0.07531200
N	-2.31078300	3.32479300	-0.64082300
N	-0.88770100	3.77454800	0.94944000
O	-3.03513700	-4.11209700	0.14539200
O	-2.61318500	-3.01087700	2.11750100
B	-2.43174200	-3.01198400	0.74057200
C	-1.42667200	2.77788900	0.21420300
C	-2.36595400	4.80171600	-0.56279000
H	-1.95557100	5.24367400	-1.47798500
C	-1.50040700	5.09488200	0.67391200
H	-0.73466000	5.85263500	0.48927100
C	0.02022600	3.60055900	2.04926500
C	1.38111300	3.90639000	1.86595900
C	2.24354100	3.76773400	2.95870200
H	3.29707500	4.00284100	2.82588000
C	1.79216700	3.33638800	4.20943200
C	0.43100700	3.05220300	4.35890500
H	0.05808000	2.72610800	5.32715500
C	-0.47266000	3.18011300	3.29923400
C	-1.93249300	2.85204700	3.50455000
H	-2.58999800	3.64167700	3.12568800
C	1.91828200	4.35255200	0.52690700
H	1.41346500	5.25172300	0.15644600
C	-3.06466600	2.60065800	-1.62784400

C	-2.49076300	2.34281600	-2.88588900
C	-1.07610800	2.76013100	-3.20650700
H	-0.90659400	3.82663100	-3.02053300
C	-3.25680200	1.65414100	-3.82887400
H	-2.81684000	1.43165900	-4.79742000
C	-4.55765800	1.22118000	-3.55241100
C	-5.09979400	1.50636500	-2.29650100
H	-6.10986200	1.17665800	-2.06481500
C	-4.37247900	2.19102300	-1.31784000
C	-4.97580000	2.44991400	0.04239300
H	-5.01236100	3.51890300	0.28334600
C	-0.97260200	-1.02368100	0.95267000
H	-1.54975200	-0.98740300	1.88330400
C	-1.57910100	-1.88297100	-1.33143800
C	-0.50296100	-1.18808600	-1.91822400
H	0.25696800	-0.74144000	-1.29021300
C	-0.37880600	-1.08668800	-3.30474200
H	0.47596900	-0.55249000	-3.71126100
C	-1.31740200	-1.67345500	-4.15228200
H	-1.21192400	-1.60585200	-5.23147500
C	-2.39117400	-2.36187000	-3.58106700
H	-3.13732800	-2.83143300	-4.21836000
C	-2.52953500	-2.46150500	-2.19859500
H	-3.36923600	-3.00232800	-1.78384200
C	-3.83210500	-4.77772200	1.15511700
C	-3.78523900	-6.28197200	0.89206300
H	-4.25651600	-6.50151800	-0.07057000
H	-4.32796100	-6.83232500	1.66819300
H	-2.75868000	-6.65051200	0.85483500
C	-5.27065000	-4.26080800	1.00870900
H	-5.32114700	-3.18282800	1.18695100
H	-5.95593100	-4.76029300	1.70057500
H	-5.61419500	-4.45230100	-0.01193400
C	-3.13786800	-4.30535600	2.49034600
C	-4.07556300	-4.12367600	3.68326500
H	-3.50535400	-3.76315500	4.54450600
H	-4.54429700	-5.07357800	3.96208900
H	-4.86072000	-3.39533800	3.47147000
C	-1.94082200	-5.17976000	2.88992100
H	-1.25372600	-5.31415600	2.05005700
H	-2.25629000	-6.16542800	3.24609700
H	-1.39228600	-4.68018700	3.69301700
C	0.40942700	-1.47307600	1.34241600
C	1.08343800	-0.81881300	2.39741400

H	0.59319300	0.01502200	2.89653700
C	2.34930300	-1.21620800	2.81645800
H	2.83053700	-0.69202200	3.63919200
C	3.00246500	-2.28629100	2.19219900
H	3.99004000	-2.59882300	2.51936000
C	2.35534800	-2.94505700	1.14681100
H	2.83580400	-3.78881600	0.65558300
C	1.08129700	-2.54606900	0.72717400
H	0.59368100	-3.08529800	-0.07826400
H	-0.84755300	2.56544600	-4.25708500
H	-0.35281800	2.20552700	-2.59947800
H	-5.99796800	2.06609700	0.08975000
H	-4.39468900	1.96154800	0.83209700
H	-2.15084100	2.71363500	4.56643900
H	-2.20508200	1.92869400	2.98022500
H	2.98411400	4.58445500	0.59976000
H	1.79653400	3.57654300	-0.23614100
C	-5.33472600	0.42932900	-4.57597900
H	-6.40021000	0.39070400	-4.33210900
H	-5.22956600	0.85573900	-5.57905400
H	-4.96351700	-0.60143900	-4.62037400
C	2.75075500	3.16106800	5.36350100
H	3.63459500	3.79550400	5.25025800
H	2.27649800	3.40475800	6.31914900
H	3.09971100	2.12314500	5.43046300
H	-3.39823900	5.14591000	-0.45459100
H	-2.09476200	5.41826200	1.53711600
C	3.53511600	0.49104600	-0.41963000
Br	2.65380900	1.36386100	-2.03196100
C	4.93884500	0.14544000	-0.72896500
C	5.37050500	-1.12586700	-0.80548600
H	4.63876900	-1.91503700	-0.63684900
H	5.61692900	0.98058600	-0.88970800
H	3.42593300	1.25703800	0.34664900
H	2.90888900	-0.36836800	-0.19010000
C	6.73516000	-1.59192200	-1.07904500
C	6.98047600	-2.97671500	-1.10606300
C	7.81817600	-0.72453400	-1.32055900
C	8.25412600	-3.48023500	-1.36516400
H	6.15646600	-3.66161800	-0.92287500
C	9.08985400	-1.22627100	-1.57924800
H	7.66465500	0.35014300	-1.30824200
C	9.31544800	-2.60638100	-1.60299900
H	8.41669600	-4.55416500	-1.38173100

H	9.91081000	-0.53913400	-1.76433100
H	10.30961400	-2.99400600	-1.80563800

L₁-TS18_g

Cu	0.26155400	0.83402000	-0.30478000
N	-1.45932500	-1.56120500	0.21567300
N	-1.74089100	3.08439300	-0.75316900
N	-0.11448500	3.73455900	0.53578700
O	-3.44870300	-3.00203800	0.74383700
O	-2.70680900	-1.52133900	2.33775200
B	-2.51774800	-2.02266200	1.05519800
C	-0.61065500	2.67539200	-0.14499100
C	-2.05477800	4.51609100	-0.53398400
H	-2.00303300	5.06517000	-1.48017900
C	-0.96475700	4.94595500	0.45979200
H	-0.38683400	5.80662400	0.11068000
C	1.03923400	3.71321000	1.38799300
C	2.26439900	4.21237000	0.90618300
C	3.36455600	4.21172300	1.77208200
H	4.31469300	4.59630100	1.40782100
C	3.27691800	3.73703700	3.08462700
C	2.03934500	3.26815600	3.53654600
H	1.94551900	2.91279800	4.56028300
C	0.90876900	3.25417600	2.71262700
C	-0.41774600	2.76728000	3.24649500
H	-1.18118700	3.55314600	3.20930600
C	2.40757600	4.72146600	-0.50803300
H	1.71289300	5.54183800	-0.72067400
C	-2.61359800	2.27870300	-1.56215400
C	-2.43653200	2.25110100	-2.95869000
C	-1.31080800	2.99882900	-3.62956800
H	-1.34064700	4.07237100	-3.40834400
C	-3.33273600	1.49633500	-3.72025100
H	-3.19762000	1.45929200	-4.79863400
C	-4.38898000	0.78875200	-3.13838400
C	-4.55119300	0.86223900	-1.75297100
H	-5.37678600	0.33139400	-1.28418800
C	-3.67753800	1.59770000	-0.94504000
C	-3.88154900	1.62833600	0.55164800
H	-3.66594900	2.61062500	0.98193400
C	-0.42364200	-0.74004900	0.88817000
H	-0.94174500	-0.10423200	1.60869100
C	-1.29841100	-1.96891900	-1.13494400

C	-0.03410800	-1.95867600	-1.74994300	H	-0.79959600	1.92250200	2.66626500
H	0.83434500	-1.63715800	-1.18957600	H	3.42023300	5.09617700	-0.67958400
C	0.12071100	-2.35289400	-3.08010500	H	2.20739700	3.92525000	-1.23330000
H	1.11168100	-2.32015300	-3.52385600	C	-5.30965700	-0.05596500	-3.98560200
C	-0.97240100	-2.78102100	-3.83014300	H	-6.28101100	-0.20170700	-3.50350200
H	-0.84815000	-3.09344600	-4.86298200	H	-5.48024500	0.39554300	-4.96798700
C	-2.23235500	-2.79735200	-3.22656300	H	-4.87201300	-1.04749700	-4.15406700
H	-3.10189400	-3.12630500	-3.79108200	C	4.49045900	3.71666700	3.98417900
C	-2.40064500	-2.38958800	-1.90586400	H	5.17482300	4.53810900	3.75158100
H	-3.38692100	-2.40388600	-1.46291700	H	4.20903800	3.79618600	5.03843900
C	-4.42457300	-3.04551300	1.81359200	H	5.05312200	2.78205900	3.86713200
C	-4.85242400	-4.49889600	2.01326100	H	-3.06748900	4.62818900	-0.13433000
H	-5.36438500	-4.85707700	1.11527800	H	-1.36704900	5.19028800	1.45001300
H	-5.54405600	-4.59196100	2.85741300	C	3.11653500	0.50162700	0.09718300
H	-3.99375100	-5.14844800	2.19098600	Br	1.82728400	1.32542900	-2.25631800
C	-5.62641700	-2.20115400	1.36755100	C	4.04562900	-0.33946600	-0.52935900
H	-5.33867700	-1.15750600	1.21433300	C	4.05125400	-1.70161300	-0.33131400
H	-6.44028700	-2.23414200	2.09840900	H	3.30306500	-2.11292000	0.34303300
H	-6.00237900	-2.59291900	0.41807500	H	4.77561400	0.12156200	-1.18856400
C	-3.62897200	-2.40651800	3.01760300	H	3.27011000	1.57061800	0.12226400
C	-4.47101100	-1.57982200	3.98813700	H	2.40405700	0.08296500	0.79716000
H	-3.82566400	-1.15514500	4.76276700	C	4.96645400	-2.65842800	-0.91640800
H	-5.22463600	-2.20327500	4.48081400	C	4.89393700	-4.00498600	-0.49457600
H	-4.97716300	-0.75594000	3.48179100	C	5.92705100	-2.31730000	-1.89643300
C	-2.78413600	-3.42825300	3.79189300	C	5.74653100	-4.96838300	-1.02284700
H	-2.16582200	-4.02314700	3.11435300	H	4.15878300	-4.27676300	0.25737400
H	-3.40749400	-4.10543500	4.38398400	C	6.77623800	-3.28269100	-2.42186700
H	-2.11450400	-2.89155700	4.46936000	H	5.99547800	-1.29583100	-2.25570600
C	0.59413800	-1.52897400	1.62411500	C	6.69196400	-4.61103800	-1.98769400
C	1.34939200	-0.92222800	2.65881400	H	5.67482700	-5.99810300	-0.68535000
H	1.16028100	0.12083400	2.90296300	H	7.50508300	-3.00476900	-3.17756600
C	2.30797700	-1.62890800	3.38003600	H	7.35767700	-5.36183800	-2.40329300
H	2.86092600	-1.12674500	4.17027900				
C	2.55419800	-2.97798200	3.10394400				
H	3.29618300	-3.53244800	3.67100300				
C	1.80936800	-3.60293700	2.09908900				
H	1.96298300	-4.65928300	1.88828200				
C	0.85376500	-2.89525100	1.36791500				
H	0.28025600	-3.40724900	0.60314600				
H	-1.37095700	2.88541200	-4.71508000				
H	-0.33524200	2.62332300	-3.30193100				
H	-4.91585000	1.37384600	0.80102200				
H	-3.23257600	0.90497400	1.05733800				
H	-0.32237700	2.44895200	4.28767100				
				L₁-19₈			
				Cu	0.56306600	0.96172400	-0.45661700
				N	-0.69523700	-1.48840800	0.38100900
				N	-2.33469300	2.20375400	-1.23709100
				N	-1.09109900	3.36473500	0.12437100
				O	-2.21581600	-3.32353700	1.15882100
				O	-1.97739200	-1.46082300	2.48425500
				B	-1.62767600	-2.08343700	1.29584700
				C	-1.22652100	2.15448900	-0.46933200
				C	-2.99712100	3.53262400	-1.23527400

H	-2.99107100	3.95439500	-2.24449500	H	-1.99048000	-5.25962400	2.95089700
C	-2.13827500	4.34085900	-0.25349000	C	-4.53857500	-3.22876600	1.76864200
H	-1.69035900	5.22443900	-0.71662900	H	-4.63445400	-2.19365800	1.43263200
C	-0.13069000	3.70792400	1.13735600	H	-5.29166200	-3.41617600	2.54007800
C	0.98204100	4.51045900	0.80975900	H	-4.74962800	-3.88172700	0.91717200
C	1.88673000	4.83325100	1.82706400	C	-2.59648500	-2.46512700	3.33120400
H	2.75431100	5.43928300	1.57621900	C	-3.67940600	-1.78904400	4.17015400
C	1.70617600	4.41211000	3.14766400	H	-3.21845600	-1.05637600	4.83896700
C	0.56072800	3.67072600	3.45016300	H	-4.20993400	-2.52124200	4.78780700
H	0.37636800	3.37166500	4.47972200	H	-4.40696400	-1.26613400	3.54704300
C	-0.37373400	3.31630800	2.46985900	C	-1.49088700	-3.01441400	4.24377100
C	-1.61993300	2.56150600	2.87374200	H	-0.68905900	-3.47704700	3.66243100
H	-2.50483200	2.91838900	2.33955500	H	-1.87870800	-3.74937600	4.95560200
C	1.19889600	5.04785200	-0.58409100	H	-1.05403500	-2.18543300	4.80689300
H	0.51134400	5.87644900	-0.79854100	C	1.23219400	-1.03939200	1.89268900
C	-3.03282800	1.10984100	-1.86091800	C	1.69219900	-0.27622200	2.98752300
C	-2.98234100	0.93303600	-3.25637100	H	1.29005100	0.72239800	3.14130800
C	-2.18568300	1.84495800	-4.15453000	C	2.63829600	-0.77873500	3.87681100
H	-2.69187200	2.81146600	-4.28218600	H	2.96813200	-0.16763800	4.71291600
C	-3.74207200	-0.10087800	-3.81616400	C	3.15321600	-2.06778200	3.70515000
H	-3.69285100	-0.25398800	-4.89167200	H	3.88703000	-2.46365200	4.40137800
C	-4.56421900	-0.92599300	-3.04617800	C	2.70069000	-2.84288100	2.63638300
C	-4.63921100	-0.68179000	-1.67181100	H	3.08219500	-3.85064900	2.49494300
H	-5.30523000	-1.28437700	-1.05828000	C	1.75598900	-2.33731100	1.74017700
C	-3.89160100	0.32977500	-1.06170300	H	1.41143200	-2.96178900	0.92387900
C	-4.04726200	0.59126700	0.41764100	H	-2.08080600	1.40444500	-5.14952000
H	-4.19422500	1.65516900	0.63139000	H	-1.18635000	2.03529000	-3.75691500
C	0.17810200	-0.47773500	1.00070300	H	-4.91832100	0.05734500	0.80742500
H	-0.44818900	0.19073500	1.58567500	H	-3.17378000	0.26615600	0.98916000
C	-0.41933600	-2.05247400	-0.89772600	H	-1.80267800	2.68239000	3.94511700
C	0.85291000	-1.96349000	-1.48298300	H	-1.54476600	1.48664000	2.67827600
H	1.65958300	-1.46462700	-0.96304300	H	2.21391200	5.44035600	-0.68819700
C	1.10176600	-2.52548900	-2.73684800	H	1.05059000	4.27979300	-1.34811900
H	2.09877300	-2.44116400	-3.15964500	C	-5.34423200	-2.05331000	-3.67943900
C	0.09533700	-3.19216700	-3.43151000	H	-6.25570900	-2.27803700	-3.11694400
H	0.29247300	-3.63201600	-4.40465400	H	-5.62886500	-1.81556500	-4.70890000
C	-1.17467500	-3.27813400	-2.85606800	H	-4.74643600	-2.97277800	-3.71269600
H	-1.97797700	-3.78519900	-3.38458600	C	2.72075000	4.74919400	4.21438300
C	-1.43663500	-2.71084500	-1.61225900	H	3.15612600	5.74040200	4.05431100
H	-2.43131200	-2.77467600	-1.19211000	H	2.27412100	4.73061700	5.21283300
C	-3.12047100	-3.52039900	2.27648700	H	3.54797900	4.02864400	4.21171800
C	-3.01901400	-4.98026100	2.71771500	H	-4.03895900	3.43423300	-0.91386700
H	-3.36942000	-5.63061100	1.91121000	H	-2.69023900	4.66698700	0.63540200
H	-3.64251200	-5.16661900	3.59856800	C	2.56353500	1.05249300	0.06297200

Br	1.15875400	1.92240500	-2.66326400	H	-0.08842000	5.64554300	-0.68370600
C	3.47058600	0.25742700	-0.72809600	C	-3.54015400	1.51891600	-0.66517700
C	4.22123100	-0.76272400	-0.22986600	C	-3.77820200	1.62340500	-2.04887900
H	4.14171300	-0.98447400	0.83218600	C	-3.10429500	2.67339300	-2.89492500
H	3.52742200	0.51772600	-1.78170800	H	-3.24664000	3.68076500	-2.48726400
H	2.54132700	2.10784800	-0.20712500	C	-4.66208300	0.70914500	-2.63400900
H	2.59930000	0.87806000	1.13293700	H	-4.84277800	0.77408100	-3.70429800
C	5.16357200	-1.59716400	-0.97131300	C	-5.32436900	-0.26861200	-1.88713200
C	5.92097200	-2.55464400	-0.26688000	C	-5.08240600	-0.32568100	-0.51064600
C	5.35748700	-1.50005100	-2.36604100	H	-5.60542000	-1.06517100	0.09134700
C	6.83443000	-3.37774400	-0.92114300	C	-4.19620300	0.55333200	0.12119900
H	5.78062400	-2.64623700	0.80717800	C	-3.95555200	0.43810600	1.60889300
C	6.27014600	-2.32263000	-3.01793500	H	-3.80908400	1.41187300	2.08390300
H	4.78712800	-0.77771400	-2.94143600	C	0.45663300	-0.74762100	0.90283700
C	7.01491000	-3.26535200	-2.30098800	H	-0.15780200	-0.12980600	1.55776000
H	7.40574100	-4.10784000	-0.35442900	C	-0.27199300	-1.80124400	-1.33250600
H	6.40221700	-2.23072000	-4.09246700	C	0.94723600	-2.07038700	-1.96621200
H	7.72608900	-3.90574200	-2.81471400	H	1.86515400	-2.09428500	-1.39470900

L₁-TS20₈

Cu	0.04537700	1.12260600	-0.41246800	H	1.94890200	-2.48364300	-3.81740100
N	-0.39118300	-1.61913500	0.08827700	C	-0.17677200	-2.25868500	-4.10466700
N	-2.70228400	2.48971800	-0.01737600	H	-0.13768000	-2.42888100	-5.17660800
N	-1.03234700	3.51052700	0.93124600	C	-1.39435400	-1.99615000	-3.47567500
O	-1.77620100	-3.66753300	0.33405300	H	-2.31212800	-1.95518100	-4.05550300
O	-1.60460500	-2.25761500	2.14658500	C	-1.44239100	-1.76104000	-2.10353700
B	-1.25805900	-2.48934400	0.82546800	H	-2.38686300	-1.53247400	-1.62120500
C	-1.38844300	2.38583900	0.26672900	C	-2.64936100	-4.22690900	1.34699200
C	-3.32113200	3.74758000	0.46625400	C	-2.46670200	-5.74444000	1.34724000
H	-3.75052300	4.30605300	-0.37099700	H	-2.79365100	-6.15103400	0.38599600
C	-2.13861000	4.47389800	1.12462100	H	-3.06758900	-6.21072000	2.13524100
H	-1.90567400	5.42814100	0.64156400	H	-1.42191900	-6.02446700	1.49181400
C	0.27434000	3.79098900	1.45564600	C	-4.08756100	-3.87528900	0.94733400
C	1.18274800	4.55299500	0.69606500	H	-4.23636500	-2.79342100	0.92072100
C	2.44046500	4.81831100	1.25085400	H	-4.81935200	-4.31420300	1.63258900
H	3.15193700	5.40078000	0.67018300	H	-4.27789900	-4.26430400	-0.05681000
C	2.80785000	4.35911300	2.51933000	C	-2.16227200	-3.49588300	2.66495700
C	1.87031700	3.62720000	3.25569000	C	-3.26777400	-3.15055900	3.66093600
H	2.12990200	3.27865500	4.25287300	H	-2.83950200	-2.60865800	4.50930500
C	0.59985000	3.33770600	2.74808600	H	-3.74241900	-4.05905200	4.04626600
C	-0.39625600	2.56429700	3.58079100	H	-4.03754500	-2.52049000	3.21197000
H	-1.28823600	3.16157900	3.80460300	C	-1.02172100	-4.22949900	3.38325500
C	0.83688200	5.05860200	-0.68336700	H	-0.20464000	-4.46439300	2.69649800
				H	-1.36709600	-5.15730500	3.84924800
				H	-0.61996400	-3.57878300	4.16462400

C	1.49320700	-1.44709200	1.70240900
C	1.93924000	-0.88473000	2.91760300
H	1.51853800	0.06195000	3.24789000
C	2.89235100	-1.52319300	3.70447000
H	3.21140400	-1.06894500	4.63869200
C	3.42751100	-2.75306300	3.30423300
H	4.16821800	-3.25511900	3.91989900
C	2.98745200	-3.33234300	2.11458400
H	3.38683900	-4.29101700	1.79525400
C	2.03437900	-2.68858600	1.32150100
H	1.68553500	-3.16677500	0.41393100
H	-3.51256300	2.66606100	-3.90895800
H	-2.02379900	2.49639900	-2.95728100
H	-4.80581400	-0.04758900	2.09695900
H	-3.06671000	-0.16554300	1.82404600
H	0.04527600	2.26648000	4.53545700
H	-0.74186500	1.66091500	3.06886200
H	1.63504800	5.70063300	-1.06477100
H	0.70003100	4.22987200	-1.38917600
C	-6.30866400	-1.21211500	-2.53829400
H	-7.33927200	-0.85554600	-2.41632000
H	-6.12092100	-1.30684300	-3.61153700
H	-6.25773800	-2.21170100	-2.09546000
C	4.18728300	4.63074600	3.07165600
H	4.89978600	3.86353300	2.74418100
H	4.57254600	5.59624400	2.73008500
H	4.18854000	4.63149500	4.16574200
H	-4.12976800	3.52314500	1.17012900
H	-2.29659900	4.66680600	2.19116000
C	2.12485200	0.79752600	0.14135800
Br	0.53387600	1.81712000	-2.74351700
C	3.03214500	0.14496000	-0.77093100
C	4.07642100	-0.62618200	-0.37053900
H	4.23476400	-0.76394300	0.69729300
H	2.83577600	0.32537800	-1.82413500
H	1.87409800	1.81767900	-0.17255100
H	2.38198600	0.75939800	1.19144100
C	5.04871500	-1.29442500	-1.23501100
C	6.07093800	-2.06157900	-0.64227500
C	5.01375900	-1.21678500	-2.64352600
C	7.01769100	-2.72685300	-1.41812400
H	6.11085500	-2.13475800	0.44169500
C	5.96063200	-1.88086200	-3.41670800
H	4.24264300	-0.63089500	-3.13360700

C	6.96766000	-2.63950400	-2.81047300
H	7.79518900	-3.31320400	-0.93611200
H	5.91563100	-1.80588400	-4.49968100
H	7.70484400	-3.15548800	-3.41886700

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C	0.49354600	1.71192400	-0.35891600
H	0.84368700	2.59277400	-0.89596300
Br	-2.62568200	-0.50767700	-0.13813300
C	-0.78351600	1.74568700	0.06895300
H	-1.38447100	2.60953100	-0.20503200
C	-1.45994200	0.74923800	0.93132700
H	-0.77658500	0.09360200	1.46554800
H	-2.16724600	1.20909700	1.61914300
C	1.51249500	0.66507600	-0.18152500
C	1.20738800	-0.70843200	-0.12766500
C	2.86424600	1.04984400	-0.10344500
C	2.21966700	-1.65323000	0.03413300
H	0.18217700	-1.03965300	-0.25467300
C	3.87234200	0.10485400	0.06555800
H	3.11870600	2.10480000	-0.16626500
C	3.55253900	-1.25267200	0.13972300
H	1.96480500	-2.70856700	0.06545000
H	4.90768200	0.42605100	0.13311100
H	4.33750000	-1.99267600	0.26447000

L₁-17₉

Cu	-0.46621500	0.61427000	1.10011900
N	-2.57105000	-0.83586200	-0.52145000
N	0.53586200	3.31338400	1.74267800
N	1.83453200	1.75078000	2.53343100
O	-4.62622900	-1.73492200	-1.61635400
O	-4.31961200	-2.13059600	0.63192000
B	-3.79881800	-1.55357800	-0.51600900
C	0.72838700	1.97895700	1.79935400
C	1.51561700	4.08221500	2.54404000
H	1.99735700	4.85204000	1.93493800
C	2.49169000	2.98811100	3.01083100
H	3.48439000	3.08999700	2.56064600
C	2.39840900	0.45684600	2.80499700
C	3.43445600	-0.03135100	1.98897600
C	3.96133100	-1.29451900	2.27984500

H	4.74668300	-1.69168000	1.64158700	C	-6.48937600	-2.91921500	1.34111900
C	3.49466000	-2.06237100	3.35005800	H	-6.08215100	-3.38928100	2.24118200
C	2.48640400	-1.52954300	4.15947900	H	-7.38902100	-3.47125400	1.04816700
H	2.11662700	-2.10980300	5.00162200	H	-6.77409000	-1.89663800	1.59550300
C	1.92286800	-0.27684000	3.90690000	C	-4.91208100	-4.37974000	0.04368300
C	0.81222500	0.25056800	4.78372100	H	-4.16324200	-4.42116900	-0.75200700
H	1.01819700	1.26337600	5.14770100	H	-5.71460300	-5.08516600	-0.19388000
C	3.97483800	0.76646300	0.82646100	H	-4.43083000	-4.70025800	0.97149800
H	4.57191000	1.62268000	1.16586000	C	-1.10000800	-2.13617800	0.99825600
C	-0.55785200	3.97751100	1.09041800	C	-0.91469200	-2.59569500	2.31795000
C	-0.34693500	4.55766600	-0.17483400	H	-1.29981800	-1.99536500	3.14016300
C	0.97465800	4.42700000	-0.89368800	C	-0.27313100	-3.80124800	2.59181400
H	1.81242800	4.80510800	-0.29765200	H	-0.16150700	-4.12678300	3.62365700
C	-1.40927200	5.24369200	-0.77186000	C	0.20282700	-4.60477100	1.55065300
H	-1.25535000	5.69724100	-1.74826200	H	0.68832700	-5.55393300	1.76072300
C	-2.65898300	5.35839800	-0.15405600	C	0.01962200	-4.17388900	0.23501200
C	-2.83034700	4.77438700	1.10433900	H	0.36343600	-4.79261700	-0.59156000
H	-3.79261900	4.85833200	1.60396200	C	-0.61904900	-2.96148600	-0.03737500
C	-1.79729800	4.08434900	1.74733600	H	-0.75829800	-2.65062500	-1.06803500
C	-2.02878600	3.45853300	3.10205500	H	0.96022500	4.98904900	-1.83085500
H	-3.00168500	3.75434100	3.50232000	H	1.20139400	3.38426900	-1.13820100
C	-1.78047400	-0.81739000	0.74069300	H	-2.00801200	2.36474900	3.03736000
H	-2.49385600	-0.65972600	1.55974500	H	-1.26328000	3.75213400	3.82866800
C	-2.12557700	-0.17563700	-1.69613800	H	0.66896500	-0.39536400	5.65358100
C	-1.69873800	1.16378300	-1.67202800	H	-0.13592900	0.29281800	4.23578700
H	-1.72457700	1.71088400	-0.73472200	H	4.62255000	0.14669600	0.20316500
C	-1.28071600	1.80408300	-2.83934200	H	3.17735600	1.15542000	0.18811300
H	-0.96971400	2.84369900	-2.79128900	C	-3.79919000	6.07085400	-0.84179700
C	-1.29064100	1.13042100	-4.06356600	H	-4.34363500	5.38766800	-1.50517600
H	-0.97861700	1.63613800	-4.97328700	H	-4.51864200	6.46700300	-0.11928700
C	-1.72663100	-0.19608300	-4.10122500	H	-3.43990100	6.90206900	-1.45615800
H	-1.74589300	-0.73694900	-5.04396100	C	4.03027300	-3.45092600	3.60280200
C	-2.13383700	-0.84283500	-2.93450300	H	5.01724900	-3.59007300	3.15268900
H	-2.47428600	-1.87131700	-2.97325000	H	4.10929100	-3.66389800	4.67373500
C	-5.87914100	-2.27027400	-1.12516600	H	3.35898800	-4.20215300	3.16898500
C	-6.44499100	-3.22040400	-2.17926700	H	1.00872100	4.58156500	3.37771400
H	-6.68226600	-2.66013400	-3.08854100	H	2.61405300	2.95980300	4.09789500
H	-7.36565900	-3.69600800	-1.82445900	C	2.49062200	-1.54868400	-1.68634000
H	-5.72775600	-4.00010200	-2.44180100	H	1.89236300	-1.98120500	-0.88584000
C	-6.83034000	-1.08166100	-0.92182700	Br	3.31492300	1.89757600	-3.18050300
H	-6.44387200	-0.39282800	-0.16517500	C	1.90550700	-0.54812900	-2.37715200
H	-7.83034700	-1.40646200	-0.61734600	H	0.92316500	-0.21971000	-2.04808500
H	-6.91706500	-0.53356300	-1.86422100	C	2.41173500	0.11823500	-3.59643800
C	-5.44163400	-2.95040600	0.22946000	H	3.17584400	-0.43880300	-4.13349900

H	1.60329000	0.42039700	-4.25817000
C	3.80202000	-2.18820900	-1.87303700
C	4.92572200	-1.53847300	-2.42242700
C	3.95400200	-3.52058100	-1.43927300
C	6.13851000	-2.21281400	-2.56457600
H	4.86393700	-0.49167400	-2.69980200
C	5.16397600	-4.19349000	-1.58935400
H	3.10468400	-4.02420100	-0.98506100
C	6.26162700	-3.54320300	-2.15911700
H	6.99373400	-1.69146700	-2.98566100
H	5.25322200	-5.22400600	-1.25691200
H	7.20786400	-4.06444700	-2.27297900

L₁-TS18₉

Cu	0.99151100	-0.07766700	0.31174100
N	-1.71160700	-1.02740800	-0.93506000
N	2.95209400	1.75418200	-1.33598700
N	1.19227600	2.88455000	-0.75410200
O	-3.82299500	-1.50792500	-2.14660300
O	-3.76326200	0.36004600	-0.80235200
B	-3.06597100	-0.73445000	-1.28115300
C	1.76484500	1.66110300	-0.68562600
C	3.23492100	3.09372300	-1.90215200
H	4.15993500	3.49829900	-1.48059900
C	1.99467700	3.88970000	-1.49353400
H	2.22756500	4.73949400	-0.84645400
C	-0.09818200	3.31180900	-0.28349300
C	-0.19177700	4.05177800	0.91191700
C	-1.45442000	4.51715000	1.29658900
H	-1.53980600	5.07683800	2.22500100
C	-2.59836500	4.29367200	0.52622900
C	-2.45755100	3.60353800	-0.68039200
H	-3.33017400	3.43492600	-1.30412000
C	-1.22129700	3.11218200	-1.10889200
C	-1.11579100	2.38679100	-2.43060100
H	-0.28812100	2.76248000	-3.04201500
C	1.01629100	4.37286100	1.75689700
H	1.69034100	5.07364600	1.24738700
C	3.93309900	0.72673200	-1.53576800
C	5.00463300	0.61341000	-0.62519400
C	5.14133900	1.54572400	0.55455700
H	5.32152200	2.57684200	0.22625900
C	5.96199700	-0.37909000	-0.85665600

H	6.78637900	-0.48156000	-0.15462500
C	5.89590800	-1.23574300	-1.96184400
C	4.85634300	-1.05230600	-2.87667500
H	4.81023800	-1.67970700	-3.76414200
C	3.87802600	-0.06643300	-2.69638400
C	2.84858400	0.17107300	-3.77717800
H	2.63732700	-0.74621900	-4.33235700
C	-1.08807600	-0.25550400	0.16177300
H	-1.11307300	0.80821200	-0.08040200
C	-1.05663800	-2.09938500	-1.61451600
C	0.13480300	-1.88576900	-2.32205400
H	0.56465200	-0.89050800	-2.32937300
C	0.76909200	-2.93502200	-2.98866000
H	1.70146100	-2.75178800	-3.51494100
C	0.20885400	-4.21410500	-2.98790200
H	0.69921300	-5.02919400	-3.51207300
C	-0.99296200	-4.42979900	-2.31136500
H	-1.44631800	-5.41736700	-2.30737700
C	-1.61667900	-3.38579800	-1.62645500
H	-2.55106500	-3.55900600	-1.10508400
C	-5.04902200	-0.78253200	-2.41306500
C	-6.18353200	-1.79382800	-2.56905700
H	-5.99958600	-2.41864000	-3.44793900
H	-7.14404400	-1.28652700	-2.70922300
H	-6.25871300	-2.44909400	-1.69958900
C	-4.84339500	-0.01701600	-3.72796200
H	-4.03809000	0.71742700	-3.63632500
H	-5.75323000	0.50219000	-4.04469900
H	-4.56293700	-0.72866600	-4.50940600
C	-5.15725900	0.15991000	-1.15247400
C	-5.80017500	1.52023000	-1.41504200
H	-5.79015600	2.11384700	-0.49643200
H	-6.84279600	1.40326900	-1.72950300
H	-5.26781800	2.07948000	-2.18679400
C	-5.83229800	-0.51260900	0.05128200
H	-5.39325900	-1.49247900	0.25590500
H	-6.90857200	-0.63611100	-0.10411000
H	-5.67654000	0.10939700	0.93646400
C	-1.71677400	-0.46130100	1.48687200
C	-1.62626200	0.55974000	2.45947600
H	-1.06493000	1.46018100	2.23224500
C	-2.25400700	0.43370700	3.69437600
H	-2.17093100	1.23815500	4.42024400
C	-2.99349000	-0.71328300	3.99966300

H	-3.49089100	-0.80675900	4.96116500			
C	-3.08382500	-1.73752700	3.05476600	Cu	0.97373300	0.31982000 0.55723700
H	-3.64637300	-2.63925500	3.28188700	N	-1.42859800	-1.47985800 -0.46550600
C	-2.45040100	-1.61717800	1.81951500	N	2.45021300	1.54223700 -1.92972900
H	-2.52923400	-2.42123400	1.09701800	N	0.74573100	2.79794600 -1.42999600
H	5.99418300	1.25528400	1.17449300	O	-3.31058500	-2.54963500 -1.66880900
H	4.24761900	1.55510100	1.18778200	O	-3.59697800	-0.37749100 -0.95866500
H	1.90800000	0.55565900	-3.38024800	B	-2.74639300	-1.46693800 -1.01697100
H	3.21871400	0.90498200	-4.50516700	C	1.33280400	1.60770400 -1.16659500
H	-2.03679700	2.50962400	-3.00570400	C	2.70832400	2.76650500 -2.72469300
H	-0.95599700	1.31260000	-2.29166100	H	3.63452600	3.24409200 -2.39057200
H	0.70895700	4.84763700	2.69226400	C	1.46921600	3.61726900 -2.43115600
H	1.58722600	3.47442300	2.00870100	H	1.71962200	4.59647100 -2.01559900
C	6.91944900	-2.32937800	-2.15445800	C	-0.55348400	3.24370400 -1.00711900
H	6.64541100	-3.22775200	-1.58765800	C	-0.67363000	4.28930900 -0.07054500
H	7.00392300	-2.61963400	-3.20570500	C	-1.96134600	4.71011800 0.28283300
H	7.90887800	-2.01701300	-1.80655900	H	-2.06188200	5.50490400 1.01845400
C	-3.95314200	4.77000400	0.99276600	C	-3.11075300	4.15062700 -0.27985100
H	-3.86916600	5.64640200	1.64243000	C	-2.95239600	3.16250500 -1.25556600
H	-4.59959700	5.03132500	0.14924500	H	-3.83006300	2.73631300 -1.73235100
H	-4.46401000	3.98637300	1.56589500	C	-1.69016200	2.70585100 -1.64379700
H	3.36093000	3.02442800	-2.98781500	C	-1.56467800	1.68248900 -2.74900200
H	1.42307400	4.26398900	-2.34929800	H	-0.82716200	1.98798100 -3.49871000
C	1.33319800	-2.16456500	0.80649200	C	0.52708000	4.98962800 0.51599400
H	1.07600900	-2.62002900	-0.14337300	H	0.92932300	5.73305800 -0.18565400
Br	2.15223600	1.08049500	2.89841800	C	3.32836900	0.42055900 -2.11645500
C	2.64812800	-1.59770900	0.83334700	C	4.56254300	0.36876500 -1.43854800
H	3.12430700	-1.43025500	-0.12920300	C	4.99166300	1.45064500 -0.47938400
C	3.35298200	-1.24104300	1.96288800	H	5.29233900	2.35749800 -1.02057500
H	3.05420600	-1.56414800	2.94911600	C	5.41507500	-0.70988500 -1.70325400
H	4.34202300	-0.81174000	1.87303100	H	6.36670800	-0.75881500 -1.17868300
C	0.65228200	-2.79445300	1.94927400	C	5.09056000	-1.71167700 -2.62246600
C	0.62080000	-2.26597500	3.25596800	C	3.87955000	-1.60343800 -3.31343000
C	0.04216000	-4.04623800	1.72294300	H	3.62288900	-2.35069100 -4.06102300
C	0.04542900	-2.99177800	4.29670300	C	2.99369800	-0.54350900 -3.08918100
H	1.01052100	-1.27125400	3.44562400	C	1.74060900	-0.42393400 -3.92672700
C	-0.52317800	-4.77119600	2.76884200	H	1.57395300	-1.33694600 -4.50350200
H	0.03525100	-4.45568400	0.71655900	C	-1.00724000	-0.33651700 0.35591300
C	-0.51713800	-4.24866500	4.06416600	H	-1.16755100	0.58888100 -0.19744500
H	0.02739200	-2.56410600	5.29488200	C	-0.64745200	-2.67313100 -0.62277100
H	-0.96954400	-5.74239800	2.57261700	C	0.59745000	-2.63603200 -1.26224300
H	-0.95823300	-4.81099300	4.88266200	H	0.98483300	-1.68335900 -1.60160500
				C	1.34465100	-3.80093000 -1.43747100
				H	2.31269000	-3.74127500 -1.92626900

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C	0.85053200	-5.02954100	-0.99587500	H	5.84911000	-3.67357000	-2.11995400
H	1.43059600	-5.93707400	-1.13550300	H	5.87100200	-3.31697200	-3.84892300
C	-0.39845300	-5.07930100	-0.37541000	H	7.06838500	-2.57920800	-2.77142200
H	-0.79929100	-6.02856900	-0.03082500	C	-4.48626000	4.59345400	0.15882800
C	-1.14027400	-3.91236300	-0.18748600	H	-4.47451900	5.61723200	0.54450600
H	-2.11743100	-3.96063300	0.28012200	H	-5.20452100	4.54891800	-0.66595000
C	-4.55689900	-2.09844000	-2.25544100	H	-4.86819200	3.94711700	0.95878000
C	-5.56135400	-3.24800900	-2.19502300	H	2.81745800	2.51564900	-3.78447400
H	-5.20790300	-4.07593000	-2.81643200	H	0.83701400	3.77298300	-3.31290400
H	-6.53985200	-2.93411900	-2.57377700	C	1.47305900	-1.42368800	1.71650100
H	-5.68446700	-3.62063300	-1.17664400	H	0.85781300	-2.14049700	1.18613300
C	-4.26219300	-1.73401300	-3.71727400	Br	2.16264300	2.05352600	1.89894600
H	-3.54597900	-0.91015400	-3.78296700	C	2.84388300	-1.43250400	1.18769300
H	-5.17060600	-1.44911100	-4.25693000	H	2.91527700	-1.60078300	0.11459200
H	-3.82356500	-2.60287800	-4.21560600	C	3.99735200	-1.33321900	1.87579900
C	-4.91145900	-0.84886900	-1.35945700	H	4.02434500	-1.20194600	2.95134400
C	-5.64216100	0.27900100	-2.08473300	H	4.94947000	-1.39549300	1.35897400
H	-5.81352300	1.10980000	-1.39427600	C	1.19881300	-1.46588400	3.16727800
H	-6.61684500	-0.06173900	-2.44977700	C	1.76331600	-0.58731100	4.11570900
H	-5.06702400	0.65316600	-2.93363600	C	0.38604500	-2.51554200	3.64605600
C	-5.66644000	-1.22071500	-0.07564000	C	1.53096100	-0.76549800	5.47677900
H	-5.16361000	-2.03044700	0.45979200	H	2.34692700	0.25651200	3.77002500
H	-6.69540900	-1.52811100	-0.28615300	C	0.16476200	-2.69811600	5.00913700
H	-5.69129100	-0.35046100	0.58533200	H	-0.04684300	-3.21146300	2.93369900
C	-1.65150500	-0.22463500	1.68699300	C	0.73555300	-1.82101400	5.93205300
C	-1.65760000	1.02805500	2.34084200	H	1.96978200	-0.07063100	6.18768800
H	-1.15216600	1.87167900	1.88069300	H	-0.45551800	-3.52292900	5.34926700
C	-2.29918400	1.19643700	3.56205700	H	0.56089200	-1.95572200	6.99612400
H	-2.28768100	2.17103800	4.04211700				
C	-2.96323700	0.12360400	4.16721400	L₁-TS20₉			
H	-3.47126900	0.25825000	5.11791200	Cu	-0.76653300	0.18431400	-0.50520900
C	-2.96785700	-1.11942500	3.53538600	N	2.30945700	-1.20173800	-0.19680800
H	-3.47909500	-1.96122500	3.99517300	N	-2.76213800	1.48891000	1.40112300
C	-2.31259900	-1.29548200	2.31664500	N	-1.16941300	2.90973300	0.99069900
H	-2.33039600	-2.26580500	1.83408100	O	3.64619400	-2.32106300	1.54522000
H	5.85684500	1.12419500	0.10338100	O	2.20203400	-0.66481100	2.23356100
H	4.19337300	1.72519400	0.21591200	B	2.70475300	-1.39149000	1.17173400
H	0.84989100	-0.23971600	-3.32234300	C	-1.53970500	1.61557300	0.83105000
H	1.82053700	0.40556300	-4.64090500	C	-3.25693400	2.72554800	2.04842900
H	-2.52388200	1.55103900	-3.25435100	H	-4.25828700	2.97664300	1.69087400
H	-1.25601000	0.70300700	-2.37180700	C	-2.20268900	3.75414600	1.63731400
H	0.24803100	5.52831300	1.42549000	H	-2.59079400	4.48913200	0.92504600
H	1.31958600	4.28347600	0.77159600	C	0.09674700	3.52201000	0.70394100
C	6.01952300	-2.87930300	-2.85733600				

C	0.23361200	4.37613900	-0.40790600	H	3.08067500	-4.47417200	2.88652100
C	1.44847200	5.05415200	-0.57027900	C	3.03515400	-0.98570400	3.39128200
H	1.56038300	5.71557600	-1.42637600	C	2.15621200	-0.97990700	4.63908500
C	2.51160900	4.91087600	0.32526600	H	1.78476100	0.03100900	4.82850700
C	2.33470800	4.06992200	1.42899600	H	2.72938200	-1.29756200	5.51632200
H	3.13855400	3.96684100	2.15483300	H	1.29602900	-1.64190100	4.52660800
C	1.13628500	3.38185400	1.64555700	C	4.10811200	0.10630600	3.48510300
C	0.96211700	2.53639800	2.88468500	H	4.75083300	0.10841400	2.60033100
H	1.77073800	2.73278200	3.59465800	H	4.73754300	-0.02507000	4.37006200
C	-0.88176000	4.57941000	-1.40183100	H	3.62097100	1.08199500	3.55247300
H	-1.68568000	5.19718700	-0.98115400	C	1.62099100	0.51708400	-1.88171800
C	-3.52176100	0.28778000	1.60567000	C	1.37241400	-0.06227500	-3.13591300
C	-4.68864300	0.07020000	0.84586600	H	0.90747500	-1.03624900	-3.20081200
C	-5.10249500	1.00655300	-0.26242700	C	1.68345500	0.61979400	-4.30818100
H	-5.43971100	1.97514100	0.12846000	H	1.46934400	0.15752700	-5.26713800
C	-5.46663600	-1.05565800	1.14204800	C	2.24803300	1.89572900	-4.25498100
H	-6.36625400	-1.23290400	0.55689000	H	2.48526700	2.42727000	-5.17229700
C	-5.12659400	-1.94960900	2.16125100	C	2.48995000	2.48854300	-3.01599500
C	-3.97458700	-1.68960600	2.90927600	H	2.91629700	3.48588800	-2.95810800
H	-3.70167700	-2.36389800	3.71790700	C	2.17445400	1.80762500	-1.84007000
C	-3.16401400	-0.57924100	2.65566600	H	2.36683100	2.27721600	-0.88083400
C	-1.93838200	-0.32768400	3.49984800	H	-5.93572100	0.58083100	-0.82765700
H	-1.91623900	0.69409300	3.89399000	H	-4.27421000	1.19450700	-0.95493000
C	1.38735100	-0.17603600	-0.57329700	H	-1.90969300	-1.01425400	4.35058800
H	1.33582200	0.53135900	0.25481400	H	-1.02180200	-0.46681600	2.91860300
C	3.00737900	-2.01862100	-1.16873800	H	0.97068400	1.46765600	2.65155200
C	2.72942200	-3.38701700	-1.26916100	H	0.01505300	2.75152600	3.39061800
H	1.96123800	-3.82439500	-0.63993400	H	-0.50955200	5.09759100	-2.28943500
C	3.44374500	-4.18421100	-2.16522200	H	-1.31908700	3.62622300	-1.71840600
H	3.21750500	-5.24418900	-2.23585900	C	-5.96823900	-3.17410700	2.43310100
C	4.44395900	-3.62455300	-2.96093300	H	-5.62336500	-4.02872100	1.83768200
H	4.99785800	-4.24534900	-3.65914200	H	-5.91752600	-3.46999800	3.48547500
C	4.73451500	-2.26350600	-2.84868200	H	-7.01848300	-3.00370800	2.17776700
H	5.51863400	-1.82067700	-3.45585200	C	3.81972900	5.63367800	0.10290400
C	4.02574500	-1.46345700	-1.95295700	H	3.66914400	6.58026000	-0.42470300
H	4.25507100	-0.40801300	-1.86020200	H	4.32449400	5.84869800	1.04981800
C	3.62428800	-2.39543100	2.99589600	H	4.50845200	5.03032200	-0.50181800
C	5.04536200	-2.66398100	3.48642100	H	-3.31240000	2.58031100	3.13451200
H	5.37222000	-3.64763500	3.13791600	H	-1.77347700	4.29524700	2.48628000
H	5.08669000	-2.66156300	4.58065800	C	-0.35236700	-1.82570800	-0.79722400
H	5.75058200	-1.92250200	3.10745800	H	0.58282800	-2.12822500	-1.23970300
C	2.70646400	-3.56759800	3.36949800	Br	-2.02368600	1.16075000	-2.44675300
H	1.68250200	-3.40184500	3.02320200	C	-0.43713700	-2.30062100	0.61551400
H	2.68636600	-3.73707300	4.45015300	H	0.30642100	-1.88604400	1.28929800

C	-1.29238800	-3.19653700	1.13232800	H	0.24025500	4.83825400	-1.10114100
H	-2.06245500	-3.68090100	0.54306600	C	-2.95572500	4.23738000	-1.63782100
H	-1.23730300	-3.46625300	2.18307100	H	-2.88886400	4.47951700	-2.69536500
C	-1.43612500	-2.27996900	-1.73201300	C	-4.21512900	4.11045100	-1.04338500
C	-1.07227200	-2.90701300	-2.93755900	C	-4.27814400	3.78897100	0.31503700
C	-2.80889700	-2.16593500	-1.44437100	H	-5.24922000	3.68635300	0.79377000
C	-2.03264200	-3.39297300	-3.82369900	C	-3.12513000	3.57966100	1.07811600
H	-0.01858700	-3.03674700	-3.17330100	C	-3.23212100	3.19841100	2.53540000
C	-3.76925600	-2.65639700	-2.32384100	H	-2.67598800	3.88342200	3.18579200
H	-3.12552400	-1.68453200	-0.52741000	C	-1.23681800	-1.23300000	0.43963400
C	-3.38871700	-3.26762900	-3.52127400	H	-1.50811000	-1.52587100	1.46019300
H	-1.72018100	-3.87333400	-4.74703500	C	-2.69432300	-0.55413300	-1.49721200
H	-4.82209000	-2.54997000	-2.07716500	C	-1.60835700	0.04271700	-2.16761700
H	-4.14125900	-3.64199200	-4.20968300	H	-0.59852600	-0.13104600	-1.81749200
L₁-17₁₀				C	-1.80615300	0.83529700	-3.29910800
Cu	-0.62633300	0.61349300	0.79365400	H	-0.93689500	1.26174700	-3.79261600
N	-2.48667500	-1.37042700	-0.35971700	C	-3.08790900	1.05934300	-3.80004700
N	-0.67836400	3.52464600	1.21626700	H	-3.23937700	1.66507300	-4.68916400
N	1.02794900	2.58815700	2.19931800	C	-4.17302700	0.47872200	-3.13838600
O	-4.54996200	-2.78677300	-0.59385500	H	-5.18389600	0.63768900	-3.50736000
O	-3.17257100	-3.13494900	1.21276000	C	-3.98716900	-0.30741200	-2.00338400
B	-3.38791700	-2.39410900	0.05796800	H	-4.84365100	-0.74817900	-1.51166100
C	-0.04779200	2.35319400	1.41977600	C	-5.25682400	-3.69848800	0.28236000
C	-0.02131300	4.67266200	1.88141000	C	-5.96290700	-4.74434400	-0.57874500
H	0.30473500	5.40787100	1.13845900	H	-6.72661400	-4.25936400	-1.19395200
C	1.15620900	4.00379400	2.61437400	H	-6.45778600	-5.49645700	0.04513100
H	2.12741600	4.40817300	2.31396500	H	-5.26367400	-5.24922600	-1.24717100
C	1.92586300	1.58742600	2.70515900	C	-6.28985600	-2.86879200	1.05896300
C	3.16395900	1.38900300	2.06866600	H	-5.80070800	-2.11537900	1.68286600
C	4.04040200	0.44015400	2.60676100	H	-6.91869000	-3.49519700	1.69919300
H	4.99558200	0.27425400	2.11458800	H	-6.93660000	-2.35066800	0.34505100
C	3.71645000	-0.30380000	3.74485900	C	-4.09460600	-4.24875100	1.19361100
C	2.47807100	-0.07778400	4.35492300	C	-4.49305500	-4.57372200	2.63262300
H	2.21043700	-0.64362300	5.24452900	H	-3.61474700	-4.91927300	3.18573600
C	1.56909700	0.85981500	3.85629100	H	-5.24515900	-5.36946900	2.66101900
C	0.23394300	1.05958500	4.53293500	H	-4.89096200	-3.69737900	3.14772400
H	0.03547200	2.11428400	4.75253400	C	-3.35247500	-5.44029500	0.57062900
C	3.54568700	2.16005400	0.82820300	H	-3.06091800	-5.22760600	-0.46153800
H	3.62600300	3.23648900	1.02193400	H	-3.96054100	-6.35031600	0.58195900
C	-1.87722400	3.70475400	0.44385800	H	-2.43994100	-5.62583700	1.14356100
C	-1.77513300	4.03701700	-0.91889900	C	-0.13236400	-2.16219900	0.02004800
C	-0.43519700	4.13862000	-1.60622700	C	0.94214500	-2.40846100	0.90264600
				H	0.95147600	-1.90977900	1.86991100
				C	1.97540800	-3.27992100	0.57251800

H	2.77402500	-3.45939600	1.28933300
C	1.98515400	-3.93824400	-0.66429800
H	2.78635000	-4.62614900	-0.91979100
C	0.93423100	-3.70666100	-1.55253100
H	0.91355500	-4.21636400	-2.51323300
C	-0.10823600	-2.83633500	-1.21662400
H	-0.92591500	-2.69014800	-1.91478100
H	-0.55746200	4.48240300	-2.63630700
H	0.06828900	3.16667700	-1.63588400
H	-4.27555800	3.20634600	2.86025200
H	-2.83237900	2.19320400	2.70948800
H	0.19261600	0.50734800	5.47514000
H	-0.58533100	0.70495900	3.89715000
H	4.51435900	1.82456500	0.44971600
H	2.81060800	2.03147900	0.02763900
C	-5.47105400	4.27286500	-1.86465200
H	-6.34731400	4.44247000	-1.23242000
H	-5.38871100	5.10973300	-2.56582700
H	-5.65657300	3.36867500	-2.45672100
C	4.66639700	-1.34380800	4.29097700
H	5.69663600	-1.14706100	3.98069400
H	4.64142200	-1.37493500	5.38482600
H	4.40035500	-2.34688100	3.93450700
H	-0.72032000	5.16965100	2.56169400
H	1.07968800	4.08618900	3.70421000
Br	2.20171400	1.25761900	-2.87820200
C	5.15745000	-1.34035500	-3.34151100
H	5.69925200	-1.57251500	-4.25809300
C	3.86055300	-1.00972300	-3.47932700
H	3.43483100	-1.03208000	-4.47997900
C	2.92988300	-0.56798200	-2.41045200
H	3.39375200	-0.43463100	-1.43787300
H	2.03481200	-1.18303900	-2.32118600
C	5.96967900	-1.41150600	-2.11245300
C	5.47609700	-1.92062600	-0.89736600
C	7.31340100	-0.99462700	-2.16167100
C	6.29154000	-1.97468500	0.23427800
H	4.46624200	-2.31536300	-0.84623000
C	8.12345300	-1.04237500	-1.02987700
H	7.71648400	-0.61848700	-3.09857800
C	7.61350000	-1.52975600	0.17651700
H	5.89386300	-2.38340500	1.15901700
H	9.15467700	-0.70581300	-1.08961000
H	8.24723300	-1.57880500	1.05747600

L₁-TS18₁₀

Cu	-0.31022300	-0.48634500	0.04023800
N	2.18664000	0.97334700	-0.79602800
N	0.70302800	-2.85772200	1.64884100
N	-0.89791500	-1.82895900	2.70245200
O	4.54621800	1.82681000	-0.93279300
O	3.37734600	2.12814300	1.02275900
B	3.34877100	1.61471000	-0.26747600
C	-0.14184400	-1.81120000	1.58087600
C	0.53730600	-3.68406200	2.86772300
H	0.23827800	-4.70262300	2.59965100
C	-0.55679100	-2.92654200	3.63751600
H	-1.43531100	-3.54517700	3.84495000
C	-1.89124600	-0.85744800	3.05952100
C	-3.24746200	-1.12642500	2.79945300
C	-4.19713500	-0.17503300	3.19339200
H	-5.24812400	-0.37669400	2.99837700
C	-3.83621500	1.01467400	3.83186100
C	-2.48011400	1.23945900	4.09434900
H	-2.18029300	2.15020400	4.60798900
C	-1.49457100	0.31819900	3.72709000
C	-0.04382100	0.58179500	4.05569300
H	0.36609900	-0.18849800	4.71950800
C	-3.68192400	-2.39512300	2.10603600
H	-3.36054300	-3.28975600	2.65144800
C	1.71554900	-3.19834600	0.68747500
C	1.42599900	-4.13516500	-0.32231500
C	0.05330900	-4.74491700	-0.46709800
H	-0.27216600	-5.25222200	0.44877200
C	2.44760600	-4.47980700	-1.21183700
H	2.23121400	-5.19428200	-2.00260200
C	3.72899500	-3.92831100	-1.12002700
C	3.98697300	-3.02099500	-0.08931000
H	4.98153500	-2.59116400	0.00597900
C	2.99901400	-2.64073300	0.82409200
C	3.31682300	-1.63632000	1.90642200
H	2.87918600	-1.90990900	2.87155000
C	0.94305800	1.18105500	-0.01418600
H	1.22345200	1.13481700	1.03957100
C	2.16099100	0.31683000	-2.05415800
C	0.96091100	0.16251800	-2.77009500
H	0.03878600	0.55467100	-2.36208100

C	0.93626400	-0.49484800	-4.00142100	H	-3.26090100	-2.45682900	1.09662800
H	-0.01382400	-0.60565700	-4.51658100	C	4.79348600	-4.27764100	-2.13155000
C	2.10576100	-1.00060900	-4.56461200	H	5.79904400	-4.15594600	-1.71760200
H	2.08601300	-1.50390800	-5.52692700	H	4.69144200	-5.30857500	-2.48453300
C	3.30485200	-0.84647900	-3.86400800	H	4.71541300	-3.62211900	-3.00744100
H	4.23264900	-1.23015800	-4.28218600	C	-4.87714000	2.03864900	4.21932100
C	3.33666100	-0.21114000	-2.62531700	H	-5.87561400	1.59512100	4.27041200
H	4.27686600	-0.11111400	-2.10071500	H	-4.65483400	2.48696000	5.19296900
C	5.49552100	2.36680200	0.01888500	H	-4.91757200	2.85701200	3.48977900
C	6.37866900	3.38106300	-0.70625600	H	1.48212000	-3.74550600	3.41752900
H	6.96776900	2.87178100	-1.47454600	H	-0.20067700	-2.51872700	4.59026100
H	7.07345500	3.86311500	-0.01016800	Br	-2.10112900	-1.67299400	-1.32697900
H	5.78228800	4.15220200	-1.19623400	C	-3.84366600	1.71497400	-2.50381300
C	6.34861400	1.19432200	0.52414400	H	-3.60634400	2.24930500	-3.42283000
H	5.73253300	0.45213500	1.03928500	C	-2.80969900	1.59495300	-1.60365000
H	7.13510200	1.52797200	1.20804800	H	-1.89137600	2.12139600	-1.84774500
H	6.82336800	0.70668800	-0.33213500	C	-2.78539000	0.82022900	-0.42942700
C	4.54945300	2.97157100	1.12793600	H	-3.63196400	0.23568600	-0.10710300
C	5.08393900	2.88557700	2.55662800	H	-2.01920000	1.01336500	0.31086700
H	4.34674500	3.30305100	3.24880000	C	-5.21182400	1.22821500	-2.43369500
H	6.00998900	3.46058400	2.66284100	C	-5.91309900	1.01041400	-1.22698900
H	5.27774900	1.85315300	2.85338100	C	-5.89808800	0.99531800	-3.64681700
C	4.09828100	4.40685700	0.82018700	C	-7.22033700	0.53393700	-1.23925700
H	3.70042300	4.48717700	-0.19505200	H	-5.44686000	1.26354200	-0.28189300
H	4.91701200	5.12408400	0.93397600	C	-7.19996200	0.50787500	-3.65553400
H	3.29821000	4.68118900	1.51294100	H	-5.38276600	1.17920000	-4.58566200
C	0.28391700	2.48987000	-0.25489600	C	-7.86618900	0.26944400	-2.44997100
C	-0.56858500	3.04485400	0.73053600	H	-7.74463900	0.38166400	-0.30018400
H	-0.71653700	2.50382400	1.66277700	H	-7.69960400	0.31877200	-4.60108000
C	-1.19370200	4.27665400	0.55001700	H	-8.88677800	-0.10179200	-2.45425400
H	-1.83267200	4.67215900	1.33614100				
C	-0.99497300	5.00890000	-0.62362900	L₁-19₁₀			
H	-1.47933000	5.97079900	-0.76431800	Cu	0.87713700	0.17290900	0.01490100
C	-0.15117900	4.48556000	-1.60685900	N	-1.76275300	-0.37133800	-1.06687800
H	0.02847800	5.04688200	-2.52088000	N	-0.51315200	1.90641100	2.39180600
C	0.47643200	3.25192700	-1.43060100	N	0.86207300	0.32522500	2.98567600
H	1.13932200	2.87576400	-2.20233800	O	-4.19111500	-0.79065300	-1.53857700
H	0.04683000	-5.48382700	-1.27258400	O	-3.18494400	-1.96449500	0.16140800
H	-0.69472200	-3.97966200	-0.70140000	B	-3.03067900	-0.99895800	-0.82192200
H	4.39868700	-1.55176600	2.04323000	C	0.17286600	0.83816900	1.93758000
H	2.93601400	-0.64233600	1.64892900	C	-0.24495300	2.21869600	3.81842100
H	0.06945600	1.54526200	4.55892500	H	0.24875900	3.19183900	3.90015300
H	0.57946900	0.59391400	3.15711700	C	0.66124000	1.06077900	4.25510800
H	-4.77154800	-2.43434000	2.02563900				

H	1.61816300	1.40331400	4.65784900	H	-5.47256100	-0.20523000	0.74231300
C	1.60762700	-0.90377200	2.98811500	H	-6.93245600	-1.15326100	0.39392800
C	3.01705600	-0.86799100	2.96274600	H	-6.45725800	0.17758300	-0.67728300
C	3.70953700	-2.08378600	2.98406100	C	-4.43208200	-2.65871900	-0.10626000
H	4.79654000	-2.06246500	2.95383100	C	-5.05789400	-3.06118600	1.22769800
C	3.05229500	-3.31552900	3.05408200	H	-4.40481100	-3.77546200	1.73752000
C	1.65699700	-3.31245500	3.13875200	H	-6.02858600	-3.54348700	1.07263100
H	1.12797700	-4.25749700	3.24113000	H	-5.19677700	-2.20134700	1.88542300
C	0.91530000	-2.12545200	3.11916100	C	-4.07629700	-3.91108100	-0.91948000
C	-0.58755100	-2.18754200	3.27292400	H	-3.60559300	-3.64890100	-1.87062300
H	-0.96566500	-1.38595100	3.91326000	H	-4.95794300	-4.52675200	-1.12181100
C	3.78200600	0.43299400	2.94391900	H	-3.35917600	-4.50928000	-0.35107300
H	3.72855300	0.93749400	3.91730800	C	-0.32772400	-2.37981400	-1.37909700
C	-1.56099300	2.64045200	1.73147400	C	0.22629900	-3.51373100	-0.74909300
C	-1.31281200	3.92349400	1.20758400	H	0.45163000	-3.47147000	0.31398900
C	0.04528000	4.57297200	1.28607400	C	0.46686600	-4.69137000	-1.45447300
H	0.24679700	4.93907100	2.30192200	H	0.88947300	-5.54963200	-0.93861200
C	-2.38585100	4.62252300	0.64396000	C	0.15436500	-4.77576400	-2.81327100
H	-2.19684400	5.60707900	0.22246700	H	0.33792600	-5.69380900	-3.36389400
C	-3.68329500	4.10616300	0.61872100	C	-0.40782700	-3.66828000	-3.45191600
C	-3.90561400	2.85662100	1.20345100	H	-0.66639200	-3.72229000	-4.50617000
H	-4.91554200	2.45368400	1.23223400	C	-0.64610800	-2.48723100	-2.74797800
C	-2.86584000	2.11210000	1.76958000	H	-1.09435700	-1.64212900	-3.25921500
C	-3.16626000	0.79075700	2.43772700	H	0.09520200	5.43696000	0.61813700
H	-2.68052000	0.70637500	3.41533400	H	0.84339000	3.88043000	1.00969800
C	-0.61699800	-1.15848900	-0.57425700	H	-4.24278500	0.68431900	2.59874000
H	-0.84030600	-1.46375200	0.44429500	H	-2.83425000	-0.06191100	1.83875300
C	-1.61158900	0.72228100	-1.96624300	H	-0.88130500	-3.14102600	3.72063500
C	-0.41723300	0.94320500	-2.66922900	H	-1.11511400	-2.10390500	2.31686200
H	0.42216800	0.27365700	-2.54504600	H	4.83943600	0.25159800	2.73438100
C	-0.28596500	2.03098600	-3.53442700	H	3.39752200	1.12200300	2.18644100
H	0.65874800	2.17678400	-4.05005300	C	-4.81055700	4.87631400	-0.02661200
C	-1.34300600	2.91508900	-3.73454800	H	-5.78512200	4.56185000	0.35863700
H	-1.24045700	3.75783200	-4.41170300	H	-4.70915600	5.95312200	0.14158600
C	-2.53499500	2.70128300	-3.03811800	H	-4.82000000	4.71874500	-1.11229600
H	-3.37201100	3.38228600	-3.17053000	C	3.82814900	-4.61122600	3.03872000
C	-2.66910500	1.63154800	-2.15820200	H	4.79949300	-4.50256600	3.53072000
H	-3.59508700	1.49775200	-1.61614000	H	3.27952400	-5.41319900	3.54154400
C	-5.24526900	-1.58374200	-0.93345800	H	4.02098700	-4.94190900	2.01057100
C	-6.11375200	-2.15178900	-2.05557700	H	-1.18369600	2.26468600	4.37884500
H	-6.59880300	-1.33141700	-2.59227500	H	0.19393000	0.40679700	5.00088400
H	-6.89682600	-2.80325800	-1.65326300	Br	2.36783500	2.09656600	-0.10458600
H	-5.52081100	-2.71910600	-2.77451200	C	3.53957300	-0.41451100	-2.98935200
C	-6.07804600	-0.63929700	-0.05685200	H	3.39150100	-0.43301200	-4.06925700

C	2.54844900	-0.98040300	-2.24767500	C	-1.49094200	-4.05092700	0.04064500
H	1.76264300	-1.47198500	-2.81763500	C	-0.17133200	-4.65231500	0.45016700
C	2.37550700	-1.00308400	-0.81118500	H	0.36029500	-5.09146500	-0.40194700
H	3.17310600	-0.56131300	-0.22605300	C	-2.67004300	-4.44110300	0.68513900
H	2.00798300	-1.94503500	-0.41259500	H	-2.60487500	-5.17326400	1.48653500
C	4.79938700	0.21123200	-2.57737400	C	-3.92135500	-3.93689300	0.31957300
C	5.52288800	-0.16758600	-1.42928300	C	-3.98083400	-3.01803200	-0.73227300
C	5.36041700	1.20096400	-3.40931100	H	-4.94914900	-2.64642200	-1.05909000
C	6.72968800	0.44915000	-1.10821500	C	-2.82997500	-2.57871100	-1.39672100
H	5.15281600	-0.97413400	-0.80641400	C	-2.94863100	-1.57716400	-2.52232000
C	6.56114400	1.82418800	-3.08326100	H	-2.25697200	-1.78834200	-3.34271800
H	4.82866200	1.49291800	-4.31130500	C	-0.51817600	1.53280200	-0.06625900
C	7.25104100	1.45383400	-1.92626900	H	-0.61210900	1.11313500	-1.06788000
H	7.27198000	0.13648600	-0.21994700	C	-1.40720500	0.49390500	2.11145300
H	6.96241200	2.59649500	-3.73360400	C	-0.55033900	1.07741800	3.05131300
H	8.19220400	1.93324500	-1.67264200	H	0.05256100	1.93296300	2.78023500
L₁-TS20₁₀				C	-0.44297800	0.54167900	4.33464600
Cu	0.68049600	-0.44867500	0.04824600	H	0.24024100	0.99912000	5.04465000
N	-1.59170000	1.02719700	0.79202400	C	-1.20158200	-0.56628100	4.70779500
N	-0.41265300	-2.73751700	-1.73885800	H	-1.11588000	-0.97905400	5.70864000
N	1.32307100	-1.71214200	-2.55128900	C	-2.05753200	-1.15106000	3.77320500
O	-4.02535800	1.38472100	1.15979800	H	-2.64183900	-2.02715900	4.04060800
O	-3.20787100	1.64604000	-0.97603300	C	-2.15235400	-0.63487400	2.48348500
B	-2.92076300	1.32114700	0.33903200	H	-2.79796700	-1.10944600	1.75241700
C	0.40290100	-1.67810700	-1.55779000	C	-5.18544200	1.63646300	0.32732400
C	-0.05127000	-3.57965200	-2.90556900	C	-6.10984200	2.59414500	1.07900400
H	0.18703600	-4.59663300	-2.57893100	H	-6.47075600	2.11035600	1.99104800
C	1.16086200	-2.84326400	-3.49145600	H	-6.97995800	2.86014800	0.46924500
H	2.06400600	-3.46099400	-3.51128300	H	-5.59198700	3.51006800	1.36812700
C	2.35815600	-0.74385400	-2.77232300	C	-5.88944600	0.29056600	0.11724000
C	3.65157100	-0.98260400	-2.27164600	H	-5.23624100	-0.42032900	-0.39332800
C	4.64783200	-0.03765600	-2.54925700	H	-6.81191500	0.40041700	-0.46114400
H	5.65265000	-0.21520900	-2.17277400	H	-6.14232600	-0.13074200	1.09407800
C	4.39297900	1.11734100	-3.29472100	C	-4.54122800	2.22647400	-0.99315100
C	3.09923700	1.31259700	-3.79087000	C	-5.23321000	1.81519500	-2.29152800
H	2.88553800	2.19566100	-4.38916100	H	-4.69050100	2.23413000	-3.14401600
C	2.07241300	0.39426200	-3.55099600	H	-6.25846700	2.19855700	-2.32357700
C	0.69655100	0.62052500	-4.13420900	H	-5.26384700	0.73100100	-2.41008800
H	0.43982800	-0.14712000	-4.87422800	C	-4.36604100	3.75086300	-0.95788400
C	3.96596500	-2.20604900	-1.44593900	H	-3.86324900	4.07661200	-0.04402000
H	3.69467100	-3.13094400	-1.96706900	H	-5.32769100	4.26788100	-1.03104000
C	-1.58573400	-3.09327900	-0.98831000	H	-3.74391400	4.05509800	-1.80390900
				C	-0.44306400	3.01628900	-0.15755000
				C	0.06387300	3.62801100	-1.32143500

H	0.40064000	3.00473200	-2.14585100	H	6.06795700	-0.26464700	4.87562700
C	0.11782900	5.01412200	-1.44554700	H	7.25001400	-1.18283500	2.88646900
H	0.50913600	5.45749300	-2.35719400				
C	-0.34176300	5.83271400	-0.41047700	L₁-7₂			
H	-0.30294000	6.91375000	-0.50714000				
C	-0.86284800	5.24489800	0.74364600	C	-1.12206000	2.12643300	-0.17244400
H	-1.23286000	5.86920000	1.55242700	C	-1.20533300	4.07172200	-1.51641500
C	-0.91491500	3.85627100	0.86993700	C	-2.63407400	3.53417200	-1.32610300
H	-1.33873400	3.41470200	1.76541100	N	-2.39906900	2.27697900	-0.57804000
H	-0.32575900	-5.44499600	1.18695000	N	-0.41307200	3.16808400	-0.65055200
H	0.48694300	-3.89427000	0.89111500	C	-4.05080000	1.56153200	1.09430200
H	-3.96310100	-1.58286600	-2.93191900	C	-3.49386500	1.43152600	-0.19247700
H	-2.74150400	-0.55864000	-2.17594500	C	-4.01351000	0.51701000	-1.12482800
H	0.64427300	1.58913200	-4.63849900	C	-5.10746900	-0.26769500	-0.74356800
H	-0.08354900	0.59241900	-3.36746000	C	-5.68425300	-0.16633600	0.52477200
H	5.03503300	-2.25356200	-1.22374500	C	-5.14154300	0.75458600	1.42738400
H	3.42011900	-2.19673400	-0.49413100	H	-5.51037300	-0.98252900	-1.45713000
C	-5.17407800	-4.36979400	1.04455600	H	-5.57647500	0.84734400	2.41998300
H	-5.09969100	-5.40579900	1.38890700	C	1.47547200	4.23382000	0.48617000
H	-5.35291800	-3.74637400	1.92942500	C	2.85532300	4.42212800	0.60247600
H	-6.05735600	-4.28649500	0.40405600	C	3.76410400	3.74588200	-0.21759900
C	5.47961100	2.13690100	-3.54317400	C	3.26157800	2.86466900	-1.17950800
H	5.34353000	2.64195800	-4.50434900	C	1.88912200	2.64696100	-1.33774300
H	5.47818600	2.91090700	-2.76572300	C	1.00466700	3.34229000	-0.49436100
H	6.47093100	1.67438700	-3.53878400	H	3.22880800	5.10752400	1.35990300
H	-0.89349900	-3.63970000	-3.60263400	H	3.95315900	2.32104900	-1.81839600
H	0.98533700	-2.47294400	-4.50760700	Cu	-0.38913900	0.63652300	0.89724100
Br	1.79108300	-1.79303900	1.75364800	C	-6.84332000	-1.04803200	0.92653800
C	3.07966200	2.15611200	2.31472600	H	-7.37299200	-1.43755300	0.05234700
H	3.04125400	2.88627400	3.12382500	H	-6.49802700	-1.90875400	1.51247800
C	2.11494300	2.27954000	1.37012800	H	-7.56392800	-0.50478900	1.54614500
H	1.47037100	3.14945200	1.47040800	C	5.25251900	3.93718500	-0.04467300
C	1.84124400	1.41462000	0.23154200	H	5.78746500	3.79492600	-0.98839700
H	2.48420600	0.53331400	0.19467500	H	5.48731700	4.93709600	0.33270500
H	1.77421700	1.91379100	-0.72829600	H	5.66021300	3.21449700	0.67306600
C	4.19965700	1.21423800	2.42353500	C	-3.41274500	0.36341500	-2.50158500
C	4.89105900	0.70113800	1.31059800	H	-3.72756500	1.17058500	-3.17618300
C	4.66345700	0.86704300	3.70707200	H	-2.32049200	0.37445500	-2.46274800
C	5.97796000	-0.15423400	1.47939300	H	-3.72199200	-0.58199100	-2.95287400
H	4.59716300	0.99939300	0.30999300	C	-3.47886900	2.52395200	2.10729200
C	5.74081500	0.00279500	3.87480400	H	-2.50044900	2.17986100	2.46242800
H	4.15272000	1.26885800	4.57834600	H	-3.33502200	3.52621200	1.68940900
C	6.40304600	-0.51477000	2.75884800	H	-4.14051900	2.61150200	2.97288900
H	6.50226100	-0.53441800	0.60680200	C	1.38712400	1.66179100	-2.36550000

H	2.19655600	1.35395200	-3.03174100
H	0.99155500	0.76176600	-1.88116500
H	0.58265700	2.08033100	-2.97996900
C	0.52443700	4.95256100	1.41317100
H	1.07574400	5.54285400	2.14934500
H	-0.14139300	5.63783600	0.87470100
H	-0.11128000	4.24355600	1.95335900
C	3.06470000	-2.04228400	-1.64181500
C	3.62938600	-1.23374000	-0.63888100
C	3.88498700	-2.51721700	-2.68229800
C	4.97203500	-0.86654000	-0.71100900
H	3.00189000	-0.91169700	0.18708700
C	5.23036200	-2.15602900	-2.73637200
H	3.47673600	-3.19574700	-3.42560300
C	5.77765200	-1.32084900	-1.75929600
H	5.39364900	-0.23501300	0.06603100
H	5.85638000	-2.53840900	-3.53826300
H	6.82764000	-1.04561500	-1.80296900
C	-0.44999400	-2.93528900	-2.44603300
C	-1.13979700	-3.28642200	-3.61797400
C	-1.13290000	-2.94923300	-1.21496900
C	-2.48072500	-3.66562900	-3.56618500
H	-0.61575800	-3.27040900	-4.57110500
C	-2.47378900	-3.31969400	-1.16934300
H	-0.61189200	-2.65533500	-0.31029800
C	-3.14941400	-3.68482600	-2.33992200
H	-3.00096000	-3.94714000	-4.47748000
H	-2.99425300	-3.31903000	-0.21637100
H	-4.19382600	-3.98198800	-2.29558400
B	0.40335400	-0.85070100	1.97138900
C	1.88101100	-1.96407400	3.38526700
O	1.72054300	-0.87093100	2.44394800
C	0.69811800	-2.92531200	2.99562700
O	-0.25177700	-2.01631900	2.37660700
C	3.28198800	-2.55313300	3.21709300
H	4.03022800	-1.80141900	3.48755700
H	3.42586500	-3.42131200	3.87026300
H	3.46942700	-2.85690600	2.18587400
C	1.74064600	-1.35804400	4.79091300
H	0.74854200	-0.92131100	4.93365300
H	1.91406200	-2.09946100	5.57818600
H	2.47819200	-0.55798900	4.90321400
C	1.08127000	-3.97049600	1.93770600
H	1.77181700	-4.72071100	2.33772300

H	0.17460900	-4.48695700	1.60746000
H	1.53431000	-3.50144700	1.06079700
C	0.00600300	-3.61462800	4.17296400
H	-0.39308300	-2.89193000	4.88700700
H	-0.82956000	-4.21597600	3.80189800
H	0.69492000	-4.28430400	4.70042400
H	-3.14422600	3.33558400	-2.27246400
H	-3.26464100	4.20980800	-0.73571700
H	-0.86090700	3.99501200	-2.55456700
H	-1.09436000	5.11280100	-1.20079900
C	0.96643500	-2.55897400	-2.53818500
N	1.70297700	-2.36986000	-1.50742000
H	1.35764900	-2.43986100	-3.56096000

L₁-TS8₂

C	-0.02073700	-1.92594300	-0.58279400
C	0.58909200	-3.98969800	-1.57345300
C	-0.93296200	-3.79396800	-1.70866900
N	-1.15717100	-2.49753800	-1.03652900
N	1.00912300	-2.75528000	-0.88267000
C	-3.04331300	-1.16820600	-1.87749300
C	-2.48832300	-1.98259800	-0.87745000
C	-3.22855700	-2.35512800	0.26169800
C	-4.54094200	-1.89660200	0.37710400
C	-5.12726400	-1.08496200	-0.60099200
C	-4.36566300	-0.73646200	-1.71750100
H	-5.11331300	-2.16357100	1.26194000
H	-4.80408100	-0.10268700	-2.48492500
C	3.21637300	-1.86483100	-1.47217500
C	4.56322700	-1.68185600	-1.13539100
C	5.08829600	-2.12496600	0.08143700
C	4.22952800	-2.77082500	0.97881100
C	2.87942500	-2.97893300	0.68768200
C	2.38301100	-2.51839900	-0.54774900
H	5.21460500	-1.17583200	-1.84397400
H	4.61945300	-3.11888400	1.93272700
Cu	0.20235200	-0.21597700	0.18408200
C	-6.53957400	-0.57945500	-0.42811700
H	-7.22873600	-1.39145900	-0.17143000
H	-6.58940900	0.15493100	0.38448700
H	-6.90833700	-0.09724800	-1.33770900
C	6.53943600	-1.89914300	0.43543500
H	7.00682900	-2.81581600	0.81089400

H	7.11417500	-1.55627500	-0.42920700	O	-1.00074500	2.14231000	-1.17053700
H	6.63900200	-1.14225300	1.22272000	C	1.57212100	4.67784600	-1.91741900
C	-2.61278300	-3.19861300	1.35191500	H	2.60355700	4.50345800	-2.23806900
H	-2.24592800	-4.16048800	0.97473700	H	1.16681400	5.50202200	-2.51522200
H	-1.76342700	-2.68086100	1.80906000	H	1.59541500	4.98090200	-0.86962000
H	-3.34300300	-3.40447800	2.13794800	C	0.92607200	2.88393400	-3.54766500
C	-2.23754800	-0.71302800	-3.06980800	H	0.34477800	1.97223500	-3.71068100
H	-1.59116800	0.12428500	-2.78364700	H	0.62249600	3.62894500	-4.29028900
H	-1.59523000	-1.50420400	-3.46776500	H	1.98129100	2.64696300	-3.71094000
H	-2.89591300	-0.37325400	-3.87426000	C	-0.96628500	4.45745300	-0.48553800
C	1.97690000	-3.66643500	1.68479600	H	-0.82131700	5.50008700	-0.78574800
H	2.52825000	-3.91825900	2.59416000	H	-1.99010400	4.34872200	-0.11610400
H	1.13423400	-3.02511800	1.96298600	H	-0.28593800	4.23147800	0.33928700
H	1.55642000	-4.59629200	1.28395300	C	-1.75124900	3.79178600	-2.77520800
C	2.67620700	-1.33803500	-2.77995200	H	-1.70963000	3.04045200	-3.56591300
H	3.48598100	-0.95146000	-3.40404400	H	-2.76585700	3.79460500	-2.36584900
H	2.15275600	-2.11201700	-3.35180700	H	-1.56333800	4.77612500	-3.21822400
H	1.96384700	-0.52495800	-2.60278500	H	-1.50696400	-4.58531100	-1.21545900
C	1.72904400	1.81815700	1.60014700	H	-1.26146800	-3.74462600	-2.75295600
C	2.88940000	1.23469300	1.08009200	H	0.85024400	-4.87262200	-0.97914200
C	1.84688100	2.84755900	2.54828900	H	1.09072900	-4.07981600	-2.54315500
C	4.14635900	1.68945900	1.48744900	C	-0.21477100	0.60591900	2.15137100
H	2.80732500	0.43815200	0.34827700	N	0.39582700	1.44022100	1.22001200
C	3.10280900	3.28927700	2.95674400	H	0.44004800	0.12816700	2.87829900
H	0.94271500	3.29347300	2.95169600				
C	4.26174200	2.71500500	2.42456800	L₁-9₂			
H	5.03679400	1.23053800	1.06629900	C	-1.60983200	-1.73737000	-0.00480800
H	3.17642700	4.08822000	3.68973900	C	-2.59277500	-3.84690000	-0.43277900
H	5.24091200	3.06234500	2.74170000	C	-3.70550300	-2.80140500	-0.25647600
C	-1.63193600	0.66565900	2.47046900	N	-2.93812800	-1.53904900	-0.14753100
C	-2.12256900	-0.07488200	3.57192800	N	-1.37889500	-3.06290200	-0.11555100
C	-2.55350000	1.45507000	1.74585700	C	-4.11582900	0.32732900	-1.20530400
C	-3.46218800	-0.01987600	3.93861600	C	-3.61207100	-0.27596100	-0.03701000
H	-1.42941300	-0.68457400	4.14804700	C	-3.80177900	0.31367000	1.22717600
C	-3.89513700	1.49988400	2.11874000	C	-4.47696300	1.53710200	1.29021700
H	-2.20410800	2.02148200	0.89097000	C	-4.96732000	2.17587600	0.14819600
C	-4.36355200	0.77037700	3.21499600	C	-4.78374900	1.54995700	-1.08855300
H	-3.80644900	-0.58843400	4.79928200	H	-4.61983000	2.00193000	2.26284200
H	-4.58273200	2.12077100	1.54896900	H	-5.16882700	2.02431900	-1.98846700
H	-5.40880700	0.82047000	3.50698100	C	0.70007300	-3.66745600	-1.27980900
B	0.22391900	1.62318600	-0.74391100	C	1.94514300	-4.30273600	-1.24932000
C	0.75365400	3.40187000	-2.11204900	C	2.42723300	-4.93219900	-0.09736800
O	1.28285800	2.38123000	-1.22559200	C	1.62528000	-4.92078600	1.04817400
C	-0.75065700	3.49376700	-1.66067600				

C	0.37365800	-4.29851800	1.06750200	H	0.38197400	0.10882600	3.78169700
C	-0.07875200	-3.67432800	-0.10844700	C	-0.29161900	3.77849100	2.78065000
H	2.55547200	-4.30074600	-2.14948700	H	0.68007700	3.30107300	0.92478200
H	1.98524800	-5.40114500	1.95496400	C	-0.70647400	3.32585800	4.03469100
Cu	-0.21957200	-0.46825300	0.43542700	H	-0.75119000	1.62381900	5.36210600
C	-5.65702400	3.51583700	0.24799600	H	-0.45905600	4.81513300	2.49660900
H	-6.25991300	3.58855100	1.15846400	H	-1.19977400	3.99751200	4.73157500
H	-4.92485200	4.33201000	0.27941300	B	1.76409100	1.57938000	-0.99547100
H	-6.31206900	3.69566700	-0.60946200	C	1.79586300	2.39484700	-3.13879500
C	3.79241900	-5.57800500	-0.08193300	O	2.48515900	2.38204600	-1.86991600
H	3.84031100	-6.39766800	0.64109100	C	0.31986900	2.03075600	-2.72093600
H	4.05890300	-5.97545200	-1.06594300	O	0.53298300	1.21263800	-1.54187300
H	4.56575800	-4.85154600	0.19629300	C	1.96961300	3.77595900	-3.76965900
C	-3.29241200	-0.32414800	2.49709800	H	3.02675400	3.94574600	-3.99363200
H	-3.34122500	-1.41615300	2.45951400	H	1.40758600	3.85334000	-4.70657500
H	-2.24877100	-0.04757600	2.68366600	H	1.63930200	4.56818700	-3.09578000
H	-3.87913000	0.01464800	3.35539200	C	2.45224600	1.32613400	-4.02639100
C	-3.96278500	-0.31997800	-2.56186600	H	2.33647400	0.32809300	-3.59382600
H	-2.97815100	-0.77885300	-2.68388000	H	2.03113800	1.31850000	-5.03658000
H	-4.71209600	-1.10617900	-2.72303800	H	3.52203900	1.53985400	-4.10281300
H	-4.09904500	0.41594400	-3.35869900	C	-0.50560700	3.24912900	-2.28412700
C	-0.45077100	-4.27619400	2.33240600	H	-0.76835500	3.88694100	-3.13404600
H	0.09370700	-4.74398600	3.15636000	H	-1.42898600	2.90060800	-1.81325200
H	-0.69451200	-3.24960300	2.62484500	H	0.03811500	3.85342600	-1.55304600
H	-1.39953100	-4.81415600	2.21779300	C	-0.45925800	1.21692800	-3.75169100
C	0.23157400	-2.96572700	-2.53218800	H	0.03389100	0.26856400	-3.97357500
H	0.90216200	-3.18139900	-3.36802400	H	-1.45914600	0.99965900	-3.36740700
H	-0.77833100	-3.27248600	-2.82614300	H	-0.57103000	1.77728200	-4.68625800
H	0.20926400	-1.87998000	-2.38525500	H	-4.29120500	-2.95986000	0.65733300
C	3.53572500	1.38525500	0.74131700	H	-4.39820100	-2.76937800	-1.10097800
C	4.61653800	1.29481600	-0.15741000	H	-2.69626100	-4.69943100	0.24384500
C	3.82883800	1.61038000	2.09905500	H	-2.53543200	-4.23363100	-1.45761200
C	5.92903800	1.44757800	0.28274200	C	1.23212800	0.59801400	1.25984400
H	4.42080500	1.10763400	-1.20568700	N	2.19562700	1.19567200	0.29901800
C	5.14715700	1.75458500	2.53146500	H	1.78795300	-0.14239700	1.84853600
H	3.02218400	1.69036000	2.81652000				
C	6.20957600	1.67801300	1.63108100	L₁-16₂			
H	6.74049300	1.37166400	-0.43702500	Cu	-0.83290200	0.00581400	-0.46942100
H	5.33885800	1.93456200	3.58634600	N	1.83500000	0.71881600	0.36943400
H	7.23468300	1.79102500	1.97211500	N	-3.75564200	0.53408400	-0.28737100
C	0.59479400	1.57168400	2.20840200	N	-3.18436200	-1.53263400	0.07407200
C	0.18261400	1.13856400	3.48855800	O	4.08220800	1.50928100	1.11043900
C	0.34755100	2.91978100	1.88544100	O	3.63500700	1.38259300	-1.14977500
C	-0.45748300	1.99444600	4.38237900				

B	3.14811400	1.20997100	0.13346500	H	5.88803700	4.12018900	0.00338900
C	-2.70510500	-0.30629300	-0.21830400	H	4.91988900	3.93422000	1.47750000
C	-5.01963000	-0.10796300	0.11593900	C	5.06748400	1.49000400	-1.01311700
C	-4.65203700	-1.58801100	0.08832100	C	5.60379700	2.36666600	-2.12581500
C	-2.32150900	-2.66569000	0.17810200	H	5.45761400	1.87641400	-3.09198600
C	-2.11085000	-3.24224900	1.44001400	H	6.67733800	2.54392000	-1.99749500
C	-1.14411700	-4.24049100	1.55197500	H	5.09423300	3.33189800	-2.15757300
H	-0.95042700	-4.67356800	2.53289700	C	5.62864300	0.07750300	-1.12035100
C	-0.39573400	-4.66710400	0.45171500	H	5.27119900	-0.54923500	-0.29724900
C	-0.66872600	-4.10472000	-0.79496100	H	6.72346400	0.06891400	-1.11579100
H	-0.08885200	-4.41934000	-1.66059500	H	5.27820700	-0.37600400	-2.05164400
C	-1.63265100	-3.11008500	-0.96049800	C	1.65784200	-1.15520800	-1.24558700
C	-1.90448100	-2.52725900	-2.31363800	C	1.40214000	-1.60496500	-2.55468500
C	-2.88470600	-2.77863900	2.63598000	H	0.81976200	-0.96560100	-3.21899600
C	-3.63347500	1.94971900	-0.40637600	C	1.87848500	-2.82441500	-3.01463300
C	-2.97268200	2.68232900	0.59428500	H	1.66728700	-3.13281800	-4.03708700
C	-2.36318400	2.02315200	1.79370000	C	2.63676400	-3.64855300	-2.17871400
C	-2.87604000	4.06487500	0.42959700	H	3.01747100	-4.60129900	-2.53804900
H	-2.36251500	4.64427100	1.19554800	C	2.90666500	-3.21931100	-0.88211200
C	-3.41235800	4.72213100	-0.67844500	H	3.50395900	-3.84217400	-0.21847400
C	-4.05802400	3.95898700	-1.65160900	C	2.42779900	-1.99456200	-0.42152600
H	-4.46534300	4.45120800	-2.53397100	H	2.66487900	-1.66944100	0.59021500
C	-4.17933300	2.57468600	-1.53776400	H	-1.36807500	1.60866600	1.57416800
C	-4.84971300	1.77616300	-2.61306500	H	-5.89747000	1.55545400	-2.37243400
C	1.11014100	0.15196800	-0.79063000	H	-1.45057500	-1.53298900	-2.42195800
H	1.22432800	0.86803400	-1.61364600	H	-3.91337400	-3.16125700	2.63193500
C	1.29824300	0.56799000	1.65542300	H	-5.83152800	0.14920100	-0.57058700
C	0.50430400	-0.54770000	1.98506500	H	-5.01510300	-2.09684700	-0.81561800
H	0.35994600	-1.34301900	1.25401700	C	0.66610400	-5.71279900	0.60100100
C	-0.05416900	-0.66875300	3.25476000	H	0.23537100	-6.71817300	0.67582400
H	-0.63815500	-1.55522700	3.48929500	H	1.34873100	-5.70384900	-0.25299000
C	0.15439400	0.30911300	4.22367300	H	1.26016500	-5.55292700	1.50612200
H	-0.28429900	0.21029100	5.21264400	C	-3.31363400	6.21126500	-0.80929100
C	0.95107800	1.40891200	3.90796100	H	-3.36746800	6.52901700	-1.85393700
H	1.12619100	2.18419800	4.65010200	H	-4.13074400	6.71360800	-0.27854500
C	1.51694300	1.53919200	2.64518900	H	-2.37974400	6.59300800	-0.38783900
H	2.13014400	2.40215500	2.40508900	H	-4.85304500	2.32014400	-3.56055600
C	5.21322300	2.08842900	0.41976800	H	-4.34866200	0.81524000	-2.77125200
C	6.48141800	1.69228500	1.14759100	H	-1.49021900	-3.16157000	-3.10094300
H	6.50234500	2.14595600	2.14228500	H	-2.97802400	-2.40044500	-2.49451200
H	7.36624200	2.03775600	0.60154000	H	-2.42330200	-3.12546000	3.56402800
H	6.55055100	0.60971300	1.26966300	H	-2.94818700	-1.68506800	2.67661200
C	5.03061900	3.60010800	0.44230500	H	-2.23814200	2.73721700	2.61173100
H	4.13181300	3.89429000	-0.10825900	H	-2.96306900	1.18359300	2.16113100

H	-5.30308000	0.23884100	1.11991800	C	0.40423100	1.90660100	0.98446400
H	-5.02240100	-2.14066400	0.95652700	H	0.07944600	0.93862400	1.35928700
L₁-17₃				C	-0.29614800	3.04865900	1.35982500
Cu	-0.44102900	-0.33672200	-0.63767100	H	-1.17296100	2.93869600	1.99483000
N	2.22775300	0.82179700	-0.22587100	C	0.12613600	4.30522100	0.93848100
N	-3.21488700	0.38038900	-1.41739000	H	-0.41858000	5.19864000	1.23332600
N	-2.78769000	-1.75389800	-1.40894000	C	1.25797800	4.39730500	0.12944600
O	4.52508500	1.81097100	-0.31235900	H	1.59881200	5.37031100	-0.21938200
O	4.24933300	-0.42461100	-0.80557000	C	1.95865600	3.26024500	-0.25857200
B	3.63034500	0.76178700	-0.44790300	H	2.83415700	3.34856000	-0.89244200
C	-2.25664400	-0.53703100	-1.17102900	C	5.79140800	1.32869500	-0.81806300
C	-4.40917800	-0.21887300	-2.04019300	C	6.90960000	1.98684300	-0.03663600
H	-5.33098900	0.19629800	-1.62550600	H	6.92211200	3.06271000	-0.23136300
C	-4.22117100	-1.69863700	-1.73106000	H	7.88225000	1.57969000	-0.33399400
H	-4.81582800	-2.02127400	-0.86420400	H	6.78676000	1.84063500	1.03810200
C	-2.02238600	-2.95750400	-1.34151900	C	5.86709100	1.71032500	-2.29022300
C	-2.15981300	-3.82456700	-0.24759700	H	5.07986900	1.21236700	-2.86422900
C	-1.36623700	-4.97182600	-0.21558900	H	6.83368600	1.44417200	-2.72964600
H	-1.45403900	-5.64313900	0.63816500	H	5.73109700	2.79030000	-2.39112200
C	-0.43467800	-5.25630100	-1.21460200	C	5.66230100	-0.21139700	-0.60767800
C	-0.32839400	-4.37285100	-2.29044700	C	6.42831900	-1.05783600	-1.60358900
H	0.39234300	-4.57740800	-3.08078100	H	6.26988400	-2.11863900	-1.39149000
C	-1.11226100	-3.22356500	-2.37820000	H	7.50363800	-0.85876800	-1.53935100
C	-0.94972800	-2.27638600	-3.52571200	H	6.10117900	-0.86654500	-2.62771000
H	-1.91369500	-1.92811700	-3.91377000	C	5.98676500	-0.63239800	0.81977900
C	-3.08788800	-3.50412000	0.88111400	H	5.46543300	0.00204100	1.54348300
H	-4.13083200	-3.74824400	0.64261600	H	7.06069300	-0.58021800	1.02608300
C	-3.02204000	1.79084900	-1.32426000	H	5.65068500	-1.66048800	0.97679300
C	-3.84584000	2.53098700	-0.46077900	C	1.59945900	-1.26880700	0.98178200
C	-4.94029900	1.89220600	0.33985900	C	1.05022400	-2.56818500	0.99606100
H	-5.90762900	1.94913700	-0.17613600	H	0.60584000	-2.95298200	0.07686500
C	-3.63019400	3.90588100	-0.35411000	C	1.04776200	-3.34475000	2.14422900
H	-4.25428900	4.48040000	0.32965000	H	0.60489100	-4.33987400	2.11497200
C	-2.63047500	4.55457900	-1.07500700	C	1.60162400	-2.85508400	3.33218000
C	-1.84180200	3.79217200	-1.93634100	H	1.59428200	-3.45751400	4.23629100
H	-1.05061000	4.27887000	-2.50502900	C	2.16626900	-1.58402400	3.33318200
C	-2.01773800	2.41833200	-2.08548800	H	2.60187300	-1.18587600	4.24769500
C	-1.14917400	1.66649200	-3.04641800	C	2.16659400	-0.79991000	2.17752200
H	-1.69072600	0.86086200	-3.55380900	H	2.60483900	0.19754400	2.19670800
C	1.48991600	-0.45473400	-0.25765800	H	-5.06545500	2.39854900	1.30080000
H	1.89482600	-1.04407900	-1.09064600	H	-4.74530800	0.83532400	0.54516800
C	1.54512400	1.98690200	0.16539300	H	-0.74426600	2.33990100	-3.80644700
				H	-0.29572800	1.19495300	-2.53643600
				H	-0.39582700	-2.74060100	-4.34493900

H	-0.39894600	-1.37777700	-3.21364900	C	-2.20878800	2.50060500	-1.81211100
H	-2.82206900	-4.07265000	1.77625800	C	-2.70982200	1.21458700	-2.39624300
H	-3.05723300	-2.43842800	1.13449500	H	-1.90188600	0.51356000	-2.62600800
C	-2.41022700	6.03012100	-0.94671700	C	1.07047400	4.34721900	-1.11542400
H	-1.34381400	6.27518100	-0.97074100	H	1.58951000	4.09008200	-2.04531000
H	-2.88440800	6.58106900	-1.76739100	C	2.74806300	-0.43504800	-2.02665200
H	-2.82501300	6.42058800	-0.01324500	C	4.05875700	-0.01761200	-1.75501400
C	0.47094300	-6.44278800	-1.09936200	C	4.43875900	1.42403500	-1.88226400
H	1.36301300	-6.19140100	-0.51302400	H	4.11080300	1.85233300	-2.83595300
H	-0.01713400	-7.28065800	-0.59386200	C	4.97669800	-0.97646400	-1.32822900
H	0.81705700	-6.78876700	-2.07691200	H	5.99435900	-0.66403900	-1.09803900
H	-4.39916900	-0.00978000	-3.12017100	C	4.62171600	-2.31865000	-1.17799100
H	-4.46019100	-2.35377600	-2.57370700	C	3.30923800	-2.69601100	-1.46369800
C	0.13031900	1.03854700	4.59694200	H	3.00545800	-3.73101800	-1.31180600
H	0.31044600	1.70120600	5.43773500	C	2.35326800	-1.77353400	-1.88887300
H	0.89100200	0.99819500	3.82005900	C	0.93950000	-2.20266200	-2.13610800
Br	-2.71320700	0.15377600	2.25533300	H	0.77442200	-2.47705900	-3.18651500
C	-0.97920900	0.30389800	4.51102100	C	-0.93717000	-0.09557400	0.62883000
H	-1.74369800	0.36881700	5.28497500	H	-1.32603700	0.19801700	-0.35539100
C	-1.25964600	-0.60902900	3.38363000	C	0.08266700	-2.25617000	1.39355500
H	-0.40742800	-0.74304000	2.71380400	C	1.44058800	-1.92439700	1.31121200
H	-1.64277700	-1.58419100	3.68875700	H	1.76417600	-1.13075300	0.63928100
L₁-TS18₃				C	2.39076800	-2.60226700	2.06535500
Cu	0.82546100	0.89671400	0.39079600	H	3.43655300	-2.31339900	1.97645300
N	-0.89777900	-1.56728500	0.64291100	C	2.00944200	-3.63602400	2.91854000
N	1.79402200	0.54677700	-2.42997100	H	2.75085300	-4.16300000	3.51308200
N	0.10688700	1.90418000	-2.29814900	C	0.66426300	-3.99091100	2.99130500
O	-1.99875500	-3.64824700	-0.16639500	H	0.34861600	-4.79828900	3.64745100
O	-2.92715800	-1.61224000	-0.73408700	C	-0.28879600	-3.30953700	2.24085800
B	-1.91374500	-2.26850100	-0.05018700	H	-1.33813700	-3.58625200	2.30259600
C	0.99710000	1.20623200	-1.56395000	C	-3.01660600	-3.90414400	-1.16089800
C	1.34576800	0.66540000	-3.82783800	C	-3.72234800	-5.19869000	-0.81490700
H	2.19307700	0.85054700	-4.49473300	H	-3.03115600	-6.04084000	-0.90694600
C	0.36749700	1.82877000	-3.74517000	H	-4.56268600	-5.37669400	-1.49469300
H	0.80516200	2.77507100	-4.09394700	H	-4.10179700	-5.18560300	0.20868500
C	-0.84317800	2.81802000	-1.75411000	C	-2.31998600	-4.01262900	-2.51106100
C	-0.38821200	4.01421000	-1.17210500	H	-1.85643100	-3.05923400	-2.78592200
C	-1.33603600	4.88004200	-0.62686000	H	-3.01601700	-4.29874300	-3.30612500
H	-0.99417600	5.80413200	-0.16241800	H	-1.53339700	-4.76965500	-2.45356100
C	-2.70278200	4.59554400	-0.66087100	C	-3.90314400	-2.62556100	-1.05888700
C	-3.11582600	3.40669700	-1.25974900	C	-4.61042500	-2.23476400	-2.34033800
H	-4.17550200	3.15521000	-1.26918800	H	-5.20528300	-1.33056900	-2.18150000
				H	-5.29031700	-3.02918400	-2.66690700
				H	-3.90013800	-2.03492200	-3.14602500

C	-4.88595700	-2.68843500	0.10337900				
H	-4.38383300	-3.01162600	1.02104500	Cu	1.07238000	0.39450900	0.72290000
H	-5.71436500	-3.37543600	-0.09684300	N	-1.21238900	-1.67359200	0.13102100
H	-5.29554400	-1.69106500	0.28360100	N	2.70141000	1.02178600	-1.65004400
C	-1.84953100	0.49234800	1.64763400	N	0.95751000	2.31447800	-1.69634400
C	-2.01942000	1.88898200	1.68253400	O	-3.22407200	-2.91933900	-0.65812000
H	-1.45796800	2.50074300	0.97408000	O	-3.26157000	-0.61271400	-0.70386400
C	-2.85494100	2.49686200	2.60797600	B	-2.53299500	-1.75211400	-0.40631300
H	-2.95824100	3.58067600	2.60259300	C	1.50398600	1.25263500	-1.07913700
C	-3.54512100	1.72834300	3.54861700	C	3.02617200	1.95735500	-2.73844300
H	-4.19127300	2.20160000	4.28301100	H	3.97058100	2.47335000	-2.53231500
C	-3.38464700	0.34623700	3.53320000	C	1.82129400	2.89716700	-2.73786800
H	-3.91251400	-0.26850300	4.25960800	H	2.08768100	3.92689500	-2.47436600
C	-2.55588800	-0.26487500	2.59389200	C	-0.35326100	2.81234400	-1.43170800
H	-2.44165500	-1.34728100	2.59662700	C	-0.53236700	4.02537800	-0.74989300
H	5.51993600	1.55663700	-1.79953800	C	-1.83953600	4.40519900	-0.43134900
H	3.96646300	2.02133900	-1.09269800	H	-1.98995600	5.32680800	0.12966100
H	0.68460200	-3.07626800	-1.52873300	C	-2.94545300	3.63653200	-0.79239700
H	0.22136200	-1.41380600	-1.88299100	C	-2.73015100	2.48683000	-1.55329400
H	-3.28504600	1.38510600	-3.31460300	H	-3.57686900	1.89023600	-1.88293900
H	-3.36623700	0.70028700	-1.68795800	C	-1.44888500	2.06288700	-1.89496200
H	1.21967000	5.41300600	-0.92584000	C	-1.25312800	0.84418600	-2.74615500
H	1.57913400	3.79215800	-0.31745900	H	-0.54620300	1.02920100	-3.56326800
C	5.62194500	-3.33442500	-0.71747000	C	0.61897800	4.91477100	-0.40106500
H	6.03149600	-3.90422300	-1.55961200	H	0.86964800	5.57359000	-1.24313900
H	6.46586500	-2.86674100	-0.20357700	C	3.48339000	-0.15008100	-1.41883500
H	5.16960500	-4.06061200	-0.03515800	C	4.64410500	-0.07072100	-0.63455800
C	-3.70192300	5.54602900	-0.07507300	C	5.05657000	1.22235000	-0.00954800
H	-4.12478600	6.20671600	-0.84090500	H	5.32909400	1.97007200	-0.76450100
H	-4.53962600	5.01345000	0.38436300	C	5.37641400	-1.24065700	-0.43552400
H	-3.24987400	6.18598500	0.68754800	H	6.27183400	-1.19561700	0.18361500
H	0.86112600	-0.26912500	-4.14662200	C	4.98508400	-2.46366500	-0.98543400
H	-0.56076500	1.66199100	-4.30064800	C	3.83792200	-2.49709200	-1.77932500
C	0.53380800	0.23323300	3.73387700	H	3.51901000	-3.44043100	-2.22120500
H	0.05994000	-0.74368600	3.75093300	C	3.07655100	-1.35201600	-2.01659900
H	-0.11709900	1.08983200	3.57088900	C	1.83732900	-1.41547500	-2.85580400
Br	2.70882800	1.93760700	1.45834100	H	1.80941200	-0.62370700	-3.61325000
C	1.86250400	0.38976300	3.94510100	C	-0.83685500	-0.33907000	0.58162200
H	2.49190600	-0.49138600	4.05953600	H	-1.02804600	0.37608800	-0.21830500
C	2.49476300	1.65290900	3.83160300	C	-0.48117200	-2.84701200	0.45874700
H	1.89012000	2.54716900	3.94504600	C	0.88433600	-2.93865800	0.17884600
H	3.54211300	1.76698000	4.09055900	H	1.39699900	-2.07607700	-0.23896500
				C	1.59191400	-4.10051600	0.46459800
				H	2.65630000	-4.13957900	0.24011900

L₁-19₃

H	-6.17726400	1.39117200	-0.25967500	C	0.69220300	-2.18445700	-0.02576300
C	-0.31308000	3.54749000	-0.77128800	C	-0.23816100	-2.95896200	-0.74730200
C	-0.13464400	4.07485000	0.51313800	H	-0.61587000	-2.57020500	-1.69408000
C	-1.20627500	3.94347400	1.54994200	C	-0.69297600	-4.18053600	-0.27465700
H	-2.08703700	4.55931200	1.32924900	H	-1.41940900	-4.74735200	-0.85544900
C	1.09626100	4.65762400	0.81431700	C	-0.21898900	-4.68870800	0.93849300
H	1.25806000	5.05377200	1.81527100	H	-0.56967700	-5.64846700	1.30860600
C	2.13948200	4.69355400	-0.10948400	C	0.70593200	-3.94349300	1.66398700
C	1.93260800	4.13008500	-1.37097400	H	1.08808100	-4.32488200	2.60870600
H	2.74535700	4.12868200	-2.09638200	C	1.15394000	-2.70898800	1.19328300
C	0.71688100	3.54923000	-1.72344300	H	1.88155100	-2.14201100	1.77158800
C	0.53032400	2.88633900	-3.05315000	H	-0.83504600	4.24108100	2.53362400
H	-0.41670300	3.16491200	-3.52944500	H	-1.54900600	2.90280200	1.62323600
C	1.10894700	-0.85713800	-0.54775200	H	1.34512900	3.13360900	-3.73749900
H	1.32404100	-0.97549300	-1.61911600	H	0.50976600	1.79319600	-2.93865600
C	2.24674700	0.59475900	1.12332700	H	-2.02244300	-1.16255600	-4.11341100
C	1.10221600	0.63802300	1.93733100	H	-1.00732500	-0.56210400	-2.79532300
H	0.31025100	-0.09107500	1.78358500	H	-5.87699800	0.36538200	1.14105900
C	0.99123000	1.56572600	2.96842600	H	-4.66646300	1.55236500	0.65193400
H	0.09042200	1.56490600	3.57898700	C	3.47061200	5.27421200	0.25443500
C	2.02202300	2.46523600	3.22499600	H	3.80756800	6.01428400	-0.47886900
H	1.93754500	3.18829300	4.03256400	H	3.44559500	5.75708300	1.23490600
C	3.16560200	2.42287600	2.42803000	H	4.23912100	4.49372600	0.29396600
H	3.97846400	3.12395900	2.60778200	C	-5.07053000	-3.93323500	-1.27026900
C	3.27901500	1.50951700	1.38675700	H	-4.81266000	-4.51352400	-2.16017600
H	4.16953400	1.49335500	0.76599400	H	-4.57715600	-4.41392300	-0.41571700
C	5.73354100	-1.59896800	-0.38483700	H	-6.14871200	-4.01870800	-1.10684700
C	6.75181100	-2.20397300	0.55997800	H	-2.53356700	4.42977100	-2.28651000
H	7.33266800	-1.41419500	1.04406300	H	-3.81016700	2.52141200	-2.99110700
H	7.44931100	-2.84992800	0.01534200	C	-2.39790300	-1.73505500	1.52023800
H	6.27163700	-2.79522100	1.34232300	Br	-2.58336400	0.04992500	2.37386100
C	6.40109900	-0.61452300	-1.33560700	C	-3.45328700	-2.64393200	2.01364300
H	5.67449600	-0.19652400	-2.03897100	C	-3.20038200	-3.80848600	2.61177000
H	7.20371800	-1.08738300	-1.91037100	H	-4.00161300	-4.46498900	2.93788100
H	6.83068700	0.20947800	-0.75971100	H	-2.17934200	-4.14353400	2.77881800
C	4.83763800	-2.63486300	-1.13195100	H	-4.48111700	-2.32043500	1.84843000
C	5.36051600	-3.06645200	-2.48643700	H	-2.46985400	-1.51824100	0.44910700
H	4.67129000	-3.78178400	-2.94282900	H	-1.38808900	-2.08140100	1.75222700
H	6.33649600	-3.55425500	-2.38899600				
H	5.46394800	-2.21746200	-3.16521600				
C	4.50223500	-3.84625900	-0.27163900				
H	4.15664000	-3.53866400	0.72023300				
H	5.36360900	-4.51077600	-0.14944100				
H	3.69144100	-4.40888500	-0.74228700				
				L₁-TS18₄			
				N	-1.82654800	0.75963200	0.47682600
				N	0.43363500	-2.55071600	-1.40536400
				N	2.40726100	-1.70755700	-1.72163400

O	-4.30135800	1.04163500	0.22218400	H	-3.76575700	-0.86044200	1.37515900
O	-2.91792100	1.71538100	-1.49273500	C	-5.15080800	1.34279600	-0.90717200
B	-2.99859200	1.14691200	-0.23061200	C	-6.41281600	2.01071900	-0.40210700
C	1.26367200	-1.56933400	-1.01649300	H	-6.99136700	1.31011100	0.20606700
C	1.05992200	-3.50607200	-2.33683100	H	-7.04412400	2.33165600	-1.23782700
H	1.24725200	-4.45817300	-1.82133700	H	-6.18510000	2.88200700	0.21456600
C	2.34417100	-2.78349100	-2.72591600	C	-5.47574400	0.01928200	-1.58678800
H	3.23305900	-3.42065900	-2.67487300	H	-4.56730400	-0.44019100	-1.99004300
C	3.44759000	-0.73361200	-1.71501900	H	-6.19422800	0.14246800	-2.40323700
C	4.67127600	-1.04268800	-1.10565100	H	-5.90276400	-0.66886600	-0.85071700
C	5.65752100	-0.05386800	-1.07803300	C	-4.22929200	2.25095400	-1.77906000
H	6.60709300	-0.27520100	-0.59260600	C	-4.47659800	2.16197900	-3.27087900
C	5.45319200	1.20974500	-1.63539200	H	-3.78717200	2.82085800	-3.80541300
C	4.23196800	1.46949900	-2.26280500	H	-5.49765200	2.47431700	-3.51510400
H	4.06212200	2.44339100	-2.72092200	H	-4.32758100	1.14527400	-3.64202500
C	3.21965800	0.51205400	-2.32347000	C	-4.23029200	3.70120900	-1.31494800
C	1.92967400	0.79319600	-3.03146000	H	-4.08906500	3.76783000	-0.23188600
H	1.08469500	0.82763900	-2.33395200	H	-5.16423700	4.21108100	-1.57237900
C	4.91103900	-2.39182100	-0.50618900	H	-3.40306900	4.23203900	-1.79281700
H	5.16360100	-3.13364900	-1.27484100	C	-0.23874700	2.64850700	0.35235900
C	-0.82312500	-2.85496700	-0.79820600	C	0.75177400	3.37986400	-0.34288700
C	-0.84638200	-3.55577100	0.41684200	H	1.23896700	2.91275000	-1.19997500
C	0.41704200	-3.84780300	1.16223300	C	1.10865600	4.66545400	0.03681000
H	0.24033300	-4.55757000	1.97383400	H	1.87966600	5.19493800	-0.51844400
C	-2.08714700	-3.93325200	0.92889200	C	0.48117200	5.28250000	1.12025100
H	-2.12238900	-4.46358100	1.87969700	H	0.75652500	6.29064400	1.41638900
C	-3.27878000	-3.62262300	0.27520300	C	-0.52069800	4.59099200	1.80210200
C	-3.21593100	-2.90442900	-0.91985700	H	-1.03315300	5.06514800	2.63627700
H	-4.13959000	-2.64851300	-1.43759700	C	-0.86908500	3.29535200	1.43585700
C	-2.00035100	-2.49731500	-1.46947900	H	-1.65231000	2.77107700	1.97903900
C	-1.96402100	-1.64781400	-2.70349700	H	0.83265500	-2.93217300	1.60505100
H	-1.09020300	-1.84811400	-3.33075200	H	1.20440100	-4.25556100	0.51729000
C	-0.54966900	1.26938800	-0.05013300	H	-2.86232100	-1.79098100	-3.31149700
H	-0.60113900	1.21817200	-1.14305000	H	-1.91969800	-0.58288400	-2.43509300
C	-1.82592400	0.02653400	1.67725700	H	1.68920100	0.01086100	-3.76100400
C	-0.72223400	0.07755800	2.54824600	H	1.97011300	1.74781100	-3.56169600
H	0.09856000	0.76460700	2.34755100	H	5.74077200	-2.36559400	0.20358900
C	-0.67589500	-0.71722600	3.69138800	H	4.02368600	-2.74651300	0.02577100
H	0.20969900	-0.67337600	4.31984900	C	-4.60234100	-3.98444100	0.87387000
C	-1.74080000	-1.54705500	4.02163700	H	-5.32406800	-4.29946900	0.11403100
H	-1.70704100	-2.16236000	4.91621400	H	-4.51056200	-4.78684700	1.61088000
C	-2.85988900	-1.56386700	3.18930300	H	-5.04319100	-3.12232200	1.39116700
H	-3.70508900	-2.20679600	3.42942700	C	6.49989700	2.27589400	-1.52834600
C	-2.90504700	-0.79982300	2.03167300	H	6.29628200	2.94125100	-0.68065200

H	7.49582800	1.85319000	-1.37319200
H	6.53286900	2.90512000	-2.42222800
H	0.39850600	-3.71191000	-3.18478100
H	2.29805400	-2.35266500	-3.73629900
Cu	0.90679300	-0.14359900	0.30368500
Br	2.75335100	-0.92067300	2.03260000
C	2.42758100	2.97186200	2.99589900
H	1.44379000	3.16057000	2.57317700
H	2.67225300	3.46803400	3.92986400
C	3.30470400	2.14256600	2.38751300
H	4.27411800	1.94798000	2.84418000
C	3.02051600	1.48941200	1.15883600
H	2.10485300	1.76039900	0.63954200
H	3.81722000	1.07066200	0.55515800

L₁-19₄

Cu	1.38960800	-0.28284500	0.61400900
N	-1.24409100	0.69381000	0.52243800
N	0.09595300	-2.52450400	-1.30593400
N	1.96578700	-1.56276800	-1.84251700
O	-3.60567600	1.43696200	0.20124500
O	-2.02718100	2.05231400	-1.36271400
B	-2.29072000	1.35102200	-0.19816800
C	0.92263100	-1.51652300	-0.98309700
C	0.64323300	-3.39496700	-2.36948300
H	0.92313100	-4.36371900	-1.93693600
C	1.84333600	-2.60567200	-2.87005600
H	2.75790800	-3.20408100	-2.92845500
C	2.98345600	-0.56140100	-1.87729200
C	4.28010500	-0.88221700	-1.44241600
C	5.22581100	0.14280400	-1.38524800
H	6.22580400	-0.09064700	-1.02235500
C	4.92188400	1.45303100	-1.75424500
C	3.64608900	1.71832100	-2.25408000
H	3.40474900	2.72527600	-2.59479500
C	2.66561800	0.72917600	-2.34249200
C	1.35427000	1.04587200	-2.99949600
H	0.54974000	0.37379500	-2.69488500
C	4.65701700	-2.28352700	-1.07871200
H	5.01400000	-2.83102200	-1.96113000
C	-1.26317800	-2.72983600	-0.90857600
C	-1.57662900	-3.65000100	0.09896200
C	-0.50838700	-4.32031900	0.89758500

H	0.04223100	-5.06003300	0.30284000
C	-2.92628700	-3.91429100	0.34417300
H	-3.18153200	-4.60964800	1.14293800
C	-3.94695900	-3.29718800	-0.37480300
C	-3.59554900	-2.40296600	-1.38874800
H	-4.37889500	-1.92964600	-1.97936600
C	-2.26382000	-2.10539200	-1.67299000
C	-1.91605300	-1.14938500	-2.77297000
H	-1.07324200	-1.49850300	-3.38057700
C	0.08190000	1.26540500	0.27546600
H	0.23664700	1.31627900	-0.80171400
C	-1.49501300	-0.10461500	1.66127100
C	-0.58778300	-0.16276400	2.72756300
H	0.29508600	0.46927600	2.72333200
C	-0.82306900	-0.99961800	3.81454700
H	-0.08549900	-1.03960900	4.61237200
C	-1.97838900	-1.77069700	3.87916400
H	-2.16126500	-2.42297700	4.72827900
C	-2.89676500	-1.69238600	2.83362700
H	-3.80305600	-2.29436600	2.85625600
C	-2.66034500	-0.88030400	1.73320200
H	-3.36530300	-0.86694000	0.90793200
C	-4.31891800	2.10374900	-0.86709100
C	-5.40538800	2.96394600	-0.25530200
H	-6.15247100	2.33212100	0.23215200
H	-5.91427100	3.55374100	-1.02538800
H	-5.00106500	3.64674500	0.49385000
C	-4.92325800	1.01775700	-1.74439100
H	-4.13813900	0.41918400	-2.21622200
H	-5.56166700	1.43404100	-2.53001300
H	-5.52762000	0.34978400	-1.12325300
C	-3.18025900	2.89943400	-1.58432700
C	-3.37087000	3.07660100	-3.07620800
H	-2.52812500	3.63158500	-3.49729200
H	-4.28477000	3.64195800	-3.28740800
H	-3.43144200	2.11508200	-3.59136500
C	-2.88208500	4.23238200	-0.91132500
H	-2.73189500	4.10369500	0.16545600
H	-3.68771800	4.95637100	-1.06756300
H	-1.95957100	4.64862500	-1.32485700
C	0.27061500	2.60837900	0.85734200
C	1.16335100	3.51034300	0.24956900
H	1.73487700	3.17313500	-0.61597000
C	1.31006000	4.80807900	0.71913900

H	1.99969800	5.48685700	0.22355600	C	-3.10287900	-0.60829800	1.23001400
C	0.56273000	5.24663100	1.81391700	C	-4.44065400	-0.20406200	1.20146200
H	0.67201000	6.26397400	2.17928600	C	-5.12304300	0.01230700	-0.00003100
C	-0.32783200	4.37002600	2.42623100	C	-4.43737200	-0.19618700	-1.20096400
H	-0.91758400	4.70008000	3.27748900	H	-4.95931000	-0.04898900	2.14434700
C	-0.47090100	3.06593900	1.95988400	H	-4.95347500	-0.03501100	-2.14422100
H	-1.18527900	2.40086300	2.43800800	C	3.10657400	-0.60424600	-1.22670100
H	-0.93505600	-4.84236700	1.75735900	C	4.44268800	-0.19166200	-1.19901300
H	0.23508900	-3.60332100	1.26083100	C	5.12329400	0.03211900	0.00115600
H	-2.76730100	-0.99717000	-3.44307700	C	4.43453200	-0.16509800	1.20322500
H	-1.63126900	-0.16480000	-2.38023100	C	3.09999300	-0.57738400	1.23180800
H	1.44626400	0.96512200	-4.08991800	C	2.45602100	-0.79349100	0.00214800
H	1.02747500	2.06849700	-2.78449300	H	4.95976700	-0.03406700	-2.14219300
H	5.46496300	-2.29409000	-0.34361500	H	4.94568200	0.01405300	2.14604800
H	3.81629000	-2.82865000	-0.64441600	Cu	-0.00406800	1.50087600	-0.00548900
C	-5.38575400	-3.53859300	-0.03694100	H	-1.38442900	-3.37540200	0.00803800
H	-6.00738900	-3.63612700	-0.93231800	H	1.39720100	-3.37036100	0.00974300
H	-5.51566400	-4.44061800	0.56680800	C	-6.55600100	0.48870400	-0.00030800
H	-5.79609100	-2.70035900	0.54106700	H	-7.09684000	0.13405200	0.88204200
C	5.92567600	2.55218600	-1.59478300	H	-6.60196400	1.58455500	0.00723100
H	5.82418000	3.31334300	-2.37357200	H	-7.09242800	0.14634600	-0.89014000
H	5.79388900	3.06079800	-0.63234700	C	6.57229200	0.45782300	0.00560000
H	6.95101900	2.17408000	-1.61920900	H	7.23368900	-0.39412100	0.20674800
H	-0.11466700	-3.57549900	-3.13863000	H	6.86693300	0.88299400	-0.95761300
H	1.67743300	-2.14306600	-3.85409400	H	6.76460900	1.20680300	0.77994300
C	2.76762100	0.93568900	1.46744000	C	-2.38562300	-0.80849600	2.54325200
Br	2.46322800	-2.21237100	1.70230600	H	-1.93529700	-1.80427600	2.61707600
C	2.60970300	1.10716200	2.89265500	H	-1.57687600	-0.07929500	2.66357300
C	2.30125900	2.27214300	3.49634100	H	-3.07561700	-0.68668400	3.38137500
H	2.17738100	2.33912400	4.57332600	C	-2.37877800	-0.79141200	-2.54132000
H	2.18961800	3.19376700	2.92891000	H	-1.91706400	-1.78187800	-2.61542300
H	2.72448100	0.20382400	3.49533300	H	-3.06929500	-0.67653900	-3.38001100
H	3.58000100	0.26296000	1.18074300	H	-1.57835500	-0.05276800	-2.66015300
H	2.75799100	1.85930800	0.88704200	C	2.37541900	-0.75542200	2.54420900
L₂CuCl				H	3.06234300	-0.62694800	3.38387400
C	0.00105600	-0.39087900	-0.00026700	H	1.57075200	-0.01957700	2.65106300
C	0.68331400	-2.56224000	0.00684400	H	1.91855100	-1.74733200	2.62861900
C	-0.67348000	-2.56468800	0.00610200	C	2.39049600	-0.80922700	-2.53984700
N	-1.07424200	-1.23254600	0.00178500	H	1.93786700	-1.80424300	-2.60906700
N	1.07934200	-1.22866800	0.00285100	H	1.58368700	-0.07863900	-2.66496600
C	-3.09944700	-0.60030400	-1.22862200	H	3.08185100	-0.69346700	-3.37771400
C	-2.45212700	-0.80121200	0.00091100	Cl	-0.01278700	3.62611900	-0.01055500
				L₂-1			

C 0.06594900 -1.17098600 -0.31734900
 C -0.59135700 -1.93220600 -2.34911300
 C 0.76605600 -1.88382800 -2.35254400
 N 1.15122900 -1.41558500 -1.10200900
 N -1.00287100 -1.49196400 -1.09684300
 C 3.24003500 -2.20871900 -0.09335500
 C 2.51514900 -1.16725900 -0.69589000
 C 3.06534400 0.10636600 -0.91772900
 C 4.38705000 0.31466900 -0.50617400
 C 5.14302000 -0.68861500 0.10713200
 C 4.55478300 -1.94395500 0.29836100
 H 4.83314200 1.29218900 -0.67159100
 H 5.13147000 -2.73808300 0.76636200
 C -3.01969100 -2.42618800 -0.06304200
 C -4.34661200 -2.25442400 0.34057400
 C -5.02896200 -1.05014100 0.13698800
 C -4.35297300 0.00086800 -0.49027500
 C -3.02415200 -0.11386300 -0.91435300
 C -2.37971800 -1.34172100 -0.68503700
 H -4.85622100 -3.08110000 0.82939200
 H -4.86936200 0.94341200 -0.65471400
 Cu 0.04462200 -0.43354900 1.42371000
 H 1.48546100 -2.12824900 -3.11758700
 H -1.29542200 -2.22743000 -3.11046800
 C 6.55366800 -0.41817100 0.57379700
 H 7.03901300 0.34614300 -0.03998600
 H 6.55966300 -0.05677800 1.60946400
 H 7.16746900 -1.32321900 0.54112500
 C -6.47154300 -0.89683900 0.55742300
 H -7.14981800 -1.10286200 -0.28003500
 H -6.72888900 -1.58828200 1.36471400
 H -6.68046900 0.12054900 0.90104100
 C 2.27791300 1.22120800 -1.56241000
 H 1.72726600 0.87472400 -2.44274000
 H 1.54320400 1.67004200 -0.87942400
 H 2.95102400 2.02031400 -1.88307000
 C 2.62511400 -3.56859600 0.13869600
 H 2.25583900 -4.01517800 -0.79101300
 H 3.35763000 -4.25304900 0.57275700
 H 1.77299000 -3.50792800 0.82493300
 C -2.32663400 1.05173400 -1.57230600
 H -3.06200900 1.78503900 -1.91336900
 H -1.64032900 1.57377700 -0.88954200

H -1.74093000 0.73648800 -2.44167000
 C -2.30303400 -3.73312600 0.18119000
 H -1.91822300 -4.16784500 -0.74795400
 H -1.44615900 -3.59896700 0.85073100
 H -2.97636900 -4.46143900 0.63901100
 Cl 0.00863700 0.66071800 3.29505700
 O -0.17587700 3.21059500 0.31513100
 C -0.27809200 4.44012700 -0.32335800
 C -0.05797700 4.28072400 -1.84703700
 H -0.79516200 3.58715100 -2.26552100
 H -0.14628000 5.23497800 -2.38128900
 H 0.93925800 3.87295600 -2.04385100
 C -1.68218200 5.04443400 -0.08464500
 H -1.85065700 5.18082100 0.99033400
 H -1.81563800 6.01621300 -0.57717100
 H -2.45147500 4.36058000 -0.46000700
 C 0.78876700 5.41421700 0.23031000
 H 1.78804600 4.98730200 0.08920400
 H 0.76172500 6.39770000 -0.25635500
 H 0.63439700 5.56309500 1.30612500
 Li -0.10535600 2.41382400 1.79679300

L₂-TS2

C -0.05034900 -0.94421500 -0.31700800
 C -0.74308900 -2.25879100 -2.03982200
 C 0.60947600 -2.34164500 -1.98722400
 N 1.01804700 -1.53372000 -0.92950500
 N -1.13060400 -1.40457300 -1.01287000
 C 2.87715600 -2.05242400 0.58724300
 C 2.39456400 -1.35847800 -0.53476000
 C 3.21711300 -0.51775300 -1.30357300
 C 4.54998100 -0.37023900 -0.90837300
 C 5.06738700 -1.02851000 0.21177600
 C 4.21816400 -1.86788700 0.93902200
 H 5.19708800 0.28177200 -1.48998400
 H 4.60694300 -2.39820900 1.80497800
 C -3.24078600 -2.01402700 0.06789700
 C -4.57287600 -1.70886400 0.35627600
 C -5.17191900 -0.52580900 -0.09143100
 C -4.40182500 0.36618500 -0.84186900
 C -3.06210800 0.11124200 -1.16164500
 C -2.50534300 -1.09105600 -0.69696800
 H -5.15293400 -2.40904200 0.95261900

H	-4.85001200	1.29297700	-1.19196800				
Cu	-0.13563100	0.21590100	1.18790800	L₂-3			
H	1.31294600	-2.89274300	-2.59033000				
H	-1.45928600	-2.71634600	-2.70332500	C	0.23107700	-0.86238000	0.00823000
C	6.50072100	-0.81909600	0.63895500	C	1.11551300	-2.96311900	0.05442800
H	7.15130300	-0.62758500	-0.21958500	C	-0.23442200	-3.09360400	0.05918300
H	6.58625600	0.04339700	1.31129500	N	-0.75977100	-1.80478400	0.03070400
H	6.89013400	-1.68963300	1.17489200	N	1.38406200	-1.59802600	0.02320200
C	-6.62329400	-0.23457600	0.20934800	C	-2.84272300	-1.44296700	-1.20940000
H	-7.28029200	-0.67618100	-0.55056500	C	-2.17163200	-1.50914100	0.02195200
H	-6.92169300	-0.64914200	1.17690100	C	-2.83253400	-1.30842900	1.24468500
H	-6.81984800	0.84121400	0.22493500	C	-4.20359800	-1.03773000	1.20755700
C	2.69291300	0.20433500	-2.52159500	C	-4.91209200	-0.96644800	0.00348200
H	2.50410500	-0.48502800	-3.35319300	C	-4.21411100	-1.17015300	-1.19106000
H	1.75193700	0.71855100	-2.30766400	H	-4.72858400	-0.87314600	2.14544200
H	3.41386700	0.94899900	-2.86639600	H	-4.74677600	-1.10854700	-2.13691200
C	1.99505300	-2.97111600	1.39856900	C	3.33260700	-0.78333700	-1.22345100
H	1.42190600	-3.65159500	0.76032300	C	4.62394600	-0.24838200	-1.20682000
H	2.59704800	-3.57321100	2.08353200	C	5.29275200	0.03376900	-0.01145900
H	1.27304800	-2.40289100	1.99565400	C	4.63626500	-0.22760400	1.19535500
C	-2.25555000	1.12220000	-1.93518600	C	3.34507600	-0.76175100	1.23432200
H	-2.91783200	1.80807500	-2.47077400	C	2.71287100	-1.03577500	0.01094500
H	-1.62476100	1.71761700	-1.25832700	H	5.11497100	-0.03998300	-2.15425800
H	-1.59761700	0.64482500	-2.66802100	H	5.13676200	-0.00249200	2.13396500
C	-2.61348600	-3.28410600	0.59156600	Cu	0.06417100	1.00568100	-0.02435700
H	-2.25913500	-3.93323900	-0.21685900	H	-0.86578200	-3.96745600	0.08043600
H	-1.75000600	-3.06287500	1.22824700	H	1.90239800	-3.70022700	0.07010200
H	-3.33375700	-3.85168600	1.18535500	C	-6.39854300	-0.69912100	-0.00319000
Cl	-0.55877200	0.97358300	3.23523300	H	-6.96779300	-1.63041500	0.10956100
O	-0.33618000	2.88967700	0.29434100	H	-6.68867900	-0.03915800	0.81962300
C	0.54103700	3.77499000	-0.33484700	H	-6.71648300	-0.23341000	-0.94029100
C	0.35410900	3.72566100	-1.86827900	C	6.69834100	0.58641500	-0.02364000
H	-0.67543500	3.99191500	-2.13048700	H	7.44072100	-0.22170100	-0.02898200
H	1.03062000	4.41270800	-2.39155700	H	6.87837600	1.19977000	-0.91125100
H	0.54344300	2.71254300	-2.23896500	H	6.89303500	1.20181100	0.85940700
C	0.26142900	5.22121700	0.14321400	C	-2.09046000	-1.35377900	2.55838600
H	0.41050000	5.29385500	1.22910400	H	-1.52303000	-2.28326200	2.67521600
H	0.91759100	5.96182200	-0.33154200	H	-1.37450100	-0.52761100	2.63106500
H	-0.77724300	5.49208600	-0.07831000	H	-2.78592600	-1.27331400	3.39714400
C	2.00357000	3.41179200	0.01048800	C	-2.11104000	-1.63141700	-2.51628800
H	2.21629100	2.38272200	-0.29701300	H	-1.35947000	-0.84766700	-2.66100300
H	2.72938800	4.07637000	-0.47584800	H	-1.58603400	-2.59200100	-2.55670200
H	2.15872400	3.47207800	1.09414200	H	-2.80738400	-1.59171100	-3.35721300
Li	-0.87860400	2.75676400	1.91056000	C	2.64954800	-1.00301400	2.55221500

H	1.77639400	-0.34965600	2.65758600	H	-2.96048100	2.93825000	2.42968400
H	2.29335500	-2.03466500	2.64495500	Cu	0.84674700	0.07949800	-0.29619700
H	3.32485000	-0.80180800	3.38718300	H	4.43114000	3.43869600	0.98571700
C	2.62426500	-1.04856700	-2.52981700	H	1.99879900	4.75534200	1.26905400
H	2.25788600	-2.07871900	-2.59525800	C	7.14304100	-2.13991100	-0.70430700
H	1.75639600	-0.38949700	-2.64331600	H	7.77263400	-1.86890800	-1.55708100
H	3.29457800	-0.87308500	-3.37454800	H	7.79245900	-2.30575400	0.16020800
O	0.06958400	2.80495200	-0.04850900	H	6.66635300	-3.09852100	-0.94310500
C	-1.00366500	3.70620200	-0.03335700	C	-4.26969500	4.47547600	0.59243500
C	-1.89607800	3.51404300	-1.27889700	H	-4.38416400	5.46892300	0.14794600
H	-1.29166200	3.62011000	-2.18602900	H	-4.89900400	3.78659600	0.01624200
H	-2.33115300	2.50750500	-1.27573000	H	-4.66919300	4.50969400	1.61009000
H	-2.71598400	4.24273400	-1.32140800	C	4.18117500	0.31084800	2.57820200
C	-0.40563400	5.12851700	-0.04766600	H	4.44961600	1.30754600	2.94718500
H	-1.18065300	5.90467300	-0.03892700	H	3.09286000	0.22337000	2.65429100
H	0.23751700	5.26859400	0.82714400	H	4.62739200	-0.42499600	3.25107200
H	0.21056900	5.26172100	-0.94268700	C	4.03719500	1.48468900	-2.36827500
C	-1.85453400	3.52223400	1.24224200	H	2.98127300	1.25915100	-2.55109400
H	-2.29036500	2.51605400	1.25950200	H	4.10390600	2.55739800	-2.15657900
H	-1.22009600	3.63341400	2.12805800	H	4.59036200	1.28556100	-3.28922200
H	-2.67228400	4.25166600	1.30759700	C	-0.48105900	1.91284300	2.73504000
L₂-4				H	-1.14147900	1.98288600	3.60322700
C	1.77696900	1.64614000	0.20263300	H	-0.45964800	0.86519700	2.41176300
C	2.23402200	3.75524200	0.94220800	H	0.53026100	2.18635700	3.05146300
C	3.41891100	3.11268500	0.80778100	C	0.24892600	4.37848400	-1.66427400
N	3.12585400	1.82913700	0.35578600	H	1.05935400	5.04734200	-1.35287500
N	1.24288200	2.85175100	0.56883300	H	0.71666200	3.50091300	-2.12264000
C	4.58482100	0.65808600	-1.22975700	H	-0.33074300	4.89400100	-2.43362500
C	4.13194400	0.83174200	0.08852500	O	-0.06799700	-1.36847000	-1.25604100
C	4.65598600	0.09206900	1.16125200	C	-0.13396800	-1.60630500	-2.68047300
C	5.64231600	-0.85804600	0.87851000	C	-0.70860300	-0.36111900	-3.37330900
C	6.10624500	-1.07869500	-0.42207900	H	-1.72595800	-0.17607700	-3.02213300
C	5.57107200	-0.30619900	-1.45825100	H	-0.09077600	0.51709100	-3.15006700
H	6.05461200	-1.44210300	1.69768000	H	-0.73162100	-0.49435300	-4.46136200
H	5.93091400	-0.45412200	-2.47359700	C	-0.99722700	-2.83844300	-2.98911900
C	-0.63967500	3.98262600	-0.50833600	H	-0.94652300	-3.06067500	-4.06125600
C	-1.97610100	4.38654400	-0.47134300	H	-0.64353400	-3.70397300	-2.42609400
C	-2.82691800	4.02796000	0.58079900	H	-2.04120400	-2.66037500	-2.72473400
C	-2.31312200	3.23072200	1.60691400	C	1.30943500	-1.85768000	-3.14166400
C	-0.98173100	2.79654300	1.61971300	H	1.35751300	-1.99287200	-4.22808300
C	-0.15887500	3.19702700	0.55495700	H	1.95118100	-1.01154200	-2.87207100
H	-2.36014400	4.99912900	-1.28358600	H	1.71071700	-2.75541600	-2.66168100
				B	-1.04568200	-1.83245500	-0.13496100
				O	-0.31344900	-1.33071300	1.07972400

O	-1.04305300	-3.28988800	0.00696200	C	0.55245400	-4.15175300	-1.16383300
C	-0.67200100	-3.63809600	1.33619600	C	1.86842600	-3.89309500	-0.97107400
C	0.28441800	-2.45902400	1.75344400	N	1.94764000	-2.61426900	-0.42917300
C	1.71674700	-2.67339200	1.23405700	N	-0.14133400	-3.02487800	-0.73546700
H	2.28853000	-1.74767600	1.35401600	C	3.87014200	-2.32806300	1.06145000
H	2.23707400	-3.46328300	1.78727900	C	3.20857700	-1.97936700	-0.12782900
H	1.70802200	-2.93156800	0.17352000	C	3.76251200	-1.08792300	-1.06005500
C	0.32222300	-2.15789000	3.25363300	C	5.02238400	-0.55098700	-0.77125900
H	0.67893300	-3.02408700	3.82277700	C	5.71966300	-0.87595500	0.39584200
H	1.00680100	-1.32507300	3.45090800	C	5.12713700	-1.76606100	1.29855800
H	-0.66510300	-1.87806400	3.62542700	H	5.46829500	0.13872400	-1.48358400
C	-0.00722400	-5.01967200	1.31048400	H	5.65255400	-2.02697400	2.21417400
H	0.81715800	-5.05422400	0.59558900	C	-2.35875900	-3.56614600	0.14936000
H	0.37143600	-5.30197300	2.29995800	C	-3.74949900	-3.51983400	0.00801400
H	-0.74394500	-5.76961700	1.00579100	C	-4.36068900	-2.85308600	-1.05925300
C	-1.93944200	-3.70684100	2.21220600	C	-3.54448300	-2.21882700	-2.00045700
H	-1.72406500	-4.06533900	3.22510700	C	-2.14913000	-2.23419900	-1.90823400
H	-2.42736100	-2.73171400	2.27436300	C	-1.57803100	-2.91959800	-0.82268200
H	-2.64113400	-4.40584600	1.74625000	H	-4.36740100	-4.02046200	0.74971500
B	-2.65944000	-1.20551000	-0.26977900	H	-4.00291600	-1.69616700	-2.83631000
C	-4.70372500	-0.51707300	-1.13010500	Cu	0.25530500	-0.25451900	0.21692900
O	-3.40972900	-1.09216100	-1.43800600	H	2.74840600	-4.48260500	-1.17263000
C	-4.83109100	-0.79514100	0.41472900	H	0.04674100	-5.01395000	-1.56794200
O	-3.44610500	-0.87685300	0.82987800	C	7.06436700	-0.25623000	0.69388300
C	-5.75661400	-1.19586000	-2.00695900	H	7.71346100	-0.94877200	1.23853300
H	-6.76332000	-0.83660000	-1.76577400	H	7.57906600	0.04421800	-0.22325100
H	-5.55955000	-0.96707700	-3.05870600	H	6.95142100	0.64093500	1.31474600
H	-5.73621800	-2.28079400	-1.89150000	C	-5.86523100	-2.79821100	-1.18109800
C	-4.62411900	0.97655900	-1.47776800	H	-6.34134100	-3.63052500	-0.65464200
H	-4.34170400	1.08068400	-2.52949700	H	-6.25879500	-1.86897300	-0.75152700
H	-5.58652400	1.47886800	-1.33184000	H	-6.18275500	-2.83069800	-2.22785500
H	-3.86619900	1.48232800	-0.87398900	C	3.03671400	-0.70465700	-2.32613600
C	-5.51779300	0.30567000	1.22353100	H	2.63038200	-1.58061600	-2.84277200
H	-6.55944500	0.43687400	0.90980200	H	2.20006800	-0.02932700	-2.11133700
H	-5.51694500	0.03287700	2.28323700	H	3.71511300	-0.19205200	-3.01309100
H	-4.99854400	1.26055700	1.12325100	C	3.24647600	-3.27023700	2.06374800
C	-5.47531000	-2.15244800	0.73571600	H	2.26366200	-2.90993600	2.38584800
H	-5.35165800	-2.35859600	1.80258000	H	3.09872400	-4.27406100	1.64960200
H	-6.54545200	-2.16229700	0.50464600	H	3.88009300	-3.36378500	2.94887000
H	-4.98979100	-2.95998800	0.18134500	C	-1.30677900	-1.52602400	-2.94006300
L₂-TS5				H	-1.90770800	-1.28525300	-3.82087300
C	0.70854600	-2.05593600	-0.27828000	H	-0.90138500	-0.58805500	-2.54191600
				H	-0.45978300	-2.13921900	-3.26498600
				C	-1.72917300	-4.28649500	1.31877600

H	-1.13227000	-5.14815700	0.99924300	H	-3.98262900	1.61513200	4.25987500
H	-1.06056300	-3.62432300	1.87884800	H	-2.29942000	1.30004500	4.71098400
H	-2.49835800	-4.64977500	2.00443400	H	-2.69592600	2.73108600	3.75340200
O	1.42146200	1.68638300	0.42720900	C	-2.88246400	-0.64029500	2.97265200
C	2.10037300	2.37485400	1.49746100	H	-2.12690500	-0.91467000	3.71489100
C	2.92167700	1.30783100	2.23406100	H	-3.86941200	-0.86769500	3.38897100
H	2.25605100	0.55950400	2.67733600	H	-2.72779800	-1.25684400	2.08399600
H	3.59931700	0.79987200	1.54326000	C	-4.83751500	0.50036900	1.12537400
H	3.51525300	1.75723500	3.03843100	H	-5.55101200	0.60096900	1.95103000
C	1.14844800	3.06512800	2.48827300	H	-5.31950300	0.87306700	0.21645900
H	1.73508800	3.54324800	3.28162800	H	-4.61409300	-0.55774400	0.97968200
H	0.55119400	3.82728700	1.98541000	C	-3.90579100	2.81048700	1.41272600
H	0.46979200	2.34227200	2.94429900	H	-4.35398200	3.08725200	0.45512700
C	3.04245500	3.41743400	0.87120600	H	-4.61815300	3.05462200	2.20719000
H	3.64837700	3.91146800	1.64022500	H	-3.00349800	3.41262800	1.54527500
H	3.71750200	2.93883400	0.15447600				
H	2.46355700	4.18438400	0.35016500	L₂-6			
B	0.11021100	1.96728500	-0.19483700	C	0.02060400	-1.63265200	0.03708300
O	0.10705300	1.58369600	-1.60876700	C	-0.63542700	-3.80977900	0.23490800
O	-0.33714200	3.34183600	-0.14194300	C	0.72096700	-3.79472400	0.24741100
C	-0.64776900	3.81005700	-1.46687300	N	1.10302500	-2.46157300	0.12499400
C	0.09344500	2.77587300	-2.40723200	N	-1.04474200	-2.48544400	0.10544100
C	1.54429200	3.17638000	-2.73206200	C	3.11591700	-1.67992500	1.28936800
H	2.02772600	2.34526300	-3.25513900	C	2.47583400	-2.01870300	0.08648600
H	1.59331700	4.05793800	-3.38081200	C	3.13262100	-1.95582600	-1.15242500
H	2.11504900	3.37466900	-1.82413800	C	4.47038900	-1.54934800	-1.16181600
C	-0.63934400	2.47081600	-3.71782400	C	5.14676900	-1.20519500	0.01250500
H	-0.73929000	3.36951300	-4.33712900	C	4.45373300	-1.27969700	1.22519800
H	-0.06988700	1.73185900	-4.29131300	H	4.99341700	-1.49594300	-2.11359800
H	-1.63388100	2.06110000	-3.53285900	H	4.96443500	-1.01467100	2.14793500
C	-0.14201500	5.25268100	-1.58362900	C	-3.08439700	-1.69880400	1.22076100
H	0.92315800	5.32827500	-1.35744500	C	-4.42955000	-1.32966600	1.12810100
H	-0.31398900	5.65234800	-2.58966500	C	-5.11264400	-1.32034400	-0.09229300
H	-0.68168200	5.88631900	-0.87286700	C	-4.41825700	-1.69842000	-1.24552600
C	-2.17320900	3.80109300	-1.65311600	C	-3.07248500	-2.07574400	-1.20757000
H	-2.46291000	4.20643400	-2.62846300	C	-2.42609800	-2.07346900	0.03851900
H	-2.57711500	2.79333700	-1.54511000	H	-4.95404200	-1.03720800	2.03462700
H	-2.62369000	4.42964300	-0.87948800	H	-4.93328900	-1.69516500	-2.20316600
B	-1.34629100	1.09972300	0.79862100	Cu	-0.00181900	0.33245500	-0.05818600
C	-2.73429700	0.85268800	2.64638500	H	1.44148800	-4.59284700	0.33067600
O	-1.37064000	1.05380400	2.19123800	H	-1.33941800	-4.62366200	0.30614900
C	-3.57103800	1.31246200	1.39478300	C	6.58134000	-0.73448800	-0.02987600
O	-2.64069200	1.09222000	0.29854600	H	7.12879700	-1.03435800	0.86889500
C	-2.94507700	1.68110500	3.91400300				

H	7.10920000	-1.13541600	-0.90006400	L ₂ -7			
H	6.63242300	0.35950200	-0.09196500				
C	-6.55639900	-0.88256600	-0.16563400	C	-0.40504500	-1.13161900	-1.25889000
H	-7.11075800	-1.17699000	0.73077400	C	-0.11103300	-2.28029400	-3.21151700
H	-6.63075700	0.20861800	-0.24953300	C	-1.42910600	-1.98465600	-3.11346400
H	-7.06197300	-1.31214800	-1.03533400	N	-1.59199300	-1.28164000	-1.92184400
C	2.41867200	-2.28763100	-2.44041800	N	0.49842700	-1.75302800	-2.07550300
H	1.95049400	-3.27714100	-2.40785300	C	-3.26510300	0.51053900	-1.92948100
H	1.62355300	-1.56117300	-2.64232700	C	-2.86647500	-0.76320400	-1.48857800
H	3.11418300	-2.26943700	-3.28287600	C	-3.69240800	-1.57090500	-0.69175200
C	2.38314800	-1.71738300	2.60836700	C	-4.93346200	-1.05380100	-0.30560700
H	1.58939100	-0.96212500	2.63233000	C	-5.35861900	0.21871600	-0.69754300
H	1.90988000	-2.68872600	2.78740400	C	-4.51615300	0.97869700	-1.51604700
H	3.06753900	-1.51553700	3.43585800	H	-5.58201300	-1.66612000	0.31593200
C	-2.33974000	-2.44698200	-2.47428800	H	-4.84133600	1.96167200	-1.84908600
H	-3.01924700	-2.43749700	-3.32984200	C	2.75851700	-0.85375000	-2.38242500
H	-1.52876400	-1.73887200	-2.67752400	C	4.13508700	-0.99450100	-2.18691800
H	-1.88824200	-3.44297800	-2.41158500	C	4.67764100	-2.07074300	-1.47588800
C	-2.36489500	-1.66462400	2.54694100	C	3.80541400	-3.02712400	-0.94918900
H	-1.84187900	-2.60416100	2.75414000	C	2.41847400	-2.93342000	-1.11353200
H	-1.61443600	-0.86594000	2.55845000	C	1.91815300	-1.84079100	-1.83722000
H	-3.06799400	-1.47911800	3.36250400	H	4.79987300	-0.24101400	-2.60285700
B	-0.02882600	2.32767000	-0.07204400	H	4.20962400	-3.87104000	-0.39519300
C	0.45258700	4.52063100	-0.66666000	Cu	0.03164300	-0.04175800	0.35005500
O	0.41914700	3.14286800	-1.11511400	C	-6.68878600	0.76762900	-0.23784300
C	-0.56576300	4.50675500	0.52904300	H	-7.39556600	-0.03487300	-0.00731000
O	-0.49770500	3.12895600	0.97389400	H	-6.57211300	1.37116800	0.67089900
C	0.07388800	5.42637000	-1.83899900	H	-7.14116300	1.41203500	-0.99801300
H	0.03060200	6.47713600	-1.52993400	C	6.17056900	-2.18067500	-1.27337100
H	0.82657200	5.33761300	-2.62844600	H	6.71393800	-2.03439900	-2.21309000
H	-0.89158100	5.14817600	-2.26553900	H	6.52847200	-1.41643100	-0.57310100
C	1.89721100	4.81335700	-0.23030600	H	6.44997400	-3.15791500	-0.87000100
H	2.56767700	4.59724100	-1.06715500	C	-3.26868500	-2.95632000	-0.27139300
H	2.03564200	5.86014400	0.06118100	H	-4.05303300	-3.43723900	0.31659400
H	2.18924800	4.17470800	0.60770200	H	-3.05495900	-3.59097900	-1.13910100
C	-0.20914000	5.41892900	1.70333400	H	-2.36470000	-2.92779000	0.34326700
H	-0.19040200	6.47090400	1.39602900	C	-2.38732600	1.34918800	-2.82693300
H	-0.95992200	5.31131000	2.49231100	H	-1.47616300	1.67167700	-2.31216200
H	0.76253900	5.16313700	2.12986400	H	-2.07509200	0.79444500	-3.71853500
C	-2.01721300	4.76462300	0.09365100	H	-2.92603800	2.24052900	-3.16010300
H	-2.68200600	4.53115400	0.93042200	C	1.49629500	-3.96122900	-0.50514600
H	-2.18132500	5.80815100	-0.19620700	H	0.90564300	-3.51015400	0.29925000
H	-2.29372800	4.12015700	-0.74512900	H	0.79375000	-4.36804900	-1.24021600
				H	2.06869200	-4.79273500	-0.08609600

C	2.20566800	0.32674900	-3.14485300	H	1.72259400	2.37717900	3.00035200
H	1.52569700	0.01238800	-3.94401300	C	4.85452900	1.17176300	2.42002600
H	1.64492600	1.00081000	-2.48722600	H	5.28892300	-0.82436500	1.72997500
H	3.01845500	0.89801600	-3.60110200	H	4.10228900	3.06772800	3.12503100
C	0.72419200	-0.01506000	2.30821400	H	5.89744600	1.47243600	2.46984300
N	0.39097300	-1.29818200	2.10088600	H	0.07840600	0.64609400	2.89196300
C	-0.86131000	-1.75839200	2.56467400	H	-2.25980000	-2.20172400	-3.76582800
C	-0.96932500	-3.14033100	2.81866600	H	0.44845500	-2.80828600	-3.96713900
C	-1.99164500	-0.94887300	2.80979600				
C	-2.14698000	-3.69081100	3.31812800	L₂-TS8			
H	-0.09577800	-3.76001500	2.63990500	C	-0.46558500	-1.53505200	-1.00673400
C	-3.17077600	-1.50947800	3.30085500	C	-0.24301900	-3.27473900	-2.46348400
H	-1.95475200	0.11623700	2.60376200	C	-1.56176800	-2.97156800	-2.39459300
C	-3.25788700	-2.87836700	3.56436500	N	-1.68443400	-1.90632900	-1.50515500
H	-2.19679800	-4.75754900	3.52097000	N	0.41372600	-2.38932800	-1.61343700
H	-4.02948900	-0.86704500	3.47843800	C	-3.45107500	-0.33809000	-2.13342400
H	-4.17632600	-3.30550900	3.95671800	C	-2.93841000	-1.26075900	-1.20569000
B	0.04235700	1.97210300	0.17211800	C	-3.62353800	-1.59494100	-0.02623900
C	-0.34906900	4.23431300	0.53638600	C	-4.84120000	-0.95041500	0.21862000
O	-0.31337700	2.90958800	1.13654300	C	-5.37750600	-0.01106800	-0.66673100
C	0.55639700	4.05139700	-0.73680400	C	-4.67247200	0.27478300	-1.84077900
O	0.42796400	2.62417400	-1.00158400	H	-5.38119100	-1.19408200	1.13014100
C	-1.81934800	4.53300100	0.20746600	H	-5.08113900	0.99236800	-2.54835200
H	-2.40847900	4.45074200	1.12526800	C	2.65356300	-1.60884800	-2.23411800
H	-1.95195800	5.54195800	-0.19674600	C	4.03656200	-1.66119300	-2.02978900
H	-2.21795000	3.81209600	-0.51131500	C	4.60729900	-2.45244900	-1.02833900
C	0.16755500	5.24564000	1.55931300	C	3.75782300	-3.19985900	-0.20489700
H	1.16378700	4.98192000	1.91868400	C	2.36945900	-3.18724900	-0.36816600
H	0.20800400	6.25318200	1.13053500	C	1.83993700	-2.39060600	-1.39811200
H	-0.50586200	5.27300900	2.42127000	H	4.68125300	-1.06147700	-2.66764900
C	0.09889700	4.81981200	-1.97614900	H	4.18355800	-3.80716800	0.59014400
H	0.12918300	5.90097600	-1.80072800	Cu	0.03274600	-0.26193800	0.30472500
H	0.76662800	4.59696700	-2.81383600	C	-6.67714500	0.69173400	-0.35290900
H	-0.91518000	4.54526800	-2.27204300	H	-7.36580900	0.03629700	0.18878300
C	2.04509800	4.32163100	-0.47587700	H	-6.50430700	1.57213900	0.27828900
H	2.40463200	3.76153300	0.39122300	H	-7.17801400	1.03493600	-1.26291400
H	2.62055300	3.99459800	-1.34678200	C	6.10629500	-2.51909900	-0.85258200
H	2.24351000	5.38635600	-0.31547600	H	6.52836200	-3.37774700	-1.38985300
C	2.15454200	0.38699700	2.30102000	H	6.59502600	-1.62026100	-1.23931000
C	3.17458500	-0.50964100	1.94600200	H	6.38069500	-2.63032100	0.20077500
C	2.50868700	1.67909800	2.72689400	C	-3.08550900	-2.60913700	0.95189300
C	4.51085400	-0.11591100	2.00175000	H	-3.87192900	-2.93263300	1.63739700
H	2.90392200	-1.51356700	1.64035900	H	-2.68851500	-3.49242100	0.44147100
C	3.84558700	2.06741000	2.78623600				

H	-2.27934300	-2.18847600	1.56112700	H	1.79568000	4.40693600	0.22264700
C	-2.72095900	-0.02392700	-3.41827600	H	2.74671100	4.12354800	-1.23177500
H	-1.66276800	0.18895800	-3.23770000	H	1.62239200	5.49526300	-1.17371600
H	-2.76044700	-0.86297900	-4.12327400	C	2.19906300	1.46936600	1.79185100
H	-3.16679000	0.84253700	-3.91288800	C	3.22624800	0.63531500	1.32754000
C	1.47612300	-3.97255900	0.56042500	C	2.54131500	2.71387900	2.33642000
H	0.90226600	-3.29457500	1.20166400	C	4.55577000	1.04559500	1.39524000
H	0.75983600	-4.59418300	0.01298800	H	2.97828900	-0.34271200	0.92924300
H	2.07004700	-4.62573700	1.20429300	C	3.87506200	3.12431300	2.41045700
C	2.06771400	-0.70364400	-3.29116100	H	1.75597000	3.36084800	2.72128700
H	1.29700200	-1.20702000	-3.88339600	C	4.88793400	2.29235800	1.93481000
H	1.60746600	0.17705200	-2.82817500	H	5.33887200	0.38639500	1.02991000
H	2.84791500	-0.35658900	-3.97347400	H	4.11936400	4.08946800	2.84637900
C	0.74927700	1.04216500	1.77127700	H	5.92659600	2.60666600	1.99005600
N	0.56249800	-0.28804900	2.25744400	H	0.13066500	1.79728500	2.26493200
C	-0.56948000	-0.54631800	3.02979500	H	-2.41919500	-3.40763700	-2.88143400
C	-0.58893200	-1.76828000	3.75329600	H	0.28799700	-4.02694400	-3.02455000
C	-1.70350000	0.29588000	3.17420900				
C	-1.65888900	-2.11929400	4.56610400	L₂-9			
H	0.27957500	-2.41569200	3.66840000	C	0.01871900	-2.07219400	-0.59697300
C	-2.77093100	-0.06697700	3.99843700	C	0.81667100	-3.78814900	-1.86559500
H	-1.76161300	1.23352700	2.62986700	C	-0.53706800	-3.85478300	-1.90651400
C	-2.76693700	-1.27134600	4.70232800	N	-1.00931000	-2.80381300	-1.12797200
H	-1.62651900	-3.06030900	5.11117000	N	1.14034000	-2.69822800	-1.06280500
H	-3.62118300	0.60688100	4.08355900	C	-3.07188700	-1.62170100	-1.73319500
H	-3.59935900	-1.54338400	5.34472300	C	-2.40690200	-2.53081100	-0.89582900
B	0.19331700	1.83074400	0.02806900	C	-3.05885700	-3.18898000	0.15970900
C	-0.74714500	3.76097900	-0.81782600	C	-4.41020500	-2.90170000	0.37119500
O	-0.77335700	2.78779200	0.26324500	C	-5.10436800	-1.98358500	-0.42341000
C	0.68691700	3.53926900	-1.44901800	C	-4.42164200	-1.36551500	-1.47534400
O	1.00964600	2.17701800	-1.03121300	H	-4.92831100	-3.39772300	1.18835700
C	-1.90087100	3.40282400	-1.76244400	H	-4.94881600	-0.65578800	-2.10807400
H	-2.83587000	3.40571700	-1.19583000	C	3.13960500	-1.33807500	-1.50662100
H	-1.99127000	4.12057700	-2.58405700	C	4.47226500	-1.04485000	-1.19865500
H	-1.76926400	2.40347400	-2.18162400	C	5.15737800	-1.69617500	-0.17030600
C	-0.98258700	5.14554600	-0.21442000	C	4.48053700	-2.67667500	0.56266400
H	-0.25130100	5.37771700	0.56140500	C	3.15054100	-3.00898400	0.29676100
H	-0.93384700	5.92283600	-0.98457600	C	2.49930200	-2.32843900	-0.74653700
H	-1.97758000	5.18065000	0.23858900	H	4.98327200	-0.27966300	-1.77796400
C	0.73475800	3.59257600	-2.97590600	H	4.99746700	-3.19208900	1.36846200
H	0.45458800	4.58661000	-3.34093100	Cu	-0.17324500	-0.51026300	0.46160700
H	1.75348700	3.38467700	-3.31581000	C	-6.54221900	-1.63547700	-0.12428900
H	0.06978300	2.85582800	-3.43029500	H	-7.08330700	-2.48672000	0.29979200
C	1.77047300	4.45468400	-0.86760600				

H	-6.59096100	-0.81785300	0.60508900	C	-0.80880100	5.69870200	-1.79762700
H	-7.07211900	-1.30592500	-1.02276800	H	0.09753100	6.21811200	-1.48126200
C	6.57965200	-1.32230500	0.16900600	H	-0.96328100	5.88176900	-2.86647800
H	7.12133100	-0.96061900	-0.71006800	H	-1.65263400	6.13429200	-1.25507700
H	6.59297600	-0.52042800	0.91690100	C	0.13768300	2.73195800	-3.48855700
H	7.13116200	-2.17044700	0.58570600	H	-0.18277600	3.45191600	-4.24934800
C	-2.32553500	-4.15632100	1.05759400	H	1.02577100	2.21709900	-3.86706900
H	-3.00697300	-4.59466700	1.79044100	H	-0.65319000	1.99148400	-3.35693500
H	-1.86565800	-4.97366600	0.49164700	C	1.71551500	4.32191800	-2.36052800
H	-1.52044700	-3.65271200	1.60418500	H	1.96523400	4.85066800	-1.43638300
C	-2.35677400	-0.92816000	-2.86724100	H	2.56418100	3.68562900	-2.62706900
H	-1.54835500	-0.29175700	-2.49095300	H	1.57696000	5.06134900	-3.15527500
H	-1.90428900	-1.64422400	-3.56238000	C	1.88834200	1.68056800	1.81898500
H	-3.05006500	-0.30097700	-3.43277400	C	2.05159000	0.72280900	2.83246200
C	2.43716800	-4.05194400	1.12342300	C	3.03928200	2.25747600	1.26622800
H	1.57078400	-3.62045400	1.63674800	C	3.32094200	0.36412700	3.28489600
H	2.06623300	-4.88151900	0.51141300	H	1.16397600	0.27107200	3.26446900
H	3.10645100	-4.46642500	1.88102400	C	4.31307600	1.90513000	1.72000600
C	2.42585000	-0.57931600	-2.59854400	H	2.94200500	2.99150900	0.47121200
H	1.75554600	-1.22165100	-3.17712800	C	4.45980900	0.95849000	2.73419400
H	1.82499900	0.23274500	-2.17229100	H	3.42191400	-0.37168200	4.07896000
H	3.14878500	-0.13336100	-3.28738000	H	5.18999100	2.37394200	1.28020900
C	0.48936000	2.15761200	1.43670300	H	5.44886200	0.69083200	3.09728500
N	-0.50502900	1.06087000	1.44348200	H	0.21663200	2.88266100	2.21940000
C	-1.75345100	1.29679100	1.99651200	H	-1.20224500	-4.53821800	-2.40976500
C	-2.61102500	0.19193200	2.25683000	H	1.57514700	-4.40028600	-2.32662800
C	-2.26684900	2.57572200	2.34233100				
C	-3.86991200	0.34946900	2.82008500	L₂-10			
H	-2.24943400	-0.80561900	2.01661900	C	-2.43546100	1.20503600	-0.30194800
C	-3.52987800	2.71818300	2.91880900	C	-4.58457000	1.89125700	-0.61883700
H	-1.69835900	3.46976700	2.11832000	C	-3.79782700	2.99547600	-0.66117400
C	-4.35042900	1.61827000	3.16779500	N	-2.49008300	2.56079800	-0.46735400
H	-4.47833200	-0.53359000	3.00565500	N	-3.73945900	0.80752800	-0.39988700
H	-3.87914500	3.71917000	3.16476600	C	-0.68723500	3.72390200	-1.65244900
H	-5.33102700	1.74144800	3.61802400	C	-1.34072000	3.43289000	-0.44481800
B	0.31956700	2.88754800	0.04372700	C	-0.91490100	3.96504200	0.78397100
C	-0.73475300	4.20149800	-1.50467800	C	0.19461000	4.81452600	0.77547100
O	-0.45234200	4.02021500	-0.09259200	C	0.87226600	5.13628000	-0.40590700
C	0.47091500	3.44198600	-2.17788800	C	0.41727100	4.58099700	-1.60559000
O	0.80671600	2.44302800	-1.17327200	H	0.54184700	5.22842100	1.71899400
C	-2.09484300	3.54056200	-1.76922900	H	0.93745500	4.81337300	-2.53160100
H	-2.83988400	3.99196600	-1.10907300	C	-4.28313800	-1.33951200	-1.45203200
H	-2.41899300	3.67776300	-2.80563400	C	-4.73288200	-2.65657900	-1.31794400
H	-2.06215700	2.47062000	-1.54592600				

C	3.80503300	-0.11929100	-0.20113200	C	-0.89552000	-1.81739300	-1.52423800
C	4.11038700	-0.79339800	0.99247700	C	-0.00064500	-2.88352700	-1.29101300
C	4.66628800	-2.07230900	0.89444000	C	-1.53676300	-1.77167700	-2.78153600
C	4.91246800	-2.67905700	-0.34162400	C	0.25040300	-3.84663400	-2.26649800
C	4.59653200	-1.97028600	-1.50490700	H	0.49407300	-2.93849100	-0.32678800
H	4.90909700	-2.60789600	1.80901800	C	-1.29037800	-2.74592400	-3.74791000
H	4.78294900	-2.42610500	-2.47410300	H	-2.22305500	-0.96154100	-2.99831700
C	0.25060800	4.23458700	-1.27855200	C	-0.39564200	-3.79078500	-3.50386200
C	-0.91837000	4.99941100	-1.27728800	H	0.94701100	-4.65398800	-2.05184900
C	-1.69106100	5.16582400	-0.12233700	H	-1.79994900	-2.68086700	-4.70645500
C	-1.26504500	4.54773300	1.05614800	H	-0.20774300	-4.54632500	-4.26148600
C	-0.10282200	3.76947700	1.11123700	B	-1.91008800	-0.91253000	1.14557000
C	0.64218100	3.63083200	-0.07063200	C	-1.61243600	-2.42364300	2.85411600
H	-1.23496700	5.47238400	-2.20376700	O	-2.29723800	-2.17772000	1.61040700
H	-1.85264400	4.66805200	1.96306500	C	-1.36666700	-0.96150600	3.38800500
Cu	0.44367900	0.32184300	-0.34330300	O	-1.21909800	-0.20661200	2.16733500
H	5.08434300	2.34073000	0.07354700	C	-2.51351000	-3.29385100	3.73134500
H	3.29077900	4.46391800	0.17391600	H	-2.63591200	-4.27709300	3.26693500
C	5.47931500	-4.07680500	-0.41872800	H	-2.07596800	-3.44153400	4.72500800
H	6.09401700	-4.30948800	0.45573100	H	-3.50549500	-2.85317200	3.84608100
H	4.67603000	-4.82250800	-0.46145200	C	-0.30476600	-3.17003300	2.54887500
H	6.09407700	-4.21082900	-1.31372200	H	0.36724700	-2.55048200	1.94967700
C	-2.96920400	5.96972000	-0.15689100	H	0.21654300	-3.46848500	3.46451900
H	-3.18125700	6.42665100	0.81413400	H	-0.53810500	-4.07074100	1.97439100
H	-2.92218600	6.76555400	-0.90609400	C	-2.58325000	-0.39093300	4.13579600
H	-3.82508100	5.33236600	-0.41077000	H	-2.72632300	-0.86430800	5.11268200
C	3.83937900	-0.17133100	2.34143100	H	-2.43090000	0.68107200	4.29292500
H	4.38749600	0.76769200	2.47745900	H	-3.49662200	-0.52009400	3.54888300
H	2.77569500	0.05845400	2.46524700	C	-0.10870800	-0.78651400	4.23956800
H	4.13499400	-0.85038400	3.14469300	H	0.79151800	-1.06240300	3.68691300
C	3.68826800	0.04034700	-2.73748400	H	-0.01201000	0.26002000	4.54638300
H	2.60188900	0.11972600	-2.85574300	H	-0.15970700	-1.39696800	5.14809900
H	4.09112900	1.05858400	-2.74967800	C	-3.68200100	-0.70255400	-0.84807600
H	4.08148300	-0.49218500	-3.60652400	C	-4.11827100	-2.04000700	-0.84279000
C	0.29053700	3.08306800	2.39658000	C	-4.49654000	0.24968200	-1.48302700
H	-0.15709800	3.59449100	3.25319400	C	-5.31723400	-2.40147800	-1.45574400
H	-0.06701500	2.04590000	2.40013900	H	-3.51811600	-2.79076300	-0.34275800
H	1.37488100	3.06470500	2.53908400	C	-5.70172800	-0.10902900	-2.08909500
C	1.04718400	4.04916500	-2.54812600	H	-4.17671100	1.28954400	-1.49927100
H	2.07001000	4.43033900	-2.45337600	C	-6.11612200	-1.44119900	-2.08153700
H	1.12317700	2.98907000	-2.81370400	H	-5.63214300	-3.44177900	-1.44073600
H	0.57077200	4.57237500	-3.38043000	H	-6.31236400	0.65121800	-2.56983300
C	-2.42468400	-0.24591900	-0.16554600	H	-7.05094200	-1.72854600	-2.55534800
N	-1.04917200	-0.82149800	-0.53376000	H	-2.37644100	0.84537400	-0.19141100

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C	1.93486100	1.52104600	-0.07853500	H	-0.35920100	3.21258500	3.41459800
C	3.10550600	3.40912900	0.40291500	H	-0.10471500	1.76857500	2.42315100
C	3.99809500	2.39067300	0.31371800	H	1.24707300	2.86114100	2.75832500
N	3.26658700	1.24490200	0.01757000	C	1.13244700	4.29271200	-2.24016700
N	1.85051000	2.86166800	0.15956800	H	2.13786800	4.68570900	-2.05285700
C	4.34298800	-0.43963800	-1.40161400	H	1.25316600	3.26852200	-2.60983100
C	3.84155100	-0.06928900	-0.14327100	H	0.68369900	4.88853400	-3.03833800
C	3.89019600	-0.92819700	0.96647600	C	-2.38780900	-0.17754500	-0.11113900
C	4.47029300	-2.18796700	0.78592100	N	-1.01487600	-0.84587500	-0.48087500
C	4.98203300	-2.59852700	-0.44900500	C	-0.91675200	-1.76227100	-1.57133800
C	4.91265000	-1.70975000	-1.52696900	C	-0.39921800	-3.05122300	-1.36785600
H	4.51991900	-2.86550600	1.63483200	C	-1.28225300	-1.38127100	-2.87440200
H	5.30593000	-2.01296900	-2.49415600	C	-0.22973400	-3.92402900	-2.44358800
C	0.26908200	4.32738700	-1.00135400	H	-0.14124800	-3.35886700	-0.36176400
C	-0.92010500	5.06132500	-0.98301700	C	-1.11804500	-2.26093900	-3.94269200
C	-1.75081400	5.09268700	0.14212200	H	-1.70400600	-0.39441300	-3.03632400
C	-1.36331100	4.37056000	1.27486200	C	-0.58639100	-3.53685100	-3.73649200
C	-0.18405300	3.61817400	1.31174300	H	0.17394200	-4.91773700	-2.26555700
C	0.61813100	3.61455400	0.15814600	H	-1.40891200	-1.94738800	-4.94204700
H	-1.20518000	5.61794700	-1.87234900	H	-0.45925000	-4.22072000	-4.57092300
H	-1.99581300	4.38767100	2.15912200	B	-1.64929000	-1.11669400	0.94260100
Cu	0.49260500	0.32749100	-0.33625000	C	-1.67828100	-2.71942100	2.63241900
H	5.06921100	2.36918100	0.43583300	O	-2.15261600	-2.40607100	1.31799400
H	3.23995700	4.45685900	0.61928200	C	-1.36104400	-1.29429600	3.22911900
C	5.56979200	-3.97873500	-0.62284900	O	-0.89857800	-0.58275400	2.07141300
H	5.99948200	-4.35200700	0.31130500	C	-2.77140900	-3.49908700	3.36829800
H	4.79986700	-4.69395400	-0.93711800	H	-2.93059200	-4.46275700	2.87403100
H	6.35294600	-3.98768900	-1.38671200	H	-2.48991400	-3.69590000	4.40919500
C	-3.04839100	5.86552300	0.12701700	H	-3.72002700	-2.95921500	3.35647600
H	-3.25529000	6.31883200	1.10126200	C	-0.41865300	-3.59508400	2.50762500
H	-3.03292200	6.66100300	-0.62338300	H	0.39287300	-3.04494700	2.02265300
H	-3.89290100	5.20682900	-0.10940700	H	-0.06383700	-3.95102600	3.48118300
C	3.32032900	-0.52653700	2.30553800	H	-0.65670800	-4.46821900	1.89253700
H	3.68194300	0.45631200	2.62577000	C	-2.62272600	-0.59087000	3.76241600
H	2.22602500	-0.47293600	2.26992400	H	-2.98736200	-1.04394100	4.69026200
H	3.59656700	-1.25378700	3.07293500	H	-2.38367200	0.45774400	3.96541500
C	4.25456500	0.48705400	-2.59050400	H	-3.42612300	-0.61814500	3.02183800
H	3.21039100	0.68838300	-2.85441700	C	-0.27010400	-1.27032100	4.30094100
H	4.72875700	1.45474000	-2.39437000	H	0.67659200	-1.65801800	3.91951300
H	4.74145800	0.04307300	-3.46180800	H	-0.10344400	-0.24164000	4.63788100
C	0.17483500	2.82323600	2.54360900	H	-0.56181100	-1.86478400	5.17407000
				C	-3.61910200	-0.51428700	-0.87397000
				C	-4.10953300	-1.82818800	-1.00760400
				C	-4.37233100	0.52545200	-1.44922200

C	-5.29556300	-2.08035700	-1.69537300	C	4.60662700	1.51033900	1.70624200
H	-3.56382700	-2.64457300	-0.54946100	H	4.84389500	2.48488600	1.26546600
C	-5.56745300	0.27459600	-2.12379500	H	3.62577600	1.60657300	2.18485600
H	-4.01121900	1.54805200	-1.35903400	H	5.34321700	1.30681900	2.48701800
C	-6.03317700	-1.03429400	-2.25570100	C	2.87880200	-0.47310900	-2.65192000
H	-5.65190700	-3.10340300	-1.78623600	H	1.82746200	-0.62000100	-2.38298400
H	-6.12965300	1.10061400	-2.55263100	H	2.95966800	0.49362900	-3.15991900
H	-6.95989800	-1.23721800	-2.78577900	H	3.13465700	-1.25713600	-3.36653200
H	-2.24993600	0.90060000	-0.03229200	C	0.70627700	4.42616100	1.79725300

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C	1.64076000	1.69883200	-0.20151000	C	-0.81085500	2.43006600	-2.63397300
C	2.22073800	3.59277700	-1.31207100	H	0.10439900	2.76556400	-3.13200600
C	3.29812400	2.76710200	-1.32681500	H	-0.68954900	1.36328100	-2.41463900
N	2.92711700	1.61462100	-0.64445100	H	-1.63604800	2.52633100	-3.34332000
N	1.21644400	2.92519600	-0.62125300	C	-2.35500800	-0.78119600	-0.20299900
C	3.77281500	-0.54547900	-1.43838100	N	-1.27431400	-1.71168000	-0.53162900
C	3.78361000	0.46536700	-0.46261400	C	-0.75683500	-2.16626400	-1.71287800
C	4.60767000	0.40905800	0.67271900	C	0.26065900	-3.15169700	-1.71888700
C	5.43180400	-0.71037300	0.82225500	C	-1.20372400	-1.67085500	-2.96016500
C	5.44630100	-1.74725600	-0.11682000	C	0.79976600	-3.60965300	-2.91674900
C	4.61707000	-1.64244900	-1.23830900	H	0.59863000	-3.55601700	-0.76893900
H	6.07799400	-0.77189900	1.69451800	C	-0.64896100	-2.13836600	-4.15043000
H	4.62016800	-2.43622600	-1.98089600	H	-2.00841800	-0.94217300	-2.97387900
C	-1.09666300	3.22236100	-1.38096100	C	0.35791700	-3.10779800	-4.14707300
C	-2.37279100	3.74586000	-1.14605800	H	1.57202300	-4.37579900	-2.89069100
C	-2.67745500	4.46845000	0.01158400	H	-1.01854500	-1.74582500	-5.09533500
C	-1.66107600	4.68221200	0.94935300	H	0.77744300	-3.47518400	-5.07895100
C	-0.36887400	4.18290100	0.76499500	B	-1.46720400	-1.58829300	0.90494100
C	-0.11210400	3.45013500	-0.40551200	C	-1.13302900	-2.63030900	2.98771900
H	-3.14844300	3.57780600	-1.88872200	O	-1.95504700	-2.56835800	1.82860000
H	-1.87760100	5.25160200	1.85000600	C	-0.54436200	-1.17184400	3.09368200
Cu	0.65208200	0.41687600	0.76027800	O	-0.37219100	-0.86516800	1.68519700
H	4.27979000	2.88385500	-1.75722300	C	-2.00224400	-3.03931000	4.18005000
H	2.07198600	4.57764700	-1.72500500	H	-2.36892400	-4.05836300	4.02582100
C	6.31934400	-2.96297500	0.08474100	H	-1.43595000	-3.02107100	5.11834000
H	6.70824300	-3.33844400	-0.86657300	H	-2.87113200	-2.38574800	4.27672600
H	7.16876400	-2.74360800	0.73786500	C	-0.03475500	-3.68615200	2.75834200
H	5.75150700	-3.77946000	0.54733600	H	0.62826700	-3.38992700	1.94041300
C	-4.07534100	4.98418000	0.25648500	H	0.57071800	-3.86371700	3.65388200
H	-4.60227800	5.17499900	-0.68270000	H	-0.51677400	-4.62636300	2.47693000
H	-4.66669200	4.25188700	0.81942400	C	-1.54632400	-0.16681400	3.67681200
H	-4.06530800	5.91119000	0.83747000	H	-1.68468500	-0.31435300	4.75230600

H	-1.17054400	0.84981200	3.51842800	H	-4.23985200	3.54786900	-0.31747500
H	-2.51552500	-0.25621400	3.18102100	C	4.57271800	3.88709300	-1.08319000
C	0.80146700	-1.06333400	3.80655100	H	4.89666800	4.73531300	-0.47212900
H	1.56833400	-1.66243100	3.31123300	H	5.12164900	3.00405800	-0.73444100
H	1.13822600	-0.02025900	3.82694900	H	4.87113800	4.07680700	-2.11804100
H	0.71366300	-1.40214000	4.84433200	C	-6.88405300	-2.28401600	0.41428800
C	-3.76502000	-1.12290300	-0.54356600	H	-7.87337400	-1.83473100	0.56635400
C	-4.20075800	-2.44962800	-0.71061300	H	-6.95397700	-2.93896800	-0.45879500
C	-4.72158000	-0.10046600	-0.67170800	H	-6.67096000	-2.90449800	1.28947900
C	-5.53625700	-2.73593600	-0.98829000	C	0.41768000	3.68580600	1.77365200
H	-3.47938000	-3.25479400	-0.61439100	H	-0.49922000	4.28230100	1.72989600
C	-6.05948100	-0.38640500	-0.94331700	H	0.15638200	2.70642100	2.18913200
H	-4.40357200	0.93445600	-0.55581200	H	1.09906400	4.16969900	2.47746900
C	-6.47693500	-1.70893300	-1.10561600	C	0.16814200	2.57683500	-3.19263500
H	-5.84585300	-3.77073800	-1.11440700	H	-0.11416700	1.51943700	-3.13456500
H	-6.77666100	0.42621300	-1.03630100	H	-0.75773400	3.15158600	-3.30045300
H	-7.51707900	-1.93596800	-1.32320300	H	0.76053700	2.71437600	-4.10028200
H	-2.12933900	0.27805500	-0.39702400	C	-3.53971700	0.94560600	2.39237200
L₂-14				H	-3.46156400	2.03552400	2.33318000
C	-1.59028200	1.60607000	-0.42083400	H	-4.09267900	0.69512500	3.30088100
C	-3.22924700	3.17926200	-0.39056400	H	-2.52385600	0.55136000	2.50855800
C	-2.04810800	3.82573200	-0.56033100	C	-4.20274100	0.71237000	-2.65084300
N	-1.05666200	2.85158600	-0.57591200	H	-4.40960800	1.78054200	-2.78052800
N	-2.93200800	1.82373500	-0.30737900	H	-3.14132000	0.56362100	-2.87591000
C	0.95576500	3.00095100	-1.97568900	H	-4.78600700	0.16608400	-3.39565200
C	0.35445500	3.13264000	-0.71405500	C	2.51174800	-0.85475100	0.39050200
C	1.07329700	3.54538400	0.42119400	N	1.77720400	-1.58531500	1.44391300
C	2.43761400	3.80326900	0.26469500	C	1.09130100	-1.00552000	2.48528100
C	3.08536000	3.65832500	-0.96708800	C	-0.03535300	-1.65380200	3.04904300
C	2.32522600	3.26943100	-2.07446600	C	1.50061200	0.21862600	3.06401300
H	3.01146900	4.11563100	1.13351300	C	-0.70525300	-1.10522300	4.13911000
H	2.80810800	3.16869300	-3.04319100	H	-0.34944800	-2.60550400	2.63096500
C	-4.54353100	0.24042100	-1.25714400	C	0.82263300	0.75265300	4.15916200
C	-5.49464700	-0.76403300	-1.05676100	H	2.37496500	0.71889900	2.65877300
C	-5.82986200	-1.21948800	0.22324400	C	-0.28813900	0.10431400	4.70786900
C	-5.18649100	-0.64417100	1.32341800	H	-1.55838700	-1.63478000	4.55799100
C	-4.22538800	0.36272000	1.18069200	H	1.17643500	1.68285700	4.59889400
C	-3.91766800	0.78481500	-0.12308800	H	-0.80617600	0.52169100	5.56629300
H	-5.98493100	-1.20048500	-1.92352000	B	1.48593500	-2.07148100	0.08545400
H	-5.43470800	-0.98698500	2.32486500	C	1.05486900	-3.67120600	-1.54836300
Cu	-0.70129200	-0.05596300	-0.44422900	O	1.75612700	-3.40815200	-0.34199000
H	-1.81866800	4.87368400	-0.66841400	C	-0.29870800	-2.89326300	-1.33884800
				O	0.17576400	-1.71685500	-0.61876300
				C	1.86840700	-3.12561400	-2.73809000

H	2.86926500	-3.56327000	-2.69692600	C	3.19629000	-3.10429500	-1.35064100
H	1.41861500	-3.38089500	-3.70363700	C	4.04033100	-3.04022500	-0.23757800
H	1.97974300	-2.03985300	-2.67510200	C	3.45943600	-3.03141200	1.03477700
C	0.88746400	-5.18636700	-1.69102100	C	2.07380600	-3.04950100	1.21678200
H	0.44092700	-5.62199200	-0.79517500	C	1.26297500	-3.07928100	0.06974600
H	0.26967900	-5.44519500	-2.55848600	H	3.63069600	-3.12688400	-2.34694400
H	1.87146800	-5.64397100	-1.82810900	H	4.10028200	-2.99341800	1.91206700
C	-0.99918300	-2.45480500	-2.62378400	Cu	-0.27853100	-0.22223400	-0.40502700
H	-1.24084900	-3.32525100	-3.24316700	H	-3.15397100	-4.24029600	0.83971600
H	-1.94081000	-1.94438900	-2.39131000	H	-0.52214400	-5.13055900	0.73369600
H	-0.37299800	-1.77864600	-3.20990300	C	-6.93046800	0.88927400	-0.10841700
C	-1.27735400	-3.64125500	-0.42529600	H	-7.43641300	1.00185900	0.85483900
H	-0.77164700	-3.98593000	0.47944600	H	-6.66258800	1.89500300	-0.45465000
H	-2.09164000	-2.96953200	-0.13423300	H	-7.64760800	0.47805500	-0.82501100
H	-1.71617900	-4.50640600	-0.93240100	C	5.53589500	-2.93753800	-0.40716000
C	3.99456400	-0.93647400	0.34863500	H	6.06844200	-3.38130900	0.43934100
C	4.72107000	-1.83190800	1.15087300	H	5.87170300	-3.43410600	-1.32239100
C	4.71576800	-0.12810600	-0.55009400	H	5.83426400	-1.88407800	-0.47202700
C	6.11052300	-1.91292700	1.05782500	C	-3.04535400	-0.81763700	2.62957900
H	4.17501900	-2.46019900	1.84756100	H	-2.72294800	-1.82715500	2.90285800
C	6.10446800	-0.21152800	-0.64548700	H	-2.14712200	-0.19279900	2.57103300
H	4.17142900	0.56787400	-1.18606200	H	-3.66260300	-0.42606000	3.44180900
C	6.81419600	-1.10547300	0.16100800	C	-3.65465400	-2.35282300	-2.18652300
H	6.64875400	-2.61273600	1.69301700	H	-2.63618200	-2.08762900	-2.48860500
H	6.63533800	0.42159800	-1.35342900	H	-3.65211400	-3.42570300	-1.96361700
H	7.89647100	-1.17188200	0.09010400	H	-4.31547600	-2.19013800	-3.04120100
H	2.13763100	0.16101100	0.19678000	C	1.48255600	-3.03659800	2.60639000
L₂-TS15				H	1.03883900	-4.00467900	2.86869500
C	-0.93793300	-1.93339400	0.06493800	H	2.25200200	-2.81382600	3.34899800
C	-0.95120700	-4.15574400	0.56593000	H	0.69237200	-2.28605600	2.70202700
C	-2.23526500	-3.72237200	0.61536800	C	0.92757300	-3.17433700	-2.45469400
N	-2.21182500	-2.36452900	0.30723700	H	0.12676100	-3.91428100	-2.35453400
N	-0.17157000	-3.05473200	0.22896500	H	0.45187000	-2.20463300	-2.63966700
C	-4.10785900	-1.53538000	-1.00000500	H	1.51973100	-3.43058100	-3.33657300
C	-3.39419500	-1.54294500	0.21137900	C	1.08729100	1.39343100	0.96023400
C	-3.81175800	-0.80387500	1.32968500	N	1.98022900	2.22007700	0.13005100
C	-4.97175700	-0.03175000	1.20031900	C	3.30378400	1.90590800	-0.12312600
C	-5.70338100	0.01703800	0.01024700	C	3.91554500	2.30405400	-1.33211200
C	-5.25875100	-0.74623800	-1.07521400	C	4.09428000	1.22435100	0.82568400
H	-5.30917100	0.54598800	2.05725500	C	5.25667300	2.02616700	-1.57654800
H	-5.82187100	-0.72980400	-2.00526700	H	3.32301200	2.83950100	-2.06733700
C	1.80426100	-3.12337700	-1.22601000	C	5.43826600	0.95562800	0.57019800
				H	3.64835900	0.93420400	1.77195000
				C	6.03452500	1.34826300	-0.63133500

H	5.70180400	2.34494000	-2.51625200	C	4.15363000	-0.13238400	-1.06734600
H	6.02947100	0.44525900	1.32748600	C	3.59791700	0.48595400	0.06666700
H	7.08393500	1.14356600	-0.82252600	C	3.76990700	-0.03614300	1.35880200
B	0.69083200	2.13413400	-0.53029800	C	4.50960500	-1.21726000	1.48872500
C	-1.13266700	3.02323200	-1.69648900	C	5.06785000	-1.87078400	0.38755100
O	-0.13300100	3.28209500	-0.71344500	C	4.88512400	-1.30825200	-0.88051000
C	-0.44100800	1.94657100	-2.61812700	H	4.64995800	-1.63425100	2.48289200
O	0.36105900	1.20145000	-1.65728100	H	5.32090500	-1.79694600	-1.74879600
C	-2.39851600	2.49648000	-0.99603200	C	-0.68330200	3.82808900	-1.64283300
H	-2.70002600	3.22406500	-0.23761600	C	-1.93758700	4.44482800	-1.68535600
H	-3.23111500	2.35518900	-1.69313000	C	-2.53490600	4.98654600	-0.54291200
H	-2.21661300	1.54602000	-0.48296100	C	-1.84051400	4.91088300	0.66916500
C	-1.46104900	4.33940800	-2.40824000	C	-0.58460300	4.30497400	0.76585100
H	-0.55869300	4.82029400	-2.78971800	C	-0.02453000	3.76823100	-0.40483900
H	-2.15791200	4.18331900	-3.23954800	H	-2.46141700	4.49807000	-2.63666200
H	-1.92981300	5.02753500	-1.69863200	H	-2.28877800	5.32915500	1.56715200
C	-1.38911200	0.99268700	-3.33850500	Cu	0.12920600	0.54572300	0.35648300
H	-2.03853900	1.54521700	-4.02617400	H	4.54334200	3.05408500	-0.37626700
H	-0.81688700	0.26827600	-3.92761100	H	2.49810300	4.91364300	-0.67216100
H	-2.02150100	0.44402100	-2.63727100	C	5.82760300	-3.16472600	0.55827500
C	0.54037800	2.56810900	-3.62106600	H	6.31928700	-3.21464800	1.53423100
H	1.20194500	3.28298600	-3.12635000	H	5.15184400	-4.02613000	0.49038800
H	1.15500000	1.77589400	-4.05797500	H	6.59146700	-3.28758000	-0.21540700
H	0.01561800	3.08512200	-4.43029100	C	-3.90792800	5.61183900	-0.60896000
C	0.65684800	1.91674700	2.28735500	H	-4.01122200	6.42955200	0.11072800
C	0.57534100	3.29677600	2.54764500	H	-4.12122200	6.00648700	-1.60662500
C	0.29241200	1.03482800	3.32018300	H	-4.68461100	4.87318400	-0.37623900
C	0.13763900	3.76618100	3.78503100	C	3.18398000	0.62624000	2.58180300
H	0.86416000	3.99128100	1.76620400	H	3.22901000	1.71725600	2.51746800
C	-0.14879800	1.50475100	4.55825000	H	2.13302500	0.34595100	2.71611400
H	0.37521700	-0.03734100	3.15249600	H	3.72386100	0.31311900	3.47923900
C	-0.23212300	2.87735000	4.79866400	C	3.97719600	0.44607800	-2.45190700
H	0.08709800	4.83805900	3.96109600	H	2.92916300	0.68639200	-2.65531500
H	-0.41391300	0.79663700	5.34022500	H	4.54858300	1.37214200	-2.58581000
H	-0.57094400	3.24862800	5.76193300	H	4.31774500	-0.26296100	-3.21042000
H	1.43302500	0.34936500	1.02611800	C	0.12931200	4.21552500	2.09277800
L₂-16				H	1.12642300	4.66757500	2.05292900
C	1.49841800	1.82424600	-0.10106000	H	-0.44139900	4.72499800	2.87276200
C	2.47413700	3.85208300	-0.48395400	H	0.26100500	3.17066400	2.39480600
C	3.47123500	2.94428700	-0.34298800	C	-0.07492200	3.23164300	-2.88898100
N	2.86179700	1.71378900	-0.11279900	H	0.93514300	3.61285500	-3.07420100
N	1.27979300	3.15417500	-0.33536000	H	0.00270300	2.14217500	-2.80351000
				H	-0.68827300	3.45890500	-3.76418700
				C	-1.35149000	-0.48675800	1.16287800

N	-2.16524400	-1.28123000	0.20518900	H	-2.01072200	0.29577700	1.55802200
C	-3.55433600	-1.41841000	0.48278900				
C	-4.50196200	-1.48381600	-0.55684400	L₂-17			
C	-4.02721400	-1.44342400	1.80811800	Cu	-0.36793100	-0.20172700	-0.72679100
C	-5.86249700	-1.59332100	-0.27661500	N	2.39903100	0.53058300	0.06499100
H	-4.16514700	-1.45250400	-1.58532100	N	-2.74877400	0.94945600	-2.14796400
C	-5.39166700	-1.54490300	2.07769700	N	-2.74364900	-1.20170200	-2.14903900
H	-3.32216200	-1.40240800	2.62926700	O	4.87218700	0.94596900	-0.09760400
C	-6.32242000	-1.62338800	1.04123800	O	4.06914000	-1.14056800	-0.62694300
H	-6.56978600	-1.64176600	-1.10106900	B	3.74531100	0.14305000	-0.21095000
H	-5.72487100	-1.56925800	3.11228500	C	-2.03980100	-0.12318800	-1.68949100
H	-7.38443200	-1.70290800	1.25529800	C	-3.86392500	0.54849100	-2.87733900
B	-1.55102500	-1.88927300	-0.91754100	C	-3.86129400	-0.80777300	-2.87771700
C	0.05045300	-2.37952000	-2.48776100	C	-2.37226500	-2.57913600	-1.92876900
O	-0.18689400	-1.79062800	-1.18633400	C	-2.95530100	-3.27849400	-0.85969500
C	-1.18983200	-3.33998900	-2.65250100	C	-2.58795800	-4.61689000	-0.68131600
O	-2.20059100	-2.67094800	-1.86583000	H	-3.03042300	-5.17311200	0.14143400
C	0.05816000	-1.23411300	-3.51099100	C	-1.67191200	-5.25352800	-1.52402800
H	0.82367200	-0.50845300	-3.22223000	C	-1.12436100	-4.52229000	-2.58369200
H	0.28527000	-1.58956200	-4.52093300	H	-0.41775800	-5.00424300	-3.25508800
H	-0.90685200	-0.71957500	-3.53222200	C	-1.45831100	-3.18384300	-2.80848700
C	1.41004500	-3.07553900	-2.46652400	C	-0.83896100	-2.41995900	-3.95393400
H	1.46793600	-3.81506100	-1.66631800	H	-1.59547500	-1.91884900	-4.56693900
H	1.60869100	-3.57476600	-3.42135800	C	-3.93151600	-2.61887200	0.08333900
H	2.19942400	-2.33853300	-2.29446800	H	-4.73533500	-2.10443300	-0.45318700
C	-1.71100100	-3.49305700	-4.08127100	C	-2.39408400	2.33204600	-1.93110600
H	-0.94960900	-3.93731800	-4.73145500	C	-3.02791500	3.04068200	-0.89828400
H	-2.58306700	-4.15342100	-4.08279500	C	-4.02845200	2.38168800	0.02035000
H	-2.01715300	-2.53443000	-4.50440600	H	-4.82823600	1.87925900	-0.53384300
C	-0.97281300	-4.72581000	-2.02634300	C	-2.68531000	4.38606200	-0.72940500
H	-0.59246600	-4.64510400	-1.00406200	H	-3.16416300	4.95008700	0.06723100
H	-1.93347900	-5.24627600	-1.98648200	C	-1.74129600	5.01801300	-1.54353800
H	-0.27385900	-5.33299500	-2.61004600	C	-1.14206200	4.27643400	-2.56645400
C	-0.78906900	-1.25393800	2.32433900	H	-0.40857900	4.75391600	-3.21146600
C	-0.43050100	-2.61389500	2.25578700	C	-1.45047000	2.93110000	-2.78178000
C	-0.56205400	-0.59764600	3.55488000	C	-0.77238700	2.15493400	-3.88497100
C	0.13294600	-3.27492800	3.34787100	H	-1.49341800	1.61832700	-4.51086200
H	-0.60365800	-3.15828100	1.33297500	C	1.39296000	-0.56864500	0.08821000
C	0.00430500	-1.25556500	4.64467300	H	1.75495300	-1.31125600	-0.63159300
H	-0.84862900	0.44870600	3.65061900	C	2.01398400	1.84913500	0.39783400
C	0.36113800	-2.60443000	4.55120100	C	0.83624100	2.09864400	1.13164300
H	0.39149500	-4.32772400	3.25742900	H	0.22171300	1.26534700	1.44875300
H	0.15429000	-0.71637100	5.57757100	C	0.45904400	3.39887400	1.47208300
H	0.79720300	-3.12228900	5.40081100				

C	2.80670300	-1.16967700	-1.83193700	C	-1.85129300	2.27206000	1.66563900
C	4.15357300	-1.28636800	-1.45133300	H	-1.20899500	2.75866800	0.93628600
C	5.04789900	-0.08030900	-1.30305800	C	-2.59725600	3.04980000	2.54510400
H	5.07159200	0.52477800	-2.21594500	H	-2.53126400	4.13388400	2.48806000
C	4.65246100	-2.57271400	-1.21418600	C	-3.43046700	2.44884300	3.49667600
H	5.69160900	-2.67918000	-0.91262500	H	-4.01232100	3.05616100	4.18418900
C	3.86000600	-3.71495800	-1.35595000	C	-3.49888900	1.05798200	3.54429800
C	2.53273100	-3.55510900	-1.76853800	H	-4.14060000	0.57011300	4.27425600
H	1.90449600	-4.43255800	-1.90090500	C	-2.74956600	0.27559700	2.66030500
C	1.98433500	-2.29453800	-2.01912800	H	-2.82400500	-0.80505200	2.71449100
C	0.55465300	-2.15827300	-2.48341200	H	6.07174600	-0.38951200	-1.07814700
H	0.48553800	-1.56617100	-3.40283600	H	4.69918700	0.56434300	-0.49011400
C	-1.07872000	0.07273600	0.73217100	H	0.12224700	-3.14233700	-2.67909200
H	-1.20883200	0.52645800	-0.25190800	H	-0.06607900	-1.66292900	-1.73023200
C	-0.85036300	-2.38478100	1.35328900	H	-2.46929700	2.40998100	-3.36200400
C	0.54247600	-2.55251000	1.32346700	H	-1.98403000	1.23620200	-2.14148300
H	1.14798900	-1.87817900	0.72619200	H	2.75863600	5.18895900	-0.24019900
C	1.15683200	-3.57533900	2.04481300	H	2.73980100	3.44483400	0.07138200
H	2.23746400	-3.68065000	1.99927000	C	4.41442400	-5.08969500	-1.06538400
C	0.39288100	-4.46578400	2.80348300	H	4.03882400	-5.47053800	-0.10788900
H	0.87177600	-5.26375300	3.36382600	H	4.11980300	-5.81078400	-1.83496300
C	-0.99413400	-4.31844800	2.82699800	H	5.50650900	-5.07826000	-1.01069300
H	-1.60586700	-5.00237400	3.40931600	C	-2.04086700	6.49673800	-0.51195200
C	-1.61000500	-3.28800300	2.11468000	H	-2.59625400	6.26308500	0.40469800
H	-2.68919800	-3.18688800	2.13306500	H	-1.43957000	7.38844600	-0.31314400
C	-4.15619500	-2.81325500	-1.42872700	H	-2.77882800	6.74681200	-1.28061700
C	-5.36517200	-3.68233900	-1.08619700	C	0.43193700	0.06523800	3.54119100
H	-5.05582500	-4.72915600	-1.01444000	H	-0.29473300	-0.72358800	3.41362100
H	-6.13331600	-3.60891700	-1.86346300	H	0.06925900	1.08244900	3.44882400
H	-5.80704000	-3.39586600	-0.13024300	Br	3.09257500	1.23652300	1.64358900
C	-3.44248700	-3.37115800	-2.66846900	C	1.70033100	-0.19659700	4.00108200
H	-2.58082500	-2.75471100	-2.93979200	H	2.02690000	-1.23058000	4.08530800
H	-4.11206300	-3.43074700	-3.53216700	C	2.65077700	0.81900100	4.13834900
H	-3.08078700	-4.37819600	-2.44271000	H	2.33600500	1.85252200	4.21932900
C	-4.44763500	-1.26577900	-1.52374700	H	3.66276000	0.60074800	4.46097900
C	-4.71447500	-0.74188800	-2.93365500	H	1.66654500	2.71529300	-4.03710200
H	-4.87792600	0.33924000	-2.89862000	H	3.02214100	0.28819100	-4.14886900
H	-5.61182700	-1.20429100	-3.35861000				
H	-3.87331300	-0.93525700	-3.60200500	L₂-19			
C	-5.55683000	-0.79987100	-0.57004700				
H	-5.38106100	-1.16110600	0.44683200	Cu	0.90353200	0.71481200	0.91096500
H	-6.54391300	-1.14130300	-0.89674200	N	-1.02790900	-1.66805300	0.57967400
H	-5.56049000	0.29295300	-0.53881400	N	2.15972700	0.81499400	-1.95540600
C	-1.90527400	0.86104600	1.69892500	N	0.61439100	2.30511100	-1.83008200

O	-2.40903300	-3.51284900	-0.35537600	C	-4.35326000	-4.78177400	-1.02284300
O	-3.00261500	-1.35087900	-0.87621000	H	-3.78836700	-5.71721600	-1.07020200
B	-2.11649700	-2.17114700	-0.19395800	H	-5.18612900	-4.85311500	-1.73051100
C	1.16273000	1.26166600	-1.12722400	H	-4.75922800	-4.68476800	-0.01440700
C	2.23683900	1.56814300	-3.12423600	C	-2.72412900	-3.88063400	-2.70765300
C	1.26751500	2.50636200	-3.04402700	H	-2.07190500	-3.04657500	-2.98210500
C	-0.56843700	3.07083600	-1.49901400	H	-3.43430500	-4.04913800	-3.52296400
C	-0.43276600	4.32670400	-0.87625500	H	-2.10381300	-4.77469900	-2.60081000
C	-1.60277500	5.03702900	-0.58570000	C	-4.10996200	-2.18797900	-1.30704600
H	-1.51261100	6.00081900	-0.09077500	C	-4.64061300	-1.65748300	-2.63705100
C	-2.87134500	4.56064800	-0.93182900	H	-5.05890300	-0.65696900	-2.49349700
C	-2.95378500	3.35295200	-1.62832800	H	-5.43714500	-2.30333000	-3.02132200
H	-3.92593700	2.98785300	-1.95153500	H	-3.85324300	-1.59099500	-3.39002400
C	-1.81869700	2.59422300	-1.93563100	C	-5.19510000	-2.08206300	-0.22673300
C	-1.97574600	1.32395700	-2.73860200	H	-4.83720300	-2.46298200	0.73363400
H	-1.06948500	1.07042700	-3.29277500	H	-6.09892600	-2.63234300	-0.50522100
C	0.91464300	4.93655500	-0.58554700	H	-5.45780100	-1.02954300	-0.09129600
H	1.45842600	5.14148800	-1.51614200	C	-1.85787100	0.36044900	1.80041800
C	2.99458300	-0.35067400	-1.77392100	C	-2.16011000	1.73709600	1.76967100
C	4.33502000	-0.19035700	-1.38329700	H	-1.73049300	2.36016200	0.99130000
C	4.93609000	1.16688000	-1.11953600	C	-2.99633500	2.31154300	2.72183500
H	4.95918800	1.77632900	-2.03107000	H	-3.21069800	3.37584900	2.67289600
C	5.12199200	-1.34483900	-1.28004000	C	-3.55915000	1.52819400	3.73516300
H	6.15756500	-1.23822600	-0.96704900	H	-4.21257100	1.97690800	4.47795000
C	4.62520800	-2.61571100	-1.57823200	C	-3.27144100	0.16493900	3.77925900
C	3.29878500	-2.72428700	-2.01101200	H	-3.70086300	-0.45720600	4.56019800
H	2.89893000	-3.70151400	-2.27028900	C	-2.42960700	-0.41239200	2.82571800
C	2.46699600	-1.60759700	-2.12503600	H	-2.22017600	-1.47486500	2.87329300
C	1.04978300	-1.75950700	-2.62406600	H	5.96407900	1.06542000	-0.76273600
H	0.84929800	-1.09232900	-3.46969200	H	4.35942600	1.71782200	-0.37045100
C	-0.94681500	-0.21105600	0.76088700	H	0.86887600	-2.78616600	-2.95141200
H	-1.16186900	0.26049100	-0.19448300	H	0.32024800	-1.52292500	-1.84326900
C	-0.16038700	-2.60773100	1.23347300	H	-2.78924500	1.44206400	-3.46136100
C	1.22218600	-2.58546400	1.01578800	H	-2.23471800	0.47115400	-2.10306000
H	1.65204300	-1.81631600	0.38536400	H	0.79598900	5.88503800	-0.05573500
C	2.05034400	-3.54684700	1.59611400	H	1.54134200	4.27548500	0.01951000
H	3.11943700	-3.50816100	1.40712800	C	5.49269600	-3.84503900	-1.44367700
C	1.51179400	-4.55256800	2.40070800	H	5.18359400	-4.45493700	-0.58622000
H	2.15711500	-5.30167800	2.85025000	H	5.42238800	-4.48256900	-2.33148500
C	0.13403500	-4.58513700	2.61852800	H	6.54340600	-3.57967600	-1.29911600
H	-0.30230500	-5.36145400	3.24092100	C	-4.11797500	5.33200800	-0.56907600
C	-0.69442300	-3.62155500	2.04312400	H	-4.55545200	4.95152600	0.36224800
H	-1.76640000	-3.66613100	2.20000400	H	-3.90376100	6.39421400	-0.42021400
C	-3.43655800	-3.61184600	-1.37473200	H	-4.88441200	5.24345600	-1.34536800

C	0.88541000	0.14405700	2.89750500
H	0.12339100	-0.62228100	2.97350300
H	0.54444300	1.09367200	3.31003300
Br	2.59100900	2.40265900	1.44517600
C	2.17729100	-0.32250100	3.41080500
H	2.44711000	-1.34751900	3.16505300
C	2.99948400	0.38444200	4.20448900
H	2.78381100	1.41280800	4.47610600
H	3.91324000	-0.05048100	4.60014500
H	0.96877300	3.28571000	-3.72641800
H	2.96346500	1.35412500	-3.89134300

L₂-TS20

Cu	-1.08889500	-0.22439000	0.68716200
N	1.67884700	1.46517200	0.26139900
N	-3.13684600	-0.66376600	-1.58864900
N	-1.32994000	-1.76821300	-1.94664000
O	3.76620600	2.51778100	-0.55595200
O	3.76451000	0.23224700	-0.28661600
B	3.04083300	1.40254400	-0.17828200
C	-1.87836400	-0.86142900	-1.07602000
C	-3.35407600	-1.42284500	-2.73567700
C	-2.21627300	-2.11800300	-2.96104800
C	-0.02407900	-2.37731200	-1.85008400
C	0.08508200	-3.64690700	-1.25256500
C	1.35430100	-4.23395200	-1.20954400
H	1.45723300	-5.21186600	-0.74570900
C	2.48317600	-3.60781100	-1.74647900
C	2.32126100	-2.36546700	-2.36536200
H	3.18284100	-1.87359100	-2.80776200
C	1.07741500	-1.73060800	-2.43452700
C	0.94743600	-0.38924500	-3.11664500
H	0.02928700	-0.31479100	-3.70657300
C	-1.10903200	-4.36140700	-0.67291300
H	-1.93238400	-4.42853500	-1.39208900
C	-4.17882100	0.17678900	-1.04846800
C	-5.07764900	-0.36766700	-0.11426100
C	-4.95734400	-1.78945800	0.37098900
H	-4.90127900	-2.49464400	-0.46569400
C	-6.11062500	0.45767000	0.34517300
H	-6.81492700	0.05208800	1.06764500
C	-6.26722400	1.77490900	-0.09818700
C	-5.37194200	2.26298900	-1.05539500

H	-5.49569200	3.27399500	-1.43634700
C	-4.32927500	1.47703200	-1.55663100
C	-3.43988600	2.00239300	-2.65823100
H	-3.64966700	1.50075900	-3.61078900
C	1.07971300	0.25083400	0.83276900
H	0.96353700	-0.52583500	0.07080000
C	0.98779400	2.71044000	0.09538200
C	-0.13182900	2.81993200	-0.73830200
H	-0.50685000	1.93009900	-1.23272700
C	-0.76240300	4.05277600	-0.92041200
H	-1.62869500	4.11951600	-1.57149000
C	-0.27741800	5.19615700	-0.28425800
H	-0.76649700	6.15462800	-0.43170600
C	0.84550800	5.09633400	0.53933000
H	1.23530900	5.97813000	1.04006200
C	1.47150500	3.86521100	0.72890000
H	2.35104800	3.79087100	1.35900400
C	5.00653100	2.04582900	-1.14140700
C	6.11420200	3.03411600	-0.78091400
H	5.90184800	4.00495500	-1.23814600
H	7.08398300	2.68888600	-1.15463100
H	6.18769100	3.17905800	0.29824500
C	4.80362900	2.01431400	-2.66253100
H	4.01423000	1.31039100	-2.94078800
H	5.72089300	1.73391000	-3.18920500
H	4.50236900	3.00983600	-2.99977200
C	5.15089200	0.60994700	-0.50086300
C	5.81021800	-0.43620000	-1.39670300
H	5.82319900	-1.40206900	-0.88380000
H	6.84565800	-0.15871900	-1.62089400
H	5.27298400	-0.55969100	-2.33866500
C	5.83352500	0.62628900	0.87372800
H	5.37738900	1.36746200	1.53513300
H	6.90288400	0.84331600	0.79014200
H	5.71196800	-0.35360800	1.34247200
C	1.80915700	-0.30039400	2.00671900
C	1.84168800	-1.69064900	2.21503000
H	1.32326900	-2.34499400	1.52337200
C	2.52035000	-2.23277400	3.30369300
H	2.52927200	-3.30972600	3.44539700
C	3.17913000	-1.40105300	4.21212400
H	3.70713600	-1.82580300	5.06131600
C	3.15308800	-0.01780100	4.01994800
H	3.66174400	0.63954900	4.72017200

C	2.47486400	0.52605900	2.93046300
H	2.47292000	1.60179300	2.78374400
H	-5.82369200	-2.05827800	0.98078800
H	-4.05292000	-1.93493100	0.97558500
H	-3.60286800	3.07242400	-2.80941600
H	-2.38092700	1.84000300	-2.44459100
H	1.79485300	-0.21750300	-3.78572200
H	0.93430600	0.42752500	-2.38723100
H	-0.83706900	-5.37732000	-0.37555800
H	-1.48096200	-3.83166900	0.21312000
C	-7.37300500	2.64838200	0.44688200
H	-7.06279900	3.14529900	1.37446900
H	-7.65291300	3.43135900	-0.26396300
H	-8.26763300	2.06236100	0.67819700
C	3.84581500	-4.25047700	-1.64595000
H	4.36907700	-3.91050800	-0.74376700
H	3.77239900	-5.34054600	-1.58937600
H	4.47514600	-3.99464400	-2.50383600
C	-0.60111000	1.10901000	2.20391100
H	0.17833700	1.85681100	2.25422400
H	-0.55148800	0.37591600	3.00343700
Br	-1.70608100	-2.16543800	2.26843000
C	-1.92267000	1.67589300	1.90881600
H	-1.93669200	2.58807800	1.31768500
C	-3.09356600	1.15075200	2.33245200
H	-3.12317600	0.22226100	2.89384000
H	-4.03446700	1.64308000	2.10904800
H	-1.94909400	-2.82304600	-3.73172500
H	-4.29178000	-1.39528400	-3.26707600

L₂-21

Cu	0.00003100	1.19442200	-0.00108100
Br	0.00015600	3.43631500	-0.00294900
C	-0.00004500	-0.70265900	0.00115000
N	-1.07673100	-1.54203600	0.00246300
N	1.07663500	-1.54204500	0.00221800
C	-0.67853000	-2.87496300	0.00432600
C	0.67842300	-2.87496900	0.00415600
H	-1.39087000	-3.68447500	0.00560100
H	1.39075700	-3.68448700	0.00525000
C	2.45303500	-1.10589700	0.00111200
C	3.10018300	-0.90602700	-1.22874000
C	3.10159400	-0.90420700	1.22990900

C	4.43585700	-0.49471300	-1.20170200
C	4.43724400	-0.49293600	1.20072300
C	5.11944100	-0.27779600	-0.00103900
H	4.95174600	-0.33426300	-2.14520300
H	4.95422200	-0.33106100	2.14338400
C	-2.45311700	-1.10584000	0.00150700
C	-3.10131500	-0.90936400	-1.22825200
C	-3.10060900	-0.90070200	1.23038200
C	-4.43702500	-0.49791400	-1.20119400
C	-4.43619700	-0.48947300	1.20121600
C	-5.11949800	-0.27765700	-0.00060000
H	-4.95372600	-0.34004800	-2.14467500
H	-4.95234900	-0.32498300	2.14388900
C	2.38398000	-1.10074100	2.54349600
H	1.58009500	-0.36617900	2.66445100
H	1.92729400	-2.09355200	2.61723000
H	3.07519600	-0.98335200	3.38126300
C	2.38107200	-1.10436200	-2.54123700
H	1.92274100	-2.09659100	-2.61238200
H	1.57826600	-0.36875300	-2.66307700
H	3.07170500	-0.98988500	-3.37989100
C	6.54979100	0.20636100	-0.00226300
H	7.09008900	-0.14083600	-0.88789200
H	6.58977300	1.30247100	-0.00427600
H	7.09053400	-0.13762600	0.88433800
C	-2.38182200	-1.09339300	2.54389200
H	-1.92112700	-2.08427600	2.61824900
H	-1.58086900	-0.35546200	2.66397600
H	-3.07322900	-0.97802500	3.38179000
C	-2.38338700	-1.11149500	-2.54082100
H	-1.92835600	-2.10532600	-2.61105000
H	-3.07399400	-0.99576400	-3.37931800
H	-1.57819300	-0.37872200	-2.66385000
C	-6.54986500	0.20645800	-0.00137500
H	-7.08575600	-0.12691200	-0.89488000
H	-7.09494800	-0.15132300	0.87715300
H	-6.58995700	1.30246000	0.01383800

L₂-22

C	0.05266100	-1.22952400	-0.50715000
C	-0.60900500	-2.03180100	-2.52179200
C	0.74874500	-1.99308700	-2.52537900
N	1.13641500	-1.49936100	-1.28545700

N	-1.01785000	-1.56043900	-1.28006000	O	-0.15227700	3.16765500	-0.06904100
C	3.21499800	-2.27928500	-0.24550300	C	-0.21900700	4.37639600	-0.75125100
C	2.50182400	-1.25136300	-0.88428200	C	-0.04813200	4.15242500	-2.27312300
C	3.06557700	0.00811600	-1.14845300	H	-0.82765300	3.48011900	-2.64717400
C	4.38837500	0.21700300	-0.74054700	H	-0.10748000	5.09070700	-2.83866600
C	5.13260400	-0.77224700	-0.09129500	H	0.92370600	3.69215200	-2.48070400
C	4.53137200	-2.01452800	0.14063400	C	-1.58888200	5.04992400	-0.49964000
H	4.84485500	1.18368400	-0.93812700	H	-1.72055300	5.23675600	0.57296900
H	5.09910700	-2.79823100	0.63637600	H	-1.69524100	6.00583000	-1.02830800
C	-3.03818300	-2.44809200	-0.21018300	H	-2.39618400	4.38472700	-0.82550500
C	-4.36226700	-2.25535500	0.18917100	C	0.90383600	5.32177100	-0.26240600
C	-5.03971100	-1.05479800	-0.05707400	H	1.87943000	4.84588600	-0.41224200
C	-4.36075300	-0.03211000	-0.72389700	H	0.90623900	6.28664100	-0.78559200
C	-3.03210300	-0.16870600	-1.14603000	H	0.78550400	5.51713300	0.81054800
C	-2.39349900	-1.38920400	-0.87275500	Li	-0.10534700	2.44122500	1.44887600
H	-4.87495200	-3.06153100	0.70847800	Br	-0.00039900	0.71068700	3.18737400
H	-4.87317900	0.90565900	-0.92306700				
Cu	0.03443300	-0.46375300	1.22820400	L₂- TS23			
H	1.46685800	-2.25981900	-3.28415800	C	0.03396900	-1.07841700	-0.40991000
H	-1.31476300	-2.33909100	-3.27679000	C	-0.58566900	-2.59570700	-1.98733200
C	6.54482000	-0.50039600	0.36980400	C	0.76564400	-2.64854700	-1.88450600
H	7.03412900	0.24901900	-0.25894900	N	1.12939400	-1.71607100	-0.91679700
H	6.55306000	-0.11902800	1.39827200	N	-1.01676500	-1.63449600	-1.07956400
H	7.15372500	-1.40927300	0.35488000	C	2.96301200	-1.99289800	0.69392800
C	-6.47951500	-0.88412100	0.36617800	C	2.49194600	-1.45951700	-0.51734600
H	-7.15904600	-1.38404100	-0.33520200	C	3.31289700	-0.70043500	-1.36844400
H	-6.65878900	-1.31838800	1.35472300	C	4.63195500	-0.46932300	-0.96681000
H	-6.76257600	0.17121700	0.40280400	C	5.13728600	-0.96694500	0.23830800
C	2.29172600	1.10739100	-1.83495400	C	4.29020200	-1.72984900	1.04793900
H	1.74848700	0.73722700	-2.71035900	H	5.27725000	0.12122800	-1.61249700
H	1.55228300	1.58178600	-1.17468600	H	4.66959500	-2.13556000	1.98267700
H	2.97330700	1.89211400	-2.17283500	C	-3.15269000	-2.11837900	0.01730800
C	2.58679300	-3.62520500	0.02865500	C	-4.49507000	-1.79365800	0.22300100
H	2.21229300	-4.09613700	-0.88684800	C	-5.09179200	-0.69212400	-0.40225400
H	3.31301900	-4.30320100	0.48293500	C	-4.30837700	0.09629700	-1.24814300
H	1.73589200	-3.53543600	0.71319300	C	-2.95691900	-0.18275800	-1.49110500
C	-2.33161600	0.96878400	-1.84854300	C	-2.40354000	-1.30103200	-0.84825700
H	-3.06466300	1.69509000	-2.20902000	H	-5.08619500	-2.41246600	0.89384300
H	-1.63603800	1.50945800	-1.19000500	H	-4.75445400	0.95834300	-1.73817200
H	-1.75484200	0.62011100	-2.71115700	Cu	-0.13386000	0.23977900	0.95914000
C	-2.32713400	-3.74898100	0.07865200	H	1.49542300	-3.25343400	-2.39816600
H	-1.93767300	-4.21295000	-0.83424200	H	-1.27417300	-3.13943600	-2.61410100
H	-1.47408100	-3.59690500	0.74929700	C	6.55406200	-0.66670300	0.66628000
H	-3.00561000	-4.46085700	0.55442400				

H	7.21441300	-0.53693200	-0.19622800	N	-1.42489100	3.04591900	-1.27729500
H	6.59722000	0.25961100	1.25221900	N	-2.77511500	1.50456300	-1.93049800
H	6.96210000	-1.46642700	1.29142400	O	4.77177500	-1.08522000	0.18592500
C	-6.55407400	-0.38262700	-0.18416500	O	3.44738100	-2.04199700	-1.43035200
H	-7.18956300	-1.00773000	-0.82395900	B	3.48209000	-1.22072100	-0.31118800
H	-6.85208600	-0.57229900	0.85169500	C	-1.58034200	1.68968400	-1.29137000
H	-6.78084800	0.66137300	-0.41720400	C	-2.49331200	3.68940400	-1.89269000
C	2.80198600	-0.14800500	-2.67769100	C	-3.34464000	2.71795600	-2.30613000
H	2.63147000	-0.94061100	-3.41579900	C	-3.38107600	0.22208800	-2.19415800
H	1.85396700	0.38135300	-2.54600200	C	-4.41952000	-0.22193200	-1.35800400
H	3.52276700	0.55266500	-3.10510900	C	-5.00631000	-1.45792200	-1.64871900
C	2.08275400	-2.82328600	1.59722000	H	-5.81392900	-1.81389800	-1.01350900
H	1.55854200	-3.60901600	1.04313800	C	-4.58643400	-2.24353900	-2.72683300
H	2.67854100	-3.29881100	2.38006500	C	-3.55734100	-1.75828200	-3.53989000
H	1.31923400	-2.20578000	2.08301900	H	-3.22607400	-2.34890300	-4.39062100
C	-2.13710300	0.72292700	-2.37383800	C	-2.93959000	-0.52705100	-3.29747800
H	-2.79005700	1.32355000	-3.01304500	C	-1.83095600	-0.03613900	-4.19687000
H	-1.52918200	1.41125100	-1.76707800	H	-2.00572400	0.99079800	-4.53460600
H	-1.45686100	0.15870000	-3.01978300	C	-4.88677100	0.58861300	-0.17282000
C	-2.52859700	-3.29422000	0.73032800	H	-5.15554700	1.61203400	-0.45390800
H	-2.11152100	-4.02702200	0.03086700	C	-0.29043000	3.73283600	-0.70688900
H	-1.70998600	-2.96895700	1.38172800	C	-0.33249800	4.10532100	0.64631100
H	-3.26902700	-3.80520000	1.35019100	C	-1.51795000	3.77810400	1.52098200
O	-0.36658900	2.80344900	-0.33091400	H	-2.46478100	4.07791100	1.05960200
C	0.54562700	3.61880800	-1.00234100	C	0.77873700	4.76976300	1.17072900
C	0.41436400	3.43080200	-2.53102200	H	0.76979600	5.05247200	2.21997600
H	-0.60278300	3.67872600	-2.85341100	C	1.90567700	5.05573800	0.39368500
H	1.11594700	4.06239700	-3.09003400	C	1.89900900	4.67983200	-0.95256800
H	0.60562500	2.38681800	-2.80203500	H	2.76515200	4.89955200	-1.57201400
C	0.26908600	5.10531800	-0.66830700	C	0.81285600	4.01339900	-1.52777500
H	0.38276300	5.27505100	0.41083800	C	0.84619000	3.59453400	-2.97827900
H	0.94987500	5.79300100	-1.18592300	H	-0.00896800	3.98731600	-3.53934700
H	-0.75813700	5.36441200	-0.94967700	C	1.01097400	-1.07125800	-0.37246300
C	1.98819500	3.27231200	-0.56779100	H	1.24384100	-1.32927200	-1.41160700
H	2.20123500	2.21982000	-0.78129700	C	2.29928100	0.28456800	1.30816500
H	2.74138000	3.88821900	-1.07610400	C	1.15412500	0.44833900	2.11265500
H	2.09817200	3.41890400	0.51286400	H	0.26854200	-0.14148900	1.91365500
Li	-1.03989900	2.85307500	1.23631300	C	1.14782800	1.34023100	3.18610900
Br	-0.71370400	1.25044600	2.98653100	H	0.24659000	1.42229100	3.78801000
				C	2.27870500	2.09450500	3.49636300
L₂-17₂				H	2.27745200	2.77735500	4.34139800
				C	3.41905500	1.94240100	2.70290300
Cu	-0.31902000	0.35396900	-0.69272100	H	4.31621700	2.51650100	2.92413500
N	2.30179500	-0.62527300	0.22446400	C	3.43284400	1.06256600	1.62294600

H	4.32927800	0.96206300	1.02621600
C	5.67685100	-1.69192100	-0.76840000
C	6.83081900	-2.33254900	0.00140000
H	7.40698000	-1.55621500	0.51359100
H	7.50717700	-2.86359600	-0.67717100
H	6.47041600	-3.03409200	0.75585400
C	6.20604200	-0.56567000	-1.66852400
H	5.39337700	-0.09298500	-2.22758400
H	6.95224200	-0.92996900	-2.38149800
H	6.67535400	0.19802500	-1.04177300
C	4.73166000	-2.69879400	-1.52904000
C	5.05805300	-2.90743300	-3.00720200
H	4.33049200	-3.59483800	-3.44868500
H	6.05471800	-3.34449500	-3.13109500
H	5.01555400	-1.96965800	-3.56434300
C	4.60150300	-4.05526700	-0.82116700
H	4.36122100	-3.92586700	0.23764500
H	5.51850300	-4.64713300	-0.90269900
H	3.78421100	-4.61646700	-1.28208000
C	0.45014200	-2.32120200	0.24866000
C	-0.58363700	-3.02288300	-0.41064200
H	-0.96609000	-2.63080600	-1.35137100
C	-1.11589200	-4.19990700	0.10590500
H	-1.90393700	-4.71628000	-0.43781100
C	-0.63873100	-4.72664800	1.31284400
H	-1.05036200	-5.64777400	1.71563000
C	0.38005300	-4.04836800	1.98181300
H	0.77611000	-4.44509800	2.91431400
C	0.91578500	-2.86520000	1.46051100
H	1.71868100	-2.36552800	1.99249400
H	-1.43488600	4.28672900	2.48444700
H	-1.57793800	2.70147400	1.71477400
H	1.75867600	3.95252900	-3.46105700
H	0.81930000	2.50325500	-3.07337600
H	-1.74051300	-0.67435400	-5.07920000
H	-0.86881800	-0.04320600	-3.67225600
H	-5.76502900	0.12685400	0.28537400
H	-4.10898900	0.66137200	0.59550500
C	3.11375500	5.71736900	1.01054800
H	3.75874700	6.16879200	0.25130800
H	2.82540500	6.49727800	1.72254300
H	3.70987900	4.97879500	1.55968100
C	-5.21459800	-3.59077600	-2.99424900
H	-5.20060300	-3.83523400	-4.06052400

H	-4.67164300	-4.38734700	-2.47071800
H	-6.25254800	-3.62424000	-2.65035600
C	-2.83354900	-1.86352100	2.65005400
Br	-2.77475200	0.07648800	3.20146700
C	-3.52817800	-2.67000000	3.68663800
C	-2.93646000	-3.65888400	4.35993300
H	-3.47947700	-4.25087700	5.09062100
H	-1.89424800	-3.91395400	4.18992100
H	-4.57391400	-2.42872900	3.86913500
H	-3.36096600	-1.83307300	1.69731600
H	-1.79594400	-2.15230300	2.49641400
H	-2.54374100	4.76346800	-1.97417400
H	-4.28793400	2.77089500	-2.82591300

L₂-TS18₂

Cu	-1.01574300	0.18844200	0.49698500
N	1.95102300	-0.16339500	0.59238000
N	-1.40132100	1.91381500	-2.08488700
N	-2.17949600	-0.07287200	-2.31599000
O	4.35132600	-0.30313300	-0.14702400
O	2.83409800	-1.77718500	-1.04305800
B	3.02768600	-0.71363800	-0.17013000
C	-1.54150600	0.73230700	-1.41108700
C	-1.93730400	1.84319500	-3.36879000
C	-2.43285300	0.59109900	-3.51485400
C	-2.57581600	-1.43607800	-2.06795300
C	-3.82133000	-1.67674400	-1.45949500
C	-4.19163900	-3.00616700	-1.23434500
H	-5.15312700	-3.20835700	-0.76793600
C	-3.37073900	-4.07728600	-1.60495300
C	-2.15565800	-3.79426000	-2.23532300
H	-1.51605400	-4.61481400	-2.55169500
C	-1.73347700	-2.48171800	-2.48104600
C	-0.41239200	-2.22694100	-3.16881200
H	-0.48153400	-1.41648600	-3.89976300
C	-4.74357600	-0.54459500	-1.07388000
H	-4.94643500	0.11382000	-1.92562400
C	-0.76708300	3.10470000	-1.57045400
C	-1.56462100	4.12474700	-1.02861000
C	-3.06590800	4.00122100	-0.94213700
H	-3.51422900	3.74564800	-1.90826200
C	-0.91724200	5.26947900	-0.55071800

H	-1.51886500	6.06528900	-0.11833900	H	0.69721100	-5.12596200	4.09566600
C	0.47156400	5.41213200	-0.60307200	C	1.54112900	-3.19076400	3.62050100
C	1.22418500	4.38586600	-1.18288700	H	2.18986900	-3.16954500	4.49310900
H	2.30474900	4.48527500	-1.24412400	C	1.55850000	-2.11579300	2.73192400
C	0.62835400	3.22344900	-1.67692900	H	2.22263000	-1.27925800	2.92029200
C	1.46400300	2.13586000	-2.30647700	H	-3.50806600	4.94155200	-0.60334600
H	1.10488800	1.88053300	-3.30993800	H	-3.34609000	3.21697300	-0.23042000
C	0.71340700	-0.98304900	0.60885000	H	2.50577100	2.45456300	-2.39046900
H	0.59313800	-1.40100300	-0.39014100	H	1.43689800	1.22086800	-1.70689600
C	2.05679600	0.99885900	1.39938600	H	-0.07750600	-3.12729800	-3.69077500
C	1.13820700	1.24566200	2.43690700	H	0.37246500	-1.95256100	-2.45490700
H	0.35464700	0.52702100	2.64318400	H	-5.69987800	-0.93531800	-0.71650400
C	1.22288700	2.40222600	3.21387900	H	-4.31190000	0.08165600	-0.28505100
H	0.48793100	2.56016400	3.99821100	C	1.15212800	6.62922500	-0.02425300
C	2.23266800	3.33745300	2.99607200	H	1.97348700	6.97254200	-0.66178700
H	2.30283200	4.23158400	3.60878400	H	0.45160500	7.45904500	0.10566500
C	3.15732000	3.09521700	1.97715800	H	1.57924900	6.39770400	0.95899300
H	3.95686200	3.80752300	1.78766200	C	-3.78579900	-5.50205800	-1.32274500
C	3.07252500	1.95327100	1.18458800	H	-3.50510900	-5.79925800	-0.30472300
H	3.80232800	1.79055700	0.40343900	H	-4.86941100	-5.62811200	-1.40910500
C	5.05700200	-1.01760300	-1.19291600	H	-3.30532400	-6.20331200	-2.01103900
C	6.47293600	-1.31299100	-0.70129000	C	-2.46722600	-1.12379400	2.39373900
H	7.01433700	-0.37384000	-0.55441100	Br	-2.81339800	1.41365900	1.80543500
H	7.02480500	-1.91074800	-1.43457100	C	-2.56896500	-0.95319200	3.81387800
H	6.46355900	-1.84716400	0.25016900	C	-1.58080800	-1.30348600	4.66662700
C	5.10678800	-0.09431200	-2.41861500	H	-1.70661100	-1.19568700	5.73983200
H	4.10137600	0.13009400	-2.78583300	H	-0.63774500	-1.70882200	4.31340200
H	5.68457900	-0.53553800	-3.23654700	H	-3.49714600	-0.54045000	4.20126200
H	5.58282300	0.84823000	-2.13348300	H	-3.37127300	-1.23535500	1.81120700
C	4.14130300	-2.28362600	-1.40668700	H	-1.58022300	-1.60805600	2.00706000
C	4.07941800	-2.80641000	-2.84088400	H	-2.93473800	0.11307100	-4.34107000
H	3.40090600	-3.66320000	-2.88925800	H	-1.91160000	2.68309500	-4.04474800
H	5.06657600	-3.13911300	-3.17887000				
H	3.71216400	-2.04563900	-3.53225800	L₂-19₂			
C	4.46234900	-3.43288200	-0.44027600				
H	4.50465100	-3.08052900	0.59391600	Cu	1.01445900	-0.75136500	0.81249100
H	5.41305400	-3.91672100	-0.68464000	N	-1.20534100	1.09364300	0.59034200
H	3.66671300	-4.17999200	-0.50444500	N	-0.16140100	-2.44725100	-1.74234200
C	0.74242800	-2.10348700	1.57699600	N	1.77873100	-1.56017100	-1.99226600
C	-0.07948200	-3.23809300	1.36436400	O	-3.13499900	2.57759400	0.00480700
H	-0.69036100	-3.28158800	0.46465000	O	-1.26233800	2.64411000	-1.32631600
C	-0.09675900	-4.30773000	2.25749400	B	-1.87577800	2.06646400	-0.22650600
H	-0.73553700	-5.16403600	2.05442400	C	0.70962400	-1.58380000	-1.13201400
C	0.70743300	-4.29191600	3.40013200	C	0.36010100	-2.94741700	-2.93347200

C	1.58334800	-2.39259800	-3.09063400	H	-3.89281500	1.88758600	-2.48288000
C	2.96764200	-0.75362700	-1.84724000	H	-4.73732800	3.40513500	-2.84558400
C	4.10357400	-1.31343500	-1.23364600	H	-5.26076100	2.39815800	-1.48371600
C	5.24286100	-0.50964600	-1.11897500	C	-2.03338000	3.82248000	-1.68354800
H	6.12570300	-0.92590300	-0.63985100	C	-2.00282900	3.97783500	-3.20288500
C	5.28447800	0.79732600	-1.61483600	H	-0.97649900	4.16646200	-3.53105200
C	4.15426000	1.29228200	-2.27268800	H	-2.61887600	4.82555600	-3.52050400
H	4.18371500	2.28964000	-2.70547100	H	-2.35914400	3.07926500	-3.70968200
C	2.98404800	0.53583400	-2.40922800	C	-1.34356200	5.02225500	-1.01954500
C	1.80617000	1.10001100	-3.17111100	H	-1.33210200	4.92559000	0.06914000
H	1.35542400	0.35287700	-3.83078100	H	-1.83087500	5.96588600	-1.28303900
C	4.12192600	-2.74263800	-0.75039400	H	-0.30477000	5.06378600	-1.35778100
H	3.94521300	-3.44042300	-1.57731600	C	0.83871500	2.38486000	1.17688900
C	-1.52235000	-2.75286800	-1.35781800	C	2.03043900	2.94751800	0.67317900
C	-1.81338200	-3.96519000	-0.70963400	H	2.52722000	2.46843000	-0.16683400
C	-0.74757600	-4.98208000	-0.39152600	C	2.57402000	4.10620500	1.22164300
H	-0.24548100	-5.33085300	-1.30203200	H	3.49045200	4.51847700	0.80749700
C	-3.15373100	-4.22872500	-0.40495000	C	1.93943200	4.74515500	2.29116600
H	-3.39333400	-5.15466000	0.11208000	H	2.35956300	5.65148400	2.71766600
C	-4.18521300	-3.35343700	-0.75411500	C	0.75395200	4.20929100	2.79625900
C	-3.85802500	-2.19807700	-1.46970500	H	0.24449900	4.69865300	3.62214200
H	-4.65071600	-1.52896900	-1.79668500	C	0.21046900	3.04413000	2.25040600
C	-2.53530100	-1.88134700	-1.79122800	H	-0.71801100	2.65273300	2.65053500
C	-2.22133200	-0.66745300	-2.63111500	H	-1.18762600	-5.85318000	0.10031200
H	-1.64124800	-0.93709500	-3.52104000	H	0.01760800	-4.56070800	0.26660700
C	0.26394800	1.17667500	0.51753400	H	-3.14555400	-0.19398900	-2.97108400
H	0.54424600	1.18917100	-0.53222800	H	-1.63767700	0.07647600	-2.08294800
C	-1.88453800	0.37767500	1.61725400	H	2.12722600	1.94407500	-3.78735000
C	-1.24924600	0.02313500	2.81648600	H	1.01147000	1.46433700	-2.51092500
H	-0.22222800	0.30958900	2.99711900	H	5.09328200	-2.98420500	-0.31185900
C	-1.93526700	-0.69122000	3.80096300	H	3.34766200	-2.93384400	0.00053000
H	-1.41165600	-0.95714700	4.71477300	C	-5.61448300	-3.64636300	-0.36562400
C	-3.26814800	-1.05342900	3.62239900	H	-6.32298400	-3.19581200	-1.06738800
H	-3.79986100	-1.60529100	4.39182600	H	-5.80872700	-4.72250700	-0.32752200
C	-3.90677100	-0.69881400	2.43147800	H	-5.83604200	-3.24067800	0.62937200
H	-4.94519000	-0.97500400	2.26684400	C	6.51978600	1.64949600	-1.44558800
C	-3.22629100	-0.00413200	1.43590300	H	6.58141900	2.42425700	-2.21540800
H	-3.73457300	0.24640400	0.51417900	H	6.51687400	2.15427500	-0.47164800
C	-3.45661900	3.49628200	-1.07142200	H	7.43186400	1.04695300	-1.49440700
C	-4.18966100	4.69393100	-0.46713800	C	2.43294500	-0.04752500	2.11216700
H	-5.13870900	4.36145800	-0.03701400	Br	1.34236300	-2.98139500	1.81387100
H	-4.40928500	5.44596200	-1.23239200	C	2.14555500	-0.13321600	3.53890000
H	-3.60709400	5.16242000	0.32745900	C	2.08598200	0.92474100	4.37131100
C	-4.38807300	2.75394200	-2.03848900	H	1.89070000	0.79327100	5.43194500

H	2.24461600	1.94047700	4.02260400	H	-0.96117200	0.35775900	0.01116100
H	1.98343000	-1.13454000	3.93152700	C	-0.17151200	-2.64784400	1.11231200
H	3.12736400	-0.81428700	1.76686100	C	1.21708700	-2.47529600	1.09218100
H	2.69448000	0.94604400	1.76309500	H	1.64052400	-1.59292400	0.62426100
H	-0.19383200	-3.63871600	-3.54816400	C	2.06054000	-3.42231500	1.67447400
H	2.32563000	-2.50229500	-3.86503200	H	3.13375000	-3.25771100	1.65575700
L₂-TS20₂							
Cu	0.87309500	0.79471700	0.88648900	C	1.53108900	-4.57504800	2.25715200
N	-1.05170100	-1.67616500	0.52879300	H	2.18733300	-5.31382400	2.70795400
N	2.58375300	0.86695900	-1.70356200	C	0.14848500	-4.77138400	2.24768400
N	1.02662900	2.34580900	-1.75726000	H	-0.27837700	-5.66638800	2.69193900
O	-2.16353100	-3.42438900	-0.84348900	C	-0.69669800	-3.81509100	1.68580900
O	-2.80687300	-1.23722300	-1.15942800	H	-1.77002000	-3.96777600	1.69009500
B	-1.98346000	-2.10753500	-0.46612100	C	-3.02625100	-3.42405300	-2.01121200
C	1.47119000	1.27879100	-1.01959600	C	-3.91107800	-4.66788500	-1.95722900
C	2.82355900	1.65687400	-2.82532000	H	-3.28963800	-5.56405200	-2.04129100
C	1.84353100	2.58907600	-2.85798200	H	-4.62698900	-4.67359900	-2.78587200
C	-0.17230300	3.11414400	-1.51171100	H	-4.46351300	-4.72865200	-1.01804400
C	-0.07990100	4.33990000	-0.82693400	C	-2.11451700	-3.47829900	-3.24495300
C	-1.26597500	5.05260300	-0.61402100	H	-1.47896200	-2.59037000	-3.30781300
H	-1.21242900	5.99643400	-0.07712400	H	-2.68985000	-3.55999400	-4.17211200
C	-2.50346700	4.59895200	-1.08029400	H	-1.46486300	-4.35412200	-3.16473100
C	-2.53857500	3.41033500	-1.81503100	C	-3.78836200	-2.05165100	-1.86003200
H	-3.48449200	3.06149800	-2.22284000	C	-4.15391200	-1.36509400	-3.17358400
C	-1.38621000	2.65468300	-2.05315000	H	-4.64060500	-0.40796100	-2.96519500
C	-1.46960600	1.39943200	-2.88862800	H	-4.85327700	-1.98053700	-3.74915000
H	-0.56208200	1.23803500	-3.47608200	H	-3.27387300	-1.17206300	-3.78877500
C	1.24018900	4.90029300	-0.36290600	C	-5.02321700	-2.14100700	-0.95286500
H	1.94603300	4.99912900	-1.19560000	H	-4.78962300	-2.64612400	-0.01186800
C	3.41866000	-0.26683200	-1.38388100	H	-5.84412700	-2.67580300	-1.44004400
C	4.64340500	-0.05546700	-0.72935400	H	-5.36023900	-1.12920600	-0.71309600
C	5.09869900	1.31992400	-0.31213800	C	-2.26918700	0.22700300	1.63174000
H	5.15904800	2.00060300	-1.16888300	C	-2.51062200	1.61545800	1.68940300
C	5.44592700	-1.17713800	-0.48086800	H	-1.80212800	2.29996200	1.22930800
H	6.39345900	-1.03198300	0.03192800	C	-3.63787700	2.12076200	2.32648800
C	5.07207600	-2.46339800	-0.87646900	H	-3.79707000	3.19508500	2.36276100
C	3.85603900	-2.62402300	-1.55160800	C	-4.56891300	1.25286100	2.91191300
H	3.55227700	-3.61595300	-1.87744700	H	-5.45518400	1.64831200	3.39996200
C	3.01543100	-1.54188200	-1.82160200	C	-4.34634600	-0.12085700	2.86079900
C	1.71472900	-1.74729400	-2.56010500	H	-5.05773500	-0.80555300	3.31487300
H	1.63759300	-1.08783000	-3.43148800	C	-3.19979900	-0.62989000	2.24232100
C	-1.06885200	-0.26100500	0.90689500	H	-3.03549500	-1.70065700	2.20740600
				H	6.08942200	1.27040400	0.14645600
				H	4.40433300	1.76474500	0.41032300
				H	1.62891000	-2.78021700	-2.90554000

H	0.85444700	-1.53434600	-1.91722200	C	3.10597700	-1.23621300	-0.39688200
H	-2.31358900	1.46788000	-3.58108400	C	2.45858000	0.00028900	-0.58959900
H	-1.63676000	0.51118600	-2.27130200	H	4.97645900	2.14139900	0.15871400
H	1.09846800	5.89131400	0.07560800	H	4.97658200	-2.14113100	0.15739100
H	1.70862300	4.25398000	0.38789600	Cu	0.00000100	-0.00087700	1.71508300
C	5.95327600	-3.65701000	-0.59069700	H	-1.39033100	0.00133800	-3.15837900
H	6.17895000	-4.21432300	-1.50673400	H	1.39032700	0.00123400	-3.15838100
H	6.90134200	-3.35535000	-0.13760800	C	-2.40423300	-2.57730200	-0.58643300
H	5.46218500	-4.35631300	0.09626100	H	-1.36947500	-2.38099600	-0.88111900
C	-3.77165900	5.37027800	-0.80107200	C	-2.40425600	2.57780300	-0.58507000
H	-3.55891100	6.40744900	-0.52736400	H	-1.36942800	2.38166500	-0.87962400
H	-4.43719100	5.37659000	-1.67036400	C	2.40432100	-2.57726800	-0.58654300
H	-4.32927500	4.91757700	0.02813700	H	1.36958500	-2.38098900	-0.88132200
C	0.30856700	0.03195700	2.88285700	C	2.40416700	2.57783600	-0.58496700
Br	2.40163700	2.39479000	2.08333600	H	1.36932000	2.38167200	-0.87943300
C	-0.30500800	-0.99772800	3.70432700	Cl	0.00000200	-0.00190400	3.84042600
C	-1.30286500	-0.75580500	4.57478500	H	6.15822600	0.00006700	0.49792200
H	-1.68166700	-1.53549000	5.22927600	H	-6.15822500	-0.00005400	0.49792800
H	-1.74378700	0.23052200	4.67987200	C	3.05419200	-3.40011400	-1.71612400
H	0.11749300	-1.99645900	3.65557200	H	3.05132800	-2.85288200	-2.66468400
H	1.38850700	-0.09751800	2.80467600	H	4.09371900	-3.65246500	-1.48145300
H	0.02199200	1.04747400	3.14080500	H	2.51069500	-4.33931600	-1.86442800
H	3.65900300	1.47525300	-3.48224700	C	2.35678000	-3.37642400	0.73062100
H	1.64333700	3.39163900	-3.54957000	H	3.36217300	-3.63893500	1.07684100
L₃CuCl				H	1.86731700	-2.80435000	1.52431200
C	0.00000000	-0.00001300	-0.17579200	H	1.80118900	-4.30952400	0.58722300
C	0.67844500	0.00096100	-2.34872400	C	-2.35680000	-3.37651900	0.73069800
C	-0.67844700	0.00092300	-2.34872300	H	-1.86750800	-2.80445600	1.52450000
N	-1.07680500	0.00038100	-1.01686900	H	-3.36222400	-3.63916100	1.07673900
N	1.07680400	0.00039200	-1.01687100	H	-1.80109900	-4.30955700	0.58733400
C	-3.10594400	1.23666000	-0.39615200	C	-3.05398800	-3.40011700	-1.71610500
C	-2.45858000	0.00025200	-0.58959600	H	-4.09355000	-3.65244600	-1.48156600
C	-3.10592900	-1.23626500	-0.39679300	H	-3.05098400	-2.85287500	-2.66465800
C	-4.44949900	-1.20587500	-0.00411700	H	-2.51049100	-4.33933100	-1.86434800
C	-5.11660800	0.00003700	0.18990300	C	-3.05383500	3.40106400	-1.71451900
C	-4.44951800	1.20605500	-0.00349500	H	-3.05065800	2.85420900	-2.66329600
H	-4.97650700	-2.14121800	0.15750800	H	-4.09344900	3.65324400	-1.48005000
H	-4.97653300	2.14131200	0.15860800	H	-2.51035400	4.34035900	-1.86229200
C	3.10589600	1.23671300	-0.39607100	C	-2.35708600	3.37646600	0.73240500
C	4.44947100	1.20613400	-0.00343500	H	-3.36256700	3.63888600	1.07843800
C	5.11660900	0.00012700	0.18989700	H	-1.86786200	2.80408800	1.52602200
C	4.44954600	-1.20579500	-0.00418800	H	-1.80143000	4.30960400	0.58951000
				C	2.35709900	3.37655500	0.73247800
				H	1.86804000	2.80418400	1.52620200

H	3.36260800	3.63910300	1.07834100	C	5.60136200	-2.88804800	0.17988700
H	1.80133400	4.30963200	0.58962000	H	5.03845200	-3.75704800	-0.17890900
C	3.05363400	3.40107300	-1.71450000	H	6.61736000	-3.21558100	0.43537900
H	4.09328100	3.65323300	-1.48015600	H	5.11712800	-2.52955000	1.09478400
H	3.05032500	2.85421100	-2.66327100	C	6.29077100	-2.31382800	-2.17051100
H	2.51015100	4.34037900	-1.86221100	H	6.29046400	-1.53988200	-2.94679200
L₃-I							
C	-1.02324100	0.35821500	0.29248300	H	7.33014400	-2.61579100	-1.98643000
C	-2.47746300	0.62649200	2.01471800	H	5.74403400	-3.18180800	-2.55674200
C	-1.49166500	1.54801500	2.16676200	C	6.36857800	-0.54898100	-0.37872400
N	-0.61087400	1.36973600	1.10848300	H	5.89054900	-0.15667400	0.52565800
N	-2.17593800	-0.09273200	0.86492600	H	7.41449500	-0.78207300	-0.14066300
C	0.51371700	3.31872300	0.12373200	H	6.35437000	0.24297000	-1.13590100
C	0.59371000	2.14895900	0.90435300	Li	2.90105300	-1.19406500	-2.06847700
C	1.79283100	1.70166700	1.49872300	H	3.79563800	4.21915900	0.36231100
C	2.93857100	2.47673700	1.28449200	H	-5.14194400	-4.09375200	-0.95185500
C	2.89100800	3.63889100	0.51880700	C	-2.03545900	-3.45413200	3.03998000
C	1.69249800	4.05414100	-0.05274900	H	-2.52045200	-4.41852600	2.85573700
H	3.88279000	2.15819400	1.71158800	H	-1.20107700	-3.62934500	3.72697900
H	1.67014400	4.95873300	-0.65262600	H	-2.76093300	-2.80778900	3.54488900
C	-4.03587900	-0.89402600	-0.52478400	C	-0.46695300	-3.70921500	1.05412300
C	-4.80695300	-1.96954600	-0.98217700	H	-0.88216200	-4.68393600	0.77700800
C	-4.53266000	-3.27418100	-0.58198300	H	-0.07523900	-3.24199400	0.14553100
C	-3.47723400	-3.53147500	0.28804900	H	0.37281000	-3.88563800	1.73407000
C	-2.67427100	-2.49571800	0.78152600	C	-5.75016300	0.97145300	-0.49653400
C	-2.97708500	-1.18583100	0.35827800	H	-6.54514200	0.34364900	-0.91264200
H	-5.63020500	-1.78088300	-1.66436600	H	-5.82380000	0.92053300	0.59475800
H	-3.26904800	-4.55354900	0.58905000	H	-5.94787900	2.00425700	-0.80211000
Cu	-0.17176900	-0.25480500	-1.28195500	C	-4.24369100	0.65467700	-2.52083800
H	-1.33691600	2.30644000	2.91677200	H	-3.24799200	0.36454700	-2.86999400
H	-3.35259700	0.41499600	2.60761300	H	-4.97579100	0.02447700	-3.03655700
C	1.85824800	0.45333200	2.37490400	H	-4.42467500	1.69066300	-2.82679900
H	1.00359800	-0.18068900	2.11692600	C	-0.66529100	3.83543600	-2.06092000
C	-0.78148700	3.79871700	-0.52446200	H	0.09159300	4.55577700	-2.38858200
H	-1.57233200	3.08417300	-0.27753200	H	-0.38919700	2.85593200	-2.46324200
C	-1.52522300	-2.81726000	1.73231500	H	-1.62061800	4.13229100	-2.50730800
H	-1.03165100	-1.87915100	2.00146200	C	-1.21620700	5.16915500	0.03160400
C	-4.36067700	0.52229300	-0.99001300	H	-1.33589900	5.14116400	1.11956100
H	-3.62448200	1.20191000	-0.55133700	H	-0.48207900	5.94740500	-0.20167900
Cl	0.83445100	-0.93225100	-3.06971200	H	-2.17224400	5.47287800	-0.40797800
O	4.28471800	-1.42161000	-1.19350100	C	3.12928800	-0.38441200	2.14744200
C	5.58664000	-1.77921600	-0.90018600	H	3.04739000	-1.32587800	2.70146000
				H	3.30237700	-0.62402400	1.09275000
				H	4.02163100	0.12703500	2.52512900
				C	1.72152800	0.83366100	3.86541800

H 2.54951200 1.47950500 4.17741800
H 0.78742100 1.36684200 4.07044900
H 1.74198200 -0.06449700 4.49183500

L₃-TS2

C -0.17100800 -0.55721700 -0.41107300
C -1.00341900 -1.35815200 -2.37322600
C 0.29563200 -1.73991700 -2.29824700
N 0.79408500 -1.23904000 -1.09945700
N -1.27289400 -0.63913200 -1.21594100
C 2.38757200 -2.46400800 0.31853500
C 2.15105900 -1.46505400 -0.64862100
C 3.19122800 -0.70699200 -1.22897000
C 4.49671700 -0.96713600 -0.79535600
C 4.75742900 -1.93249900 0.17262400
C 3.71381500 -2.67155500 0.71922800
H 5.31996100 -0.40130300 -1.21872400
H 3.92907900 -3.42994000 1.46547900
C -3.48275100 -0.94265900 -0.19061000
C -4.74544800 -0.41631400 0.10555800
C -5.09160900 0.87906300 -0.26829600
C -4.17911100 1.67611200 -0.95231200
C -2.90116500 1.20343300 -1.27792600
C -2.57823900 -0.10964000 -0.88221400
H -5.46498200 -1.03003000 0.63855100
H -4.45971600 2.68414600 -1.24057200
Cu -0.21462400 0.15869700 1.35449200
H 0.90586600 -2.31681400 -2.97327700
H -1.75290900 -1.52695800 -3.12933600
C 2.94817600 0.33122600 -2.32224500
H 1.88248500 0.58029200 -2.32068200
C 1.28641500 -3.35147300 0.89234700
H 0.32372600 -2.97253400 0.54054200
C -1.94292400 2.09665000 -2.05899700
H -0.97666300 1.58756300 -2.12072200
C -3.14784400 -2.37386300 0.21937900
H -2.09530200 -2.55692800 -0.01415300
Cl -0.82069700 0.29794900 3.48841500
O 0.37755100 3.11224900 1.67749400
C 1.55880700 3.80897000 1.44762600
C 1.61584400 4.30271100 -0.01585300
H 0.78570600 4.98964400 -0.21081600
H 2.55393800 4.82353800 -0.24595700

H 1.51319100 3.45320200 -0.69919100
C 1.63896700 5.03971800 2.38340100
H 1.62456600 4.71409100 3.43140700
H 2.54899100 5.63318900 2.22739500
H 0.77226100 5.68879500 2.21604200
C 2.77449400 2.89354700 1.72657600
H 2.71073100 1.99287100 1.10569600
H 3.73488600 3.38763200 1.52896300
H 2.76802600 2.57081000 2.77455300
Li -0.48441200 2.46092200 2.97592800
H 5.77809600 -2.11168000 0.49832200
H -6.07651900 1.26815700 -0.02599700
C -1.69909600 3.44347200 -1.35308000
H -1.24609100 3.30811700 -0.36580700
H -1.01307700 4.05340900 -1.95029600
H -2.62827900 4.01364000 -1.24117600
C -2.44794900 2.30354400 -3.50199900
H -2.58596900 1.35035100 -4.02402900
H -3.40825600 2.83055500 -3.51529200
H -1.73138000 2.90296300 -4.07343200
C 3.29688300 -0.24498300 -3.71147600
H 3.09066500 0.49236300 -4.49469400
H 4.35912000 -0.50701500 -3.76737000
H 2.72255200 -1.14791300 -3.94052000
C 3.72059300 1.64174200 -2.08646400
H 4.80174300 1.50237700 -2.19211000
H 3.41751900 2.38936000 -2.82662500
H 3.52522100 2.05117300 -1.09341600
C 1.24782800 -3.31686400 2.43143700
H 0.41687900 -3.92821800 2.79895100
H 2.16853400 -3.71598500 2.87018100
H 1.10634600 -2.29864800 2.80468300
C 1.42934500 -4.79713500 0.37290200
H 0.60938700 -5.41963300 0.74695300
H 1.41232500 -4.83458000 -0.72137900
H 2.36997700 -5.24841000 0.70654800
C -3.32021900 -2.59565000 1.73435200
H -4.36610900 -2.48819100 2.04144200
H -3.00343000 -3.60936500 2.00320600
H -2.72384400 -1.88389000 2.31213400
C -3.98004000 -3.38981000 -0.58899800
H -5.05127600 -3.26985900 -0.39453500
H -3.82329600 -3.27284400 -1.66650800
H -3.70411500 -4.41399300 -0.31571500

L₃-3

O	0.03524600	2.79421500	1.28254700
C	-1.00090000	3.64927600	1.68231400
C	-1.95327600	3.94984900	0.50469900
H	-1.38355100	4.36236300	-0.33494200
H	-2.43728300	3.02529100	0.16782000
H	-2.73825000	4.66716900	0.77638500
C	-0.35009000	4.96443100	2.15976100
H	-1.09438400	5.69727800	2.49436600
H	0.33417700	4.75913700	2.98926800
H	0.23224300	5.40679200	1.34500000
C	-1.80405100	3.02571300	2.84440500
H	-2.27087500	2.08956000	2.51580100
H	-1.13231500	2.79736900	3.67861400
H	-2.59523800	3.69300700	3.20986200
C	0.16947900	-0.53845700	-0.24848600
C	-0.25195600	-2.55981800	-1.21606400
C	1.09527300	-2.41661600	-1.15168700
N	1.33689800	-1.18151700	-0.56012400
N	-0.80248300	-1.40863800	-0.66181400
C	3.28107500	-0.94566400	0.92159700
C	2.65931600	-0.65423900	-0.30904600
C	3.27965000	0.12011100	-1.30962700
C	4.56976500	0.59748200	-1.04858500
C	5.21135400	0.31940900	0.15465800
C	4.57073600	-0.44137200	1.12810900
H	5.07434200	1.20170700	-1.79638800
H	5.07580800	-0.64253100	2.06788700
C	-2.88230000	-1.61043700	0.62597000
C	-4.26170800	-1.38463600	0.71060200
C	-4.95341800	-0.75587600	-0.32051300
C	-4.27652400	-0.33915600	-1.46309400
C	-2.89717200	-0.53730100	-1.60172400
C	-2.22295700	-1.17416700	-0.54064700
H	-4.79911100	-1.70413600	1.59835200
H	-4.82591100	0.15116100	-2.26093900
Cu	-0.00945700	1.15286900	0.54281200
H	1.89616500	-3.06634600	-1.46588600
H	-0.86540600	-3.35996700	-1.59759500
C	2.59826100	0.46715300	-2.62943400
H	1.61835800	-0.01809800	-2.64337500
C	2.59870500	-1.75235200	2.02187400

H	1.62725200	-2.08540200	1.64570500
C	-2.19035800	-0.07724200	-2.87330500
H	-1.11906600	-0.25864500	-2.75058000
C	-2.15855700	-2.30835000	1.77322500
H	-1.09725200	-2.37054500	1.51758400
C	2.32970600	-0.87742300	3.26255700
H	1.79497800	-1.45458700	4.02505500
H	3.26438600	-0.52103700	3.70885100
H	1.72497900	-0.00259800	3.00541700
C	3.40275200	-3.01374800	2.39032600
H	3.57113300	-3.65223400	1.51679200
H	4.38159000	-2.76014300	2.81100000
H	2.86397500	-3.60112800	3.14147700
C	-2.66860100	-3.75055500	1.96344000
H	-3.72624300	-3.76851900	2.24728600
H	-2.56101700	-4.33783500	1.04552000
H	-2.10405300	-4.25308800	2.75611100
C	-2.26219900	-1.50252100	3.08230700
H	-1.86175900	-0.49240700	2.95727600
H	-3.30060700	-1.41512900	3.41970100
H	-1.69623500	-1.99888400	3.87813200
C	-2.36767700	1.43424000	-3.11183400
H	-1.80161500	1.74526300	-3.99657300
H	-3.41729900	1.69583800	-3.28356400
H	-2.01064200	2.01442100	-2.25637900
C	-2.65759900	-0.89243300	-4.09569400
H	-2.49069900	-1.96499200	-3.95092000
H	-3.72569100	-0.74571500	-4.28898100
H	-2.11132900	-0.58231500	-4.99298000
C	3.39047100	-0.06768100	-3.83795300
H	4.38109700	0.39412500	-3.90693400
H	3.53275700	-1.15177800	-3.77688700
H	2.85802900	0.15274500	-4.76934700
C	2.35552800	1.98514800	-2.74514600
H	1.76069800	2.35500500	-1.90463700
H	3.29995800	2.53967600	-2.75924600
H	1.82085000	2.21436200	-3.67354100
H	-6.02326600	-0.58918200	-0.23309500
H	6.21131800	0.70252300	0.33715100

L₃-4

C	2.01375500	0.13318600	0.49957000
C	3.83606800	0.97137400	1.59304900

C	3.73805300	-0.33997800	1.91760200	B	-2.29837300	-0.55364100	-1.13193800
N	2.62994600	-0.83896000	1.24270000	O	-1.60240000	-1.63519500	-0.38997300
N	2.78357400	1.24526200	0.72930900	O	-2.88883600	-1.20147300	-2.30269300
C	2.95148100	-3.16223000	0.52868300	C	-2.90807700	-2.60948700	-2.10324000
C	2.26226700	-2.23522500	1.33837400	C	-1.66523400	-2.85008400	-1.16111800
C	1.30840000	-2.62356500	2.29894800	C	-0.35082200	-3.00873200	-1.94574800
C	1.06118100	-3.99508900	2.43974500	H	0.48182900	-2.98395400	-1.23638200
C	1.72944800	-4.93411100	1.65981500	H	-0.30472900	-3.96083300	-2.48669900
C	2.66015600	-4.51941800	0.71144200	H	-0.22193300	-2.19325800	-2.66115900
H	0.33244100	-4.32876000	3.17141700	C	-1.82405000	-4.03606900	-0.20503400
H	3.17247600	-5.26013500	0.10517400	H	-1.97857200	-4.96921700	-0.75971200
C	3.26259400	2.87190600	-1.04356800	H	-0.92166200	-4.15233600	0.40158100
C	3.09578900	4.16400500	-1.55611600	H	-2.67085500	-3.88950500	0.46818800
C	2.28920000	5.09643900	-0.90969900	C	-2.81286600	-3.30162000	-3.46878500
C	1.63610200	4.75664100	0.27113200	H	-1.93960600	-2.96669400	-4.03253900
C	1.76918600	3.48060000	0.83319900	H	-2.76285500	-4.39153500	-3.36193200
C	2.58190100	2.55445300	0.15010900	H	-3.70363200	-3.06271400	-4.05849200
H	3.60464900	4.44283200	-2.47362800	C	-4.24580600	-3.00186900	-1.44388300
H	1.01633900	5.49475100	0.77045700	H	-4.35510300	-4.08757800	-1.34323900
Cu	0.41617000	0.09456600	-0.53019000	H	-4.35902800	-2.53702300	-0.46298000
H	4.34267900	-0.96411000	2.55518400	H	-5.05972200	-2.63204100	-2.07459100
H	4.54380700	1.72873300	1.88835500	B	-3.40586900	0.30264000	-0.09965400
C	0.57582900	-1.62727500	3.19124900	C	-5.42789100	0.89851600	0.86143000
H	0.81184000	-0.61985400	2.83770700	O	-4.70309800	-0.12825000	0.14836600
C	4.00701200	-2.74725500	-0.49408500	C	-4.26493100	1.74285200	1.50623900
H	4.01750700	-1.65493600	-0.54810800	O	-3.15545400	1.48016500	0.60880500
C	1.09038600	3.16216000	2.16172300	C	-6.37625800	0.22475000	1.85446000
H	1.21833300	2.09476100	2.36147200	H	-6.91987300	0.96633200	2.45058500
C	4.18376500	1.88498600	-1.75652700	H	-7.11129300	-0.37173700	1.30606000
H	4.05792500	0.90523700	-1.28716600	H	-5.84305800	-0.44494700	2.53190100
O	-1.14071500	0.40955400	-1.60635100	C	-6.24318600	1.67597600	-0.18370300
C	-1.26229600	1.32057100	-2.72869400	H	-6.88893100	0.97349100	-0.71783900
C	-0.35069400	2.52067200	-2.45672400	H	-6.87325300	2.44455000	0.27567700
H	-0.65876000	3.03865300	-1.54399900	H	-5.59067000	2.15300200	-0.91998200
H	0.68964100	2.20363000	-2.33559000	C	-4.50801000	3.25165400	1.55655500
H	-0.39014000	3.23186800	-3.28940300	H	-5.38036800	3.48941600	2.17550200
C	-2.71188400	1.81187200	-2.88026500	H	-3.63871800	3.75183600	1.99422200
H	-2.77356700	2.50928000	-3.72326300	H	-4.66666300	3.66607200	0.55923100
H	-3.38866000	0.97689100	-3.07049100	C	-3.85149800	1.23508500	2.89551800
H	-3.03276400	2.33698400	-1.97663900	H	-2.92853300	1.73800100	3.19731500
C	-0.81856000	0.58385800	-4.00267700	H	-4.61773400	1.44131400	3.64987400
H	-0.87150400	1.24329000	-4.87720200	H	-3.65945800	0.15914900	2.87701100
H	0.21573200	0.23511900	-3.89938300	H	2.17247200	6.09291200	-1.32613700
H	-1.46510100	-0.27984300	-4.16616800	H	1.52080800	-5.99236500	1.78802900

C	1.06432000	-1.73314000	4.65028500	C	3.77042200	-4.24611600	-0.98565700
H	0.85006800	-2.72258800	5.06885300	C	4.04880100	-3.07703900	-1.68846300
H	2.14386600	-1.56489600	4.72991700	H	2.93452800	-5.09955800	0.79711400
H	0.55843900	-0.99012500	5.27615700	H	4.54155000	-3.13823200	-2.65403800
C	-0.95312700	-1.78887700	3.09619500	C	1.77692900	3.73252100	0.39623400
H	-1.44418600	-1.00094400	3.67744200	C	1.12283200	4.96820300	0.48473000
H	-1.29300700	-1.72318000	2.05838800	C	0.06125600	5.15654600	1.36361000
H	-1.28223600	-2.74984400	3.50756900	C	-0.37187100	4.10901100	2.17270700
C	-0.42399500	3.43736800	2.13174200	C	0.24196500	2.85131400	2.12900400
H	-0.86116400	3.19021500	3.10540200	C	1.31297200	2.68946500	1.22646200
H	-0.63931000	4.49401900	1.93862600	H	1.45513800	5.79222800	-0.13938300
H	-0.93610100	2.83800100	1.37398900	H	-1.20216300	4.27031500	2.85052300
C	1.77092800	3.93194300	3.31287300	Cu	-0.02622600	-0.18385600	-0.19936700
H	2.84126300	3.70745200	3.37128700	H	4.71115500	-0.37047500	1.73216800
H	1.66574200	5.01455300	3.18258200	H	3.71073300	2.13700400	2.39682000
H	1.31592800	3.66479100	4.27256000	C	2.13632700	-2.91823300	2.20416900
C	5.41368400	-3.20063900	-0.05412800	H	1.89607200	-1.87768800	2.43961300
H	5.67722800	-2.79929800	0.92990300	C	4.08822600	-0.55909700	-1.94022100
H	5.47777700	-4.29238100	0.00520900	H	3.64963200	0.29849100	-1.42333000
H	6.16801100	-2.86039100	-0.77173300	C	-0.20305400	1.73565300	3.07014400
C	3.68195000	-3.26352800	-1.90865800	H	0.00996300	0.78114000	2.58012400
H	3.68732600	-4.35768800	-1.95261600	C	2.97095600	3.58499600	-0.54654400
H	2.69896400	-2.92028400	-2.24179600	H	3.30021500	2.54312300	-0.52283100
H	4.43129100	-2.90277900	-2.62161700	O	-1.01963600	-2.10951400	-0.84849000
C	3.82892400	1.71842200	-3.24582200	C	-1.08522200	-2.86016700	-2.08073500
H	2.78957600	1.40415800	-3.37602400	C	0.36827900	-3.17139900	-2.45137200
H	3.97129600	2.64861900	-3.80577400	H	0.92000400	-2.24511700	-2.63426300
H	4.47331100	0.95957800	-3.70222200	H	0.86521500	-3.70835400	-1.63928100
C	5.66136100	2.29352700	-1.58693800	H	0.41836500	-3.78518700	-3.35765400
H	5.85669900	3.26974300	-2.04378200	C	-1.75504800	-2.07348100	-3.21812200
H	5.94222900	2.35959900	-0.53077200	H	-1.72500000	-2.66340400	-4.14207600
H	6.31960700	1.56125700	-2.06676200	H	-2.79717600	-1.85633500	-2.97732900

L₃-TS5

C	1.71818800	0.29852000	0.51676200	H	-1.37285200	-4.74486800	-1.03015500
C	3.29328600	1.33576600	1.80933800	H	-2.88092800	-3.97019700	-1.57173900
C	3.78217700	0.11632900	1.48384800	B	-2.07814700	-1.28521900	-0.21650400
N	2.81942000	-0.50006000	0.69376100	O	-2.06847100	-1.39960700	1.23157400
N	2.04512100	1.44023600	1.20670000	O	-3.43326900	-1.55886800	-0.64912700
C	3.71279800	-1.82166700	-1.16833100	C	-4.27306000	-1.81495800	0.49401300
C	3.07567000	-1.78974500	0.08985100	C	-3.23790500	-2.11359000	1.65417300
C	2.78705100	-2.95380700	0.82612300	C	-2.90124300	-3.60950900	1.79829800
C	3.14575000	-4.18240200	0.25609200	H	-2.09225800	-3.71828600	2.52540600

H	-3.75897300	-4.18709900	2.15995200	H	1.80745100	3.25843000	-2.36966200
H	-2.56324300	-4.03984400	0.85508700	C	3.52034200	-0.55299300	-3.37161200
C	-3.65751600	-1.58369200	3.03007600	H	3.78059000	0.38455600	-3.87463600
H	-4.57575400	-2.06837100	3.38108200	H	3.92426200	-1.37286300	-3.97475700
H	-2.86724100	-1.79970300	3.75668100	H	2.43079100	-0.64436300	-3.36686000
H	-3.81547900	-0.50490700	3.01436700	C	5.61755200	-0.35936900	-1.95382400
C	-5.20086400	-2.98601100	0.14648800	H	6.02536700	-0.31031300	-0.93894600
H	-4.64614500	-3.88374400	-0.13021500	H	6.12035800	-1.18159900	-2.47423400
H	-5.85670600	-3.23161800	0.98961600	H	5.87868100	0.57148700	-2.46898300
H	-5.83427700	-2.70700300	-0.70140900	C	0.81122500	-3.69975000	2.22064400
C	-5.13970100	-0.57691900	0.76981100	H	0.34713400	-3.62458300	3.20994400
H	-5.82194300	-0.74487200	1.60968800	H	0.11123300	-3.29823500	1.48455200
H	-4.52299700	0.29824600	0.97677800	H	0.96856300	-4.76366900	2.00993500
H	-5.74473800	-0.36405500	-0.11592700	C	3.10541400	-3.42599400	3.29047400
B	-1.97541100	0.60007400	-0.81615300	H	3.37387900	-4.47556700	3.12819700
C	-2.32571500	2.25009100	-2.42368100	H	4.03396400	-2.84503400	3.30896800
O	-1.79871300	0.92520500	-2.15815500	H	2.63998500	-3.35131600	4.27899700
C	-3.26056400	2.50274800	-1.17785100	C	-1.71273700	1.75308300	3.35428000
O	-2.71857300	1.58843100	-0.18126900	H	-2.00911800	2.62153500	3.95416800
C	-3.03547500	2.21811300	-3.77872000	H	-2.28465400	1.74994800	2.42316400
H	-3.49203900	3.18719300	-4.00824500	H	-1.98431800	0.85943800	3.92224300
H	-2.30739400	1.99412800	-4.56411300	C	0.60241700	1.78710000	4.38615500
H	-3.80909300	1.44963100	-3.81097300	H	0.30230300	0.96663300	5.04675000
C	-1.12663800	3.20273700	-2.49652800	H	1.67972900	1.70021200	4.21195200
H	-0.44493200	2.84922900	-3.27584900	H	0.42349300	2.72956400	4.91650500
H	-1.43321500	4.22326900	-2.74797200				
H	-0.58137200	3.22614600	-1.55084200	L₃-6			
C	-3.21121900	3.91932900	-0.60498800	C	-1.28821800	0.05300000	-0.03446100
H	-3.56869100	4.65067800	-1.33846200	C	-3.42830400	0.83449000	-0.17209400
H	-3.86286100	3.97817900	0.27216400	C	-3.49486200	-0.52047600	-0.14392800
H	-2.20369000	4.19707800	-0.29324300	N	-2.18406900	-0.97916400	-0.05989900
C	-4.71986800	2.10484000	-1.43357100	N	-2.07893000	1.16577600	-0.10443900
H	-5.28208500	2.17638300	-0.49926000	C	-1.74155200	-2.99815600	1.26426600
H	-5.18980000	2.76923000	-2.16571200	C	-1.82248900	-2.37720300	0.00200700
H	-4.79222800	1.07581100	-1.79142800	C	-1.57324500	-3.06643900	-1.20115500
H	4.04232600	-5.20962400	-1.40731500	C	-1.23796500	-4.42304300	-1.11047000
H	-0.43072300	6.12351200	1.42079700	C	-1.15254800	-5.06319200	0.12225400
C	4.15665300	4.45170200	-0.07538100	C	-1.40055000	-4.35581700	1.29501300
H	3.90376500	5.51707600	-0.09848500	H	-1.03447700	-4.98181700	-2.01892800
H	4.45561900	4.20595500	0.94866700	H	-1.32120900	-4.86263000	2.25184900
H	5.02437600	4.30045900	-0.72645800	C	-1.41007500	3.17797100	1.13321400
C	2.61025200	3.90558900	-2.00877600	C	-0.93275200	4.49400800	1.10550400
H	2.28561800	4.94440100	-2.13015500	C	-0.63981900	5.12872200	-0.09803900
H	3.48435200	3.75724800	-2.65229800				

C	-0.81717900	4.45611700	-1.30366400	H	-4.03416800	-2.95360800	2.85276000
C	-1.29104700	3.13896600	-1.33578600	H	-2.83002300	-3.90552100	3.73083100
C	-1.58122200	2.52291700	-0.10238100	H	-3.27705200	-2.30089000	4.31661400
H	-0.78295300	5.02487600	2.04076900	C	-0.39168300	2.28249900	3.26516500
H	-0.57690400	4.95737400	-2.23644100	H	-0.60116700	1.75429700	4.20193200
Cu	0.67693700	-0.03830800	0.04170900	H	0.32608700	1.69021400	2.68954400
H	-4.33728600	-1.19283400	-0.17417700	H	0.08490400	3.23577300	3.51850600
H	-4.20089800	1.58428800	-0.23173300	C	-2.73145100	3.28503900	3.30024800
C	-1.63398900	-2.39165200	-2.56760900	H	-2.36387400	4.27921800	3.57540800
H	-1.94565300	-1.35389000	-2.41968100	H	-3.66861300	3.41750300	2.74949900
C	-1.97704700	-2.24701100	2.57104100	H	-2.95623700	2.74935100	4.22875200
H	-2.30285000	-1.23230400	2.32548500	C	-2.40924200	3.17070600	-3.61556800
C	-1.44748600	2.42212900	-2.67309600	H	-3.39440200	3.30771900	-3.15745900
H	-1.88392200	1.43788500	-2.48149100	H	-2.02589300	4.16135800	-3.88189200
C	-1.69463500	2.50304700	2.47147400	H	-2.54268200	2.60855400	-4.54599000
H	-2.12107500	1.51655300	2.26907200	C	-0.07670100	2.18911800	-3.33874700
B	2.66944700	-0.11905100	0.08455000	H	0.41615200	3.13801300	-3.57743300
C	4.85052300	-0.60915400	-0.55166800	H	0.58814600	1.61859800	-2.68287800
O	3.48309300	-0.44420300	-1.00451400	H	-0.19802100	1.63161700	-4.27406500
C	4.85944500	0.21300800	0.78762400	C	-0.24284600	-2.35703200	-3.23085700
O	3.47034100	0.14722000	1.19814900	H	0.48687700	-1.84985200	-2.59249000
C	5.79018200	-0.09589600	-1.64344400	H	0.12885600	-3.36794900	-3.43087200
H	6.83771900	-0.15660000	-1.32647500	H	-0.29144900	-1.82478100	-4.18727800
H	5.67422100	-0.70869700	-2.54271700	C	-2.67779300	-3.05579300	-3.48599300
H	5.56664500	0.93798600	-1.91289400	H	-2.41646300	-4.09582500	-3.70843700
C	5.07322000	-2.11523700	-0.34160600	H	-3.67330200	-3.05362200	-3.02974500
H	4.84819600	-2.63833100	-1.27561000	H	-2.74006900	-2.52045600	-4.43947200
H	6.10686200	-2.34238900	-0.05960900				
H	4.40552300	-2.50525300	0.43135900	L₃-7			
C	5.72588100	-0.36539600	1.90706000	C	1.67274200	1.16902300	0.22464700
H	6.78373500	-0.38487100	1.62069600	C	2.51926500	3.19961400	0.82870900
H	5.63028800	0.25750700	2.80173500	C	3.49900000	2.28087400	1.02184500
H	5.41763000	-1.37865900	2.17120600	N	2.96604000	1.05039100	0.65358000
C	5.19571900	1.69904700	0.58628600	N	1.41519900	2.50623600	0.34537000
H	4.97944000	2.23786300	1.51337100	C	4.33956300	-0.68696300	-0.41794500
H	6.25127600	1.85181000	0.33715500	C	3.69454000	-0.19598900	0.73550100
H	4.58202200	2.13503500	-0.20654300	C	3.74937600	-0.85976100	1.97800300
H	-0.88709000	-6.11554900	0.16957500	C	4.48879300	-2.04704700	2.04441100
H	-0.26806900	6.14948100	-0.09624100	C	5.13868000	-2.55370900	0.92297400
C	-0.66923200	-2.12248600	3.37781700	C	5.06132700	-1.88032800	-0.29257500
H	-0.28867300	-3.10679100	3.67186000	H	4.55192900	-2.58217600	2.98712000
H	0.10857200	-1.62126000	2.79369800	H	5.56972800	-2.28589100	-1.16152700
H	-0.83947700	-1.54317400	4.29203600	C	-0.06855800	3.55362700	-1.30803600
C	-3.09505400	-2.89172400	3.41256200				

C	-1.30233600	4.15067000	-1.59572600	C	0.12325700	-4.55895600	-3.75456100
C	-2.27047800	4.31425300	-0.61031700	H	-0.56446600	-5.20620300	-4.31054000
C	-2.02086300	3.89269900	0.69263000	H	1.00911600	-4.39581900	-4.37589400
C	-0.80572200	3.29099100	1.03909600	H	0.43971700	-5.08147500	-2.85036100
C	0.15177700	3.12788500	0.01638600	C	-0.77163200	-2.42706800	-4.72504800
H	-1.50761500	4.48458200	-2.60836900	H	-1.23599100	-1.45977400	-4.51514500
H	-2.78764500	4.02034100	1.44923500	H	0.19043000	-2.24064800	-5.21100000
Cu	0.58344400	-0.23698700	-0.62116800	H	-1.40929200	-2.97734000	-5.42479100
H	4.50941900	2.38292300	1.38381700	C	-4.35482800	0.29739600	0.18657000
H	2.50413800	4.26628000	0.98463700	C	-5.20444800	1.13496600	0.93116400
C	3.05350400	-0.33149400	3.22963300	C	-4.21198000	0.51556700	-1.19376100
H	2.46073700	0.54231600	2.94569300	C	-5.89776900	2.16484800	0.30397400
C	4.30903000	0.04255200	-1.75773100	H	-5.30876000	0.94912400	1.99513300
H	3.56630800	0.84184100	-1.68983800	C	-4.90646100	1.55205400	-1.81826500
C	-0.53937300	2.87663900	2.48378900	H	-3.54770800	-0.13053000	-1.76155200
H	0.32569500	2.20689300	2.48633700	C	-5.75192100	2.37616300	-1.07299900
C	0.96928500	3.39281100	-2.41461800	H	-6.56036800	2.80299300	0.88273500
H	1.85350500	2.91443900	-1.98423100	H	-4.79079100	1.71407300	-2.88635400
C	-3.62298700	-0.81516100	0.80833000	H	-6.30085100	3.17735200	-1.56086500
N	-3.66432000	-1.02937500	2.07490700	H	-3.05259200	-1.44515300	0.11511700
C	-2.93394600	-2.09479500	2.63750200	C	2.07768300	-1.36269900	3.82603500
C	-3.42669000	-2.63276600	3.83843800	H	2.59988600	-2.26031000	4.17416000
C	-1.74229500	-2.61797700	2.09766900	H	1.55447000	-0.93287800	4.68676100
C	-2.77416900	-3.69152400	4.46607700	H	1.32548900	-1.67160700	3.09533400
H	-4.33479200	-2.20658300	4.25364300	C	4.08080400	0.13096700	4.28244300
C	-1.08902600	-3.67051800	2.73805800	H	4.70694700	-0.70226800	4.61941800
H	-1.32285600	-2.19761100	1.18824500	H	4.74561800	0.90445600	3.88378000
C	-1.60103300	-4.21651800	3.91863000	H	3.57092500	0.54175200	5.16046500
H	-3.17751000	-4.10273900	5.38756600	C	-1.71070900	2.10252700	3.11405000
H	-0.17014700	-4.06417400	2.31125500	H	-2.59535100	2.73496000	3.24405200
H	-1.08512400	-5.03585300	4.41122100	H	-2.00392700	1.23935300	2.51203400
B	-0.30563000	-1.66834700	-1.69773100	H	-1.42429600	1.74090900	4.10731900
C	-1.78702300	-3.28640400	-2.49532500	C	-0.17848200	4.10814000	3.34096100
O	-1.65045600	-2.07113300	-1.70524700	H	0.69588000	4.63535000	2.94552100
C	-0.52639500	-3.21411600	-3.42843900	H	-1.01091200	4.81982900	3.37009800
O	0.40040000	-2.43345500	-2.62946100	H	0.04429900	3.80816800	4.37070500
C	-1.74949200	-4.46715300	-1.51365500	C	3.87590900	-0.87490300	-2.91691400
H	-2.53416700	-4.33529100	-0.76353500	H	3.80591500	-0.29188100	-3.84200700
H	-1.91623500	-5.42313000	-2.02078700	H	4.60332800	-1.67504800	-3.09321000
H	-0.79143500	-4.51330100	-0.98916400	H	2.90089400	-1.33338800	-2.72865400
C	-3.13563800	-3.25381600	-3.21370100	C	5.67356300	0.70071500	-2.04840300
H	-3.24973400	-2.35267400	-3.81934000	H	5.96057800	1.39948800	-1.25535400
H	-3.25578500	-4.12733700	-3.86432300	H	6.46605800	-0.05123300	-2.13161200
H	-3.94562200	-3.27020500	-2.47814500	H	5.63818900	1.25538000	-2.99238200

C	1.41511900	4.75980000	-2.97005000	H	1.64410600	-1.31033500	-2.40607500
H	0.58368400	5.29244800	-3.44400000	C	-0.00173500	2.45360200	0.44342400
H	1.81335500	5.40344800	-2.17866300	N	0.37091700	1.85859900	1.66097200
H	2.19726900	4.62779600	-3.72546200	C	-0.46227800	1.93895500	2.76836800
C	0.45822300	2.47190300	-3.53915000	C	0.00024600	1.34597600	3.97276500
H	0.18780000	1.48700000	-3.14604500	C	-1.70957100	2.61115500	2.83778500
H	-0.42270200	2.89516500	-4.03401700	C	-0.71197600	1.44331600	5.16115600
H	1.23409500	2.33570200	-4.30071300	H	0.95154400	0.82481300	3.94472000
H	-3.22722100	4.76391100	-0.85796200	C	-2.41756000	2.70259500	4.03673800
H	5.70568400	-3.47754400	0.99578900	H	-2.14211100	3.05159300	1.94708700

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C	0.60796800	-1.43287600	0.01981300	H	-2.48870300	2.20862600	6.14199300
C	1.93761600	-3.28943200	-0.02689900	B	-1.37059800	1.63564300	-0.75326100
C	0.65714400	-3.71497700	0.06962700	C	-3.65205200	1.73632700	-1.13326400
N	-0.14535700	-2.57677700	0.08732500	O	-2.60687500	1.51489900	-0.14350900
N	1.89701300	-1.89905000	-0.05503200	C	-2.87072600	2.45916100	-2.30224300
C	-2.14530100	-3.03545600	-1.23823200	O	-1.48642700	2.05654100	-2.06181700
C	-1.58588200	-2.68112700	0.00765700	C	-4.21041700	0.36356500	-1.51751900
C	-2.36103300	-2.52378000	1.17465800	H	-4.57814800	-0.13387900	-0.61725000
C	-3.73913800	-2.74835100	1.06162300	H	-5.03856000	0.44957000	-2.22846900
C	-4.31679400	-3.11732700	-0.15051700	H	-3.43949900	-0.27416500	-1.95222800
C	-3.52797900	-3.25299900	-1.28836900	C	-4.75337000	2.56959900	-0.47525700
H	-4.36738400	-2.63756600	1.93829000	H	-4.37094100	3.50858500	-0.07154200
H	-3.98974400	-3.53033900	-2.23134000	H	-5.55230300	2.79594600	-1.18983800
C	3.47821100	-0.69597800	-1.50108200	H	-5.18940700	2.00262800	0.35178000
C	4.71432200	-0.05331000	-1.63747400	C	-3.25544700	2.01710900	-3.71327600
C	5.54012800	0.16374300	-0.53905500	H	-4.30093800	2.26258600	-3.92864000
C	5.13578200	-0.24245600	0.72885700	H	-2.62856000	2.53814400	-4.44270300
C	3.90805000	-0.88660700	0.92711400	H	-3.11410100	0.94439500	-3.85340700
C	3.10239500	-1.11363500	-0.20721100	C	-2.91315100	3.99078700	-2.21314500
H	5.03393200	0.27755800	-2.62043700	H	-2.59449900	4.34811400	-1.22990400
H	5.78279800	-0.05932300	1.58083600	H	-2.23691900	4.41258600	-2.96214900
Cu	0.10413900	0.40344800	0.17943500	H	-3.91852400	4.37649700	-2.40792900
H	0.23620700	-4.70613800	0.11461500	C	1.17456800	3.01570700	-0.34183100
H	2.86721400	-3.83209100	-0.07924100	C	2.48617000	2.81608200	0.11394600
C	-1.73826100	-2.18203200	2.52580700	C	0.98247200	3.81854200	-1.47860400
H	-0.82520300	-1.60868500	2.33859800	C	3.57097500	3.38509600	-0.55592700
C	-1.31424300	-3.18827000	-2.51158800	H	2.62978600	2.23203100	1.01427300
H	-0.26241700	-3.03998000	-2.25592400	C	2.06561600	4.39087600	-2.14373800
C	3.50469000	-1.33056500	2.32990700	H	-0.02067800	3.99117300	-1.84789800
H	2.45519200	-1.63716300	2.29842900	C	3.36846500	4.17365100	-1.68828100
C	2.62100700	-0.94926200	-2.73770200	H	4.57677000	3.21609600	-0.18170400

H	1.89020300	5.01471100	-3.01647400	N	2.93835700	-0.73578800	-0.43693800
H	4.21213500	4.62410300	-2.20446900	C	-0.52972100	-2.40150600	-2.51412000
H	-0.80139500	3.20815700	0.49191300	C	0.14462900	-2.75931300	-1.32887900
C	-2.64185500	-1.30220500	3.40431400	C	-0.34282400	-3.73824200	-0.43927900
H	-3.52813100	-1.84411400	3.75409100	C	-1.55155100	-4.36284300	-0.77045900
H	-2.08804600	-0.97133800	4.28584700	C	-2.24002500	-4.03047600	-1.93367200
H	-2.96665100	-0.40407300	2.87285800	C	-1.73265300	-3.06110500	-2.79427700
C	-1.33911900	-3.47108200	3.27627000	H	-1.95690600	-5.12140400	-0.10877800
H	-2.22047700	-4.08867500	3.48366300	H	-2.27672200	-2.81282100	-3.70012000
H	-0.63200400	-4.07787300	2.70141800	C	3.95254700	1.45501100	-0.85905100
H	-0.86909600	-3.22218100	4.23358100	C	4.65328600	2.56407000	-0.36999600
C	3.60668100	-0.17794700	3.34562200	C	5.01557900	2.65233200	0.97061100
H	4.64168500	0.15140900	3.48722700	C	4.69088200	1.62512400	1.85195300
H	3.01284000	0.68075900	3.02292100	C	3.99427600	0.48989700	1.41955900
H	3.23301600	-0.50495600	4.32184000	C	3.62942900	0.43483100	0.05902700
C	4.33658900	-2.54433800	2.79168000	H	4.91663000	3.36809000	-1.04973100
H	4.22950200	-3.39416700	2.10967400	H	4.98720100	1.70159300	2.89298300
H	5.40196100	-2.29451300	2.84573300	Cu	0.24184600	0.10125600	0.46415100
H	4.01806800	-2.87024600	3.78769700	H	2.69790500	-3.60803100	-1.97332500
C	-1.67276700	-2.11218400	-3.55498600	H	4.66333800	-1.81144900	-1.17679200
H	-1.05859600	-2.23677500	-4.45367900	C	0.41563800	-4.16229500	0.81538200
H	-2.72310800	-2.18083600	-3.85894300	H	1.19334100	-3.41674700	1.00642100
H	-1.49422200	-1.10736400	-3.16051700	C	0.02058700	-1.37150300	-3.49601200
C	-1.43939800	-4.60382900	-3.10724900	H	0.86264800	-0.86534600	-3.01675800
H	-1.14968600	-5.37093600	-2.38157700	C	3.71858400	-0.65227100	2.39334100
H	-2.46445900	-4.82007500	-3.42600200	H	2.97195000	-1.31019800	1.93953000
H	-0.79185100	-4.70580400	-3.98459000	C	3.61195800	1.36712800	-2.34477500
C	3.24591700	-2.04503000	-3.62507100	H	2.92935000	0.52456600	-2.48677800
H	4.22942000	-1.73934900	-3.99862400	C	-1.78619900	2.16330100	1.00241200
H	3.37561700	-2.98315800	-3.07517700	N	-1.07529600	0.96543100	1.51022700
H	2.60727900	-2.24593800	-4.49221000	C	-1.44641300	0.45317200	2.73884700
C	2.36852600	0.33988800	-3.54180400	C	-0.65620200	-0.57455300	3.32994400
H	1.92677500	1.12080000	-2.91741600	C	-2.57168700	0.87614200	3.49989800
H	3.29252200	0.73737500	-3.97500400	C	-0.95054100	-1.11686300	4.57413200
H	1.68128500	0.13384100	-4.36955000	H	0.21859700	-0.92407500	2.78508100
H	6.49954000	0.65620000	-0.67078400	C	-2.84993300	0.32711100	4.75207100
H	-5.38712200	-3.29503400	-0.20806000	H	-3.25969000	1.60719600	3.09606800
L₃-9				C	-2.05250100	-0.67037700	5.31314500
C	1.58299300	-0.92902000	-0.41257600	H	-0.30325500	-1.89316500	4.97784800
C	3.59154300	-1.78953800	-1.06510200	H	-3.72333400	0.68697200	5.29270800
C	2.63274000	-2.66657500	-1.45258500	H	-2.28050900	-1.09010900	6.28820600
N	1.41640100	-2.13069700	-1.04694600	B	-3.07204700	1.66665900	0.21956300
				C	-5.19076200	0.82274100	0.02244800
				O	-4.30902800	1.65056400	0.82504300

C	-4.51326900	0.90839100	-1.39624000	H	5.78718700	-0.87962800	3.07346200
O	-3.11374800	1.13645100	-1.05689700	H	4.79399100	-2.33112900	3.28307400
C	-5.15081400	-0.58632000	0.63033300	C	-1.01087700	-0.28375300	-3.84716700
H	-5.42738600	-0.52316500	1.68579000	H	-0.54136200	0.48676900	-4.46843800
H	-5.84784200	-1.26385300	0.12715800	H	-1.85007900	-0.69453500	-4.41987000
H	-4.14544200	-1.01259200	0.57701200	H	-1.41346300	0.19462200	-2.95029000
C	-6.60450200	1.39530500	0.10819000	C	0.55665900	-2.05928800	-4.76828300
H	-6.63423700	2.44786400	-0.18008800	H	1.33496900	-2.79274000	-4.53292400
H	-7.29350500	0.83612800	-0.53400400	H	-0.24403700	-2.58362700	-5.30137200
H	-6.96592000	1.31876400	1.13760300	H	0.98479900	-1.31860200	-5.45231300
C	-4.62088600	-0.36150700	-2.23712700	C	4.87746800	1.08067200	-3.17938300
H	-5.67098100	-0.61011100	-2.42617300	H	5.60373900	1.89555200	-3.08732700
H	-4.13246200	-0.20857700	-3.20361400	H	5.37326300	0.15788300	-2.86083200
H	-4.14150600	-1.21037100	-1.74735900	H	4.62175900	0.97852600	-4.23956600
C	-4.97328500	2.12229800	-2.21505700	C	2.88799800	2.62221000	-2.86333300
H	-4.91236700	3.04258000	-1.62755700	H	1.98633800	2.83680300	-2.28523700
H	-4.32063300	2.23065200	-3.08609600	H	3.52999400	3.50871400	-2.82153300
H	-6.00165400	2.00469200	-2.57027000	H	2.60072000	2.47898000	-3.91086300
C	-0.84123300	3.12319900	0.28445100	H	5.55784800	3.52254900	1.32965700
C	0.32946000	3.54070500	0.94109000	H	-3.17452200	-4.53093400	-2.17148300
C	-1.13733300	3.69396000	-0.95998900				
C	1.16234800	4.50902900	0.38444900	L₃-10			
H	0.57103800	3.09890700	1.90335400	C	-2.20354400	0.52088900	-0.39863800
C	-0.30468800	4.66794500	-1.52219000	C	-4.37851700	0.72498300	-1.04548200
H	-2.02412900	3.37426900	-1.49709700	C	-3.78450400	1.92880000	-1.24190600
C	0.84403600	5.08402000	-0.85046400	N	-2.45976900	1.78871100	-0.84333800
H	2.05713200	4.82129300	0.91643100	N	-3.40280400	-0.12246700	-0.53111200
H	-0.55915800	5.10144600	-2.48619400	C	-0.71004900	2.99733200	-2.07132300
H	1.48676600	5.84618000	-1.28313600	C	-1.48013300	2.85007100	-0.89971500
H	-2.15444200	2.73797300	1.86754500	C	-1.34152700	3.70305200	0.21392800
C	-0.47987900	-4.21073400	2.06634900	C	-0.39980400	4.73540400	0.12238600
H	-1.26041900	-4.97414000	1.98117100	C	0.36950000	4.90953500	-1.02431000
H	0.12459200	-4.46436900	2.94382400	C	0.21530100	4.04774400	-2.10659500
H	-0.95961800	-3.24740200	2.25779000	H	-0.26594400	5.40757800	0.96420000
C	1.11631800	-5.51876500	0.59052500	H	0.82484500	4.18852000	-2.99399300
H	0.38486400	-6.30997500	0.39247700	C	-3.44377200	-2.50010000	-1.14912200
H	1.80521800	-5.48363600	-0.25994600	C	-3.70685600	-3.82476800	-0.77827500
H	1.68996500	-5.80607000	1.47823900	C	-4.13846100	-4.14164900	0.50644900
C	3.13764500	-0.16992700	3.73447400	C	-4.31651400	-3.13591300	1.45185300
H	3.85041500	0.44757700	4.29131300	C	-4.07463800	-1.79345700	1.13599600
H	2.22039200	0.40692800	3.59117300	C	-3.64087300	-1.50257400	-0.17311700
H	2.89383000	-1.03099500	4.36517400	H	-3.56481600	-4.61847300	-1.50519700
C	4.99780400	-1.48636900	2.61617100	H	-4.64347300	-3.39585500	2.45398900
H	5.38871600	-1.88544000	1.67430300				

Cu	-0.55222300	-0.15737400	0.21102100	H	7.34739100	-0.31248800	-2.08750600
H	-4.17150700	2.86037200	-1.62208800	C	2.62062400	0.81100300	2.11961300
H	-5.38971600	0.39347800	-1.21811800	C	3.57713600	1.83544400	2.20747300
C	-2.16494900	3.54254300	1.48828900	C	2.00857600	0.37784200	3.30228400
H	-2.80007600	2.65977900	1.37351100	C	3.91200600	2.40586100	3.43453100
C	-0.85060800	2.07182700	-3.27592800	H	4.07215600	2.18265900	1.30445600
H	-1.58392900	1.29995800	-3.02707900	C	2.34538500	0.94513900	4.53477000
C	-4.26410900	-0.71887200	2.20197100	H	1.26777200	-0.41191200	3.24738400
H	-4.08325700	0.25508500	1.73850300	C	3.29700200	1.96191300	4.60826300
C	-2.96246600	-2.19152200	-2.56381400	H	4.65659500	3.19715800	3.47534200
H	-2.74437600	-1.12154400	-2.62145700	H	1.86125100	0.58657100	5.43993300
C	2.21978600	0.24626400	0.75119900	H	3.55939900	2.40274600	5.56632400
N	1.12965500	-0.74206500	0.75727100	H	1.81987900	1.11693900	0.20286600
C	1.42639900	-2.05309700	1.07078900	H	1.09457300	5.71694200	-1.07300800
C	2.67573900	-2.48878000	1.58750300	H	-4.33167900	-5.17670100	0.77332300
C	0.44204000	-3.06219100	0.88436200	C	0.47278500	1.35067200	-3.59791400
C	2.91588600	-3.83611700	1.86713700	H	0.32826900	0.65743200	-4.43389400
H	3.45343000	-1.76649500	1.80916500	H	1.25415400	2.06058600	-3.89047100
C	0.69135300	-4.39602400	1.17414600	H	0.84128700	0.77793500	-2.74183100
H	-0.52897500	-2.76826000	0.49051200	C	-1.38433600	2.83209800	-4.50620400
C	1.93747200	-4.80856800	1.66508700	H	-2.34716000	3.31001500	-4.29701500
H	3.88752900	-4.12036300	2.26629400	H	-0.68816600	3.61470400	-4.82665000
H	-0.09648000	-5.12783700	1.00734800	H	-1.52252900	2.14555200	-5.34832900
H	2.13165600	-5.85321600	1.88884600	C	-4.05725400	-2.49534400	-3.60563600
B	3.42559100	-0.20142200	-0.19639700	H	-4.31913800	-3.55886800	-3.61054600
C	4.46006500	-0.73931900	-2.16978400	H	-4.97248400	-1.92884000	-3.40399600
O	3.19259000	-0.68151800	-1.46478600	H	-3.71106200	-2.23342300	-4.61122900
C	5.51313000	-0.71195000	-0.99006200	C	-1.65565800	-2.93779800	-2.89509600
O	4.76519000	-0.06693800	0.07896900	H	-1.80454300	-4.02272300	-2.91319600
C	4.47763500	-2.00531600	-3.02539400	H	-1.29196500	-2.63889600	-3.88413000
H	3.69081900	-1.94380300	-3.78300200	H	-0.87361700	-2.71908200	-2.16251500
H	5.43719900	-2.11738500	-3.54170200	C	-1.26841400	3.29753700	2.71743000
H	4.29527300	-2.89721500	-2.42415600	H	-0.62093600	4.15629500	2.92318100
C	4.52099800	0.50274400	-3.06984400	H	-1.88647200	3.13044300	3.60632700
H	4.48404000	1.42272100	-2.47944900	H	-0.62728300	2.42244400	2.57814800
H	5.42915400	0.51809700	-3.68019600	C	-3.09542300	4.75183500	1.70869100
H	3.65662900	0.49710900	-3.73971700	H	-2.52423500	5.67589800	1.84840800
C	5.89983900	-2.10676300	-0.48018500	H	-3.76759000	4.90257000	0.85733400
H	6.51538700	-2.64464100	-1.20798500	H	-3.70906500	4.60230000	2.60342200
H	6.47795300	-1.99550400	0.44162400	C	-3.23677000	-0.87987100	3.33971500
H	5.01570500	-2.70646300	-0.25091800	H	-3.35487000	-0.07725700	4.07595800
C	6.77155000	0.11248400	-1.25846400	H	-3.36634100	-1.83400700	3.86159100
H	6.53503200	1.15162400	-1.49476600	H	-2.21334700	-0.84352900	2.95473900
H	7.40675800	0.10659600	-0.36807100	C	-5.70523400	-0.70204000	2.74712100

H -6.43645100 -0.56387100 1.94384900
H -5.95281700 -1.63429100 3.26555700
H -5.82990500 0.11628400 3.46416700

L₃-TS11

C 2.01446300 0.54777100 -0.02114400
C 3.83439700 1.91169000 0.09710400
C 4.28879900 0.64272600 -0.05774200
N 3.16801000 -0.17740200 -0.12778000
N 2.44675800 1.83739900 0.11694500
C 3.18580200 -2.15050700 -1.59448400
C 3.23815000 -1.61264100 -0.29250300
C 3.38917900 -2.41388400 0.85692100
C 3.49202400 -3.79768000 0.67021500
C 3.44595600 -4.35743000 -0.60320400
C 3.29339100 -3.54111600 -1.71999300
H 3.60749200 -4.44373500 1.53532500
H 3.25400200 -3.98878400 -2.70785400
C 1.15922200 3.63606800 -0.94812100
C 0.33160800 4.75697100 -0.80909900
C -0.05916300 5.21245100 0.44676300
C 0.37015700 4.55189100 1.59410400
C 1.19577500 3.42339300 1.51646400
C 1.57735900 2.98764600 0.23173400
H -0.01113300 5.27675700 -1.69862600
H 0.05570000 4.91339400 2.56802400
Cu 0.21400600 -0.01528200 -0.15482600
H 5.28969700 0.24753100 -0.12173300
H 4.35828900 2.84900700 0.19248200
C 3.44214600 -1.83659500 2.26807400
H 3.32928000 -0.75124400 2.19737600
C 3.04758700 -1.28614100 -2.84416000
H 2.84243200 -0.26050700 -2.52496100
C 1.65609100 2.73153900 2.79544700
H 2.18358900 1.81567800 2.51366000
C 1.56718600 3.16899500 -2.34212200
H 2.19953900 2.28346400 -2.23411800
C -2.65040800 0.59292000 -0.14496500
N -1.59345600 -0.49011900 -0.44245300
C -1.75752600 -1.43576200 -1.48184900
C -1.39367000 -2.77899900 -1.24372600
C -2.19313800 -1.10528200 -2.78413300
C -1.45519000 -3.73907600 -2.25171100

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H -2.46671600 -0.08194100 -3.01083400
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H -1.16527400 -4.76352700 -2.02986800
H -2.60533400 -1.78551800 -4.77641200
H -1.95712400 -4.14803900 -4.31618700
B -2.65985300 -0.34577900 1.09744100
C -3.33214400 -1.95840000 2.59756200
O -3.60347800 -1.36364000 1.31380400
C -2.61487800 -0.78061900 3.35919500
O -1.93407100 -0.09056800 2.29034900
C -4.66168200 -2.41147900 3.20308200
H -5.08498700 -3.21645400 2.59451400
H -4.52445900 -2.79373700 4.22072200
H -5.38652100 -1.59587200 3.22877700
C -2.41778500 -3.17520300 2.38696800
H -1.44541700 -2.87048300 1.99215000
H -2.25821800 -3.73121900 3.31684200
H -2.88419100 -3.84430000 1.65869000
C -3.60963700 0.21008600 3.98803700
H -4.12133400 -0.21657900 4.85702200
H -3.06311900 1.09997900 4.31388400
H -4.36254800 0.52289900 3.25948600
C -1.59209500 -1.21697200 4.40822300
H -0.79212800 -1.81356200 3.96666900
H -1.13846000 -0.33568200 4.87231500
H -2.06865500 -1.80513100 5.20044800
C -3.84706700 0.81153300 -1.02416600
C -4.85185900 -0.15577300 -1.20831200
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C -5.96404400 0.11465300 -2.00477900
H -4.76041900 -1.11374100 -0.71045900
C -5.12591800 2.32984700 -2.44923600
H -3.24525300 2.81798700 -1.52371500
C -6.10845400 1.35567900 -2.62999800
H -6.72697600 -0.64882400 -2.13391900
H -5.22619800 3.30246100 -2.92461300
H -6.97896000 1.56165600 -3.24707000
H -2.13360300 1.54357300 0.00219500
H 3.52655000 -5.43377300 -0.72565500
H -0.70247900 6.08358300 0.53170700
C 0.46992200 2.31429100 3.68565900
H 0.83950800 1.76791800 4.56075200

H	-0.08058800	3.18606600	4.05641200	H	-2.93369100	-4.77039300	-1.22943300
H	-0.23218000	1.66914400	3.14946200	H	-3.10207600	-3.93337500	2.96666000
C	2.65138800	3.61750100	3.57213300	C	-1.48625500	3.67584300	0.57428100
H	3.52335900	3.87660900	2.96200600	C	-0.72694600	4.82997300	0.34622600
H	2.18144800	4.55341100	3.89352400	C	-0.30127100	5.17054400	-0.93463200
H	3.00680700	3.09775200	4.46831900	C	-0.62878200	4.36117500	-2.01846800
C	4.80099800	-2.11290800	2.94102700	C	-1.38228300	3.19277700	-1.85069300
H	4.83517500	-1.65223800	3.93400700	C	-1.79562600	2.87276200	-0.54188600
H	4.97565200	-3.18670700	3.06703700	H	-0.46578800	5.46831500	1.18469400
H	5.63053700	-1.70894000	2.35131600	H	-0.29084100	4.63577900	-3.01269700
C	2.27679900	-2.35607700	3.13122300	Cu	-0.22805300	-0.00056500	0.14633500
H	2.33163500	-3.44095800	3.27117400	H	-5.29784900	-0.11925500	-0.07719100
H	2.30103200	-1.89101100	4.12252400	H	-4.55937700	2.51252500	-0.59405800
H	1.31316300	-2.12276200	2.66950500	C	-3.01820000	-2.22962800	-2.18483100
C	1.86739700	-1.72733900	-3.72975000	H	-3.14146600	-1.14301200	-2.20772300
H	1.76095100	-1.04071600	-4.57645900	C	-3.23024300	-1.22282100	2.86760600
H	2.02189400	-2.73032700	-4.14124000	H	-3.12900400	-0.20720800	2.47428100
H	0.92490100	-1.73503400	-3.17626800	C	-1.73714100	2.33968600	-3.06456600
C	4.36605300	-1.26521300	-3.64429500	H	-2.24912500	1.44064600	-2.70972700
H	5.20130800	-0.90160900	-3.03633200	C	-1.93662200	3.33487800	1.99173700
H	4.62750700	-2.26639100	-4.00399000	H	-2.53783600	2.42220100	1.94836500
H	4.27220100	-0.61094700	-4.51767400	C	2.59804800	0.78748400	0.08845000
C	2.40255700	4.23953300	-3.07172400	N	1.62497900	-0.39445100	0.44371100
H	1.82518900	5.15518400	-3.23801100	C	1.81331200	-1.17851400	1.62164100
H	3.29623300	4.50994600	-2.49958900	C	1.84792500	-2.57997300	1.52923600
H	2.72528900	3.86867400	-4.05037500	C	1.90780100	-0.58788500	2.89444600
C	0.34127100	2.75237200	-3.17790000	C	1.95191100	-3.36504400	2.67749200
H	-0.33075400	3.59922300	-3.35383200	H	1.79532800	-3.04006600	0.54995600
H	0.65927100	2.37316200	-4.15505800	C	2.02060700	-1.37875600	4.03763400
H	-0.23083400	1.96573400	-2.67703200	H	1.90416500	0.49375000	2.97758500
L₃-12				C	2.03936200	-2.77222500	3.93900700
C	-2.05807800	0.44494200	-0.05810400	H	1.97437100	-4.44781200	2.58258200
C	-3.96895800	1.63495000	-0.38573200	H	2.09652900	-0.90067900	5.01095600
C	-4.32940300	0.35112700	-0.13241100	H	2.12776500	-3.38564100	4.83116100
N	-3.15267100	-0.36161400	0.06466900	B	2.50625300	-0.47799700	-0.87477500
N	-2.58088600	1.67553700	-0.33581700	C	3.50803900	-2.04015300	-2.27928700
C	-3.13009100	-2.19709000	1.69766900	O	3.57494600	-1.42739800	-0.98652000
C	-3.10215400	-1.77840400	0.35236700	C	2.69216600	-0.98059600	-3.11539800
C	-3.03967800	-2.68124700	-0.72757200	O	1.78353600	-0.46100400	-2.13216900
C	-2.99066800	-4.04700200	-0.42191000	C	4.93681800	-2.29152900	-2.76888800
C	-3.01215900	-4.49098100	0.89689300	H	5.42339100	-3.02559400	-2.11868100
C	-3.08500400	-3.57504400	1.94228800	H	4.94528600	-2.68791600	-3.79077300
				H	5.53133100	-1.37654500	-2.74096500
				C	2.76653400	-3.38243000	-2.14962800

C	2.70126000	3.43878000	1.34833100	H	-4.10840600	2.77274300	-0.85340900
H	3.16517300	2.47215500	1.13299200	C	-7.05982600	1.10311700	-0.59346500
C	0.39401600	2.28631400	-3.11610400	H	-7.25756900	-0.91459700	0.13988800
H	1.08035400	1.43940500	-3.02798000	H	-6.52503500	3.08271400	-1.26445000
C	-2.83319000	0.65749600	0.18223500	H	-8.12264700	1.23095500	-0.78033800
N	-2.03339200	-0.59681900	-0.14248300	H	-2.29748300	1.56186700	-0.11741900
C	-2.45660900	-1.62636900	-0.98517600	C	2.05076100	3.32826600	2.73954800
C	-2.21297100	-2.97080100	-0.63098800	H	1.59015700	4.27277800	3.04770300
C	-3.09051600	-1.37665400	-2.21997800	H	1.27493200	2.55754500	2.74737500
C	-2.57946900	-4.01392500	-1.47971800	H	2.80356300	3.06739500	3.49147100
H	-1.74269700	-3.18185600	0.32362700	C	3.82222000	4.49742100	1.34040800
C	-3.45161800	-2.42664300	-3.06196200	H	4.31733200	4.54910200	0.36518100
H	-3.31433700	-0.35330600	-2.50024900	H	3.43115200	5.49499900	1.56712900
C	-3.19913500	-3.75401600	-2.70529100	H	4.58051700	4.25758200	2.09353200
H	-2.38446400	-5.03998000	-1.17598200	C	5.86521700	-1.04253300	1.39071000
H	-3.94350300	-2.20332700	-4.00581200	H	6.08865200	-0.73802000	0.36352300
H	-3.48901300	-4.56846200	-3.36280200	H	6.30576500	-0.30056000	2.06553600
B	-2.23489200	-0.30759100	1.31363200	H	6.36542400	-2.00052000	1.56975800
C	-2.21290300	-1.31621000	3.43170700	C	4.06211600	-1.49098200	3.10989100
O	-3.00198900	-1.03864900	2.27617400	H	2.99061400	-1.59790400	3.29744200
C	-1.13299800	-0.16318000	3.42258100	H	4.55625700	-2.41516300	3.42728300
O	-0.94106900	0.01810900	1.99892600	H	4.44058400	-0.68690900	3.74971200
C	-3.13062300	-1.30380100	4.65745200	C	-1.03020100	1.70862200	-3.20729800
H	-3.84455600	-2.12960600	4.58341600	H	-1.27936400	1.12659200	-2.31686100
H	-2.56273300	-1.42956200	5.58636100	H	-1.77858400	2.50106100	-3.31599400
H	-3.70210500	-0.37573200	4.71390200	H	-1.11582700	1.04966800	-4.07769900
C	-1.58082400	-2.71174100	3.27714000	C	0.77312500	3.04709600	-4.40254400
H	-0.86764200	-2.73315300	2.44817100	H	1.79913100	3.42797800	-4.35938500
H	-1.06598000	-3.03978900	4.18671000	H	0.69274900	2.38517000	-5.27118400
H	-2.37702800	-3.42765600	3.05554600	H	0.10867800	3.90045500	-4.57410700
C	-1.67578300	1.15976200	3.98205800	C	0.70078200	-3.06651500	-3.16813500
H	-1.80342200	1.11699800	5.06809400	H	0.95097100	-4.10348200	-3.41824600
H	-0.96981900	1.96339600	3.75154500	H	-0.04172200	-3.07660700	-2.36759200
H	-2.63616400	1.40747300	3.52404200	H	0.23004900	-2.62778500	-4.05328600
C	0.19550600	-0.51563300	4.08370400	C	2.99589300	-2.30834100	-3.91934600
H	0.66057100	-1.38203600	3.60893600	H	3.86640200	-1.67913500	-3.70807700
H	0.88974000	0.32843100	4.01644100	H	3.35386000	-3.33326500	-4.06691500
H	0.04869300	-0.74184300	5.14528900	H	2.55512100	-1.96759500	-4.86228500
C	-4.29008000	0.76094600	-0.10481500	H	3.42818700	-5.53550600	0.21658900
C	-5.20974400	-0.27103300	0.16786300	H	-0.65781900	6.07376300	-0.57370200
C	-4.79989300	1.96267000	-0.62969700				
C	-6.57081900	-0.10050100	-0.07866600				
H	-4.85399800	-1.20266900	0.59272600				
C	-6.16401800	2.13859400	-0.86320300				
				L₃-14			
				C	1.70887000	-0.99266500	0.00106200

C	3.69162400	-2.01698000	0.44435800	B	-2.24337700	1.82141700	-0.46888600
C	2.75748500	-2.98838000	0.29425800	C	-1.78341700	3.17760200	-2.32386800
N	1.55295100	-2.34962700	0.02809900	O	-2.73559400	2.86107600	-1.32264700
N	3.03910200	-0.80556100	0.25687700	C	-0.41511500	2.95641800	-1.58150400
C	-0.13605300	-3.28090900	-1.49829000	O	-0.73586100	1.78872800	-0.76328400
C	0.31064900	-3.06420300	-0.17949400	C	-1.96772400	2.22329900	-3.51987500
C	-0.37587700	-3.55547000	0.95107600	H	-3.00829200	2.28556400	-3.84910200
C	-1.56077900	-4.26496300	0.72308600	H	-1.32113100	2.48095000	-4.36589800
C	-2.03896700	-4.47651900	-0.56695300	H	-1.77468000	1.18698900	-3.23006400
C	-1.33168000	-3.99153000	-1.66283500	C	-2.01686300	4.62114300	-2.77947000
H	-2.11894800	-4.65315200	1.56884700	H	-2.03110300	5.30756100	-1.93081900
H	-1.71056400	-4.16768400	-2.66470500	H	-1.25010700	4.94966900	-3.49043500
C	4.42815600	0.91683700	-0.80712700	H	-2.98914700	4.68754500	-3.27626800
C	5.07640100	2.15398300	-0.71324100	C	0.76947700	2.64492000	-2.49224000
C	5.00656100	2.91783100	0.44914800	H	0.93719300	3.47217100	-3.19064300
C	4.29350700	2.45323400	1.54981100	H	1.68478300	2.52070800	-1.90317600
C	3.62909800	1.21976400	1.51841400	H	0.60159300	1.73596300	-3.07486800
C	3.70340300	0.47809300	0.32202800	C	-0.06334800	4.10525600	-0.62837600
H	5.64498200	2.52274900	-1.56099900	H	-0.92409500	4.37061200	-0.01089300
H	4.25366200	3.05272700	2.45359400	H	0.75338600	3.79311800	0.03026200
Cu	0.43883900	0.36647800	-0.34243200	H	0.26157500	4.99522800	-1.17657800
H	2.83147400	-4.06189900	0.35274200	C	-4.33426000	0.01504500	-0.40791500
H	4.74485500	-2.06986600	0.66657400	C	-5.43751800	0.87905700	-0.29480200
C	0.14463500	-3.38591900	2.37643500	C	-4.55558600	-1.26326000	-0.94944900
H	0.97130700	-2.66948000	2.35493600	C	-6.70635900	0.47906100	-0.71086500
C	0.63202100	-2.80954300	-2.72992100	H	-5.27967100	1.86663100	0.12655900
H	1.52397600	-2.27397600	-2.39286400	C	-5.82457900	-1.66198300	-1.36975400
C	2.90586000	0.71907500	2.76550000	H	-3.71795000	-1.95266300	-1.03548300
H	2.37572100	-0.20132000	2.50630300	C	-6.91122200	-0.79252400	-1.25362400
C	4.56617700	0.07926000	-2.07725100	H	-7.54365600	1.16575500	-0.60953100
H	3.83910600	-0.73676900	-2.02625000	H	-5.96731800	-2.65845700	-1.78268500
C	-2.96098600	0.43806600	-0.01686600	H	-7.90174100	-1.10161000	-1.57663500
N	-2.79437800	1.60033900	0.86920700	H	-2.31013300	-0.41713400	0.22577800
C	-2.50062300	1.59669500	2.20969600	H	-2.96542400	-5.02249700	-0.71797700
C	-1.89679500	2.72538800	2.81477800	H	5.51528700	3.87630100	0.49822100
C	-2.82965200	0.50228200	3.04212400	C	-0.91697800	-2.81691500	3.33374000
C	-1.63647900	2.74880000	4.18132400	H	-1.76463100	-3.49976300	3.45413900
H	-1.66068100	3.58448100	2.19402100	H	-0.47841100	-2.66474200	4.32559800
C	-2.56283100	0.54110500	4.41005300	H	-1.30178800	-1.85507100	2.98690700
H	-3.32872100	-0.35511700	2.60064600	C	0.70188900	-4.72197700	2.91180200
C	-1.96033300	1.65753700	4.99642200	H	-0.08627000	-5.48035300	2.96959500
H	-1.17970200	3.63410800	4.61870800	H	1.49589800	-5.12028800	2.27116400
H	-2.84128200	-0.31015600	5.02770000	H	1.11357000	-4.58899700	3.91784400
H	-1.76258400	1.68497000	6.06399900	C	1.85013300	1.71862900	3.27043600

H	1.30912600	1.30216000	4.12508300	C	-0.43403200	2.96500000	0.19313500
H	2.30555800	2.66070100	3.59481500	H	-2.39527600	3.93861000	-2.39601400
H	1.10902100	1.94865900	2.50043400	H	-3.21518200	4.05367200	1.79983800
C	3.91728800	0.36747000	3.87583000	Cu	0.12314400	-0.26841100	-0.35622900
H	4.64127300	-0.38250500	3.53969900	H	4.03799800	2.56498200	1.29423800
H	4.47860100	1.25115800	4.19789800	H	1.84053700	4.24979400	1.12222400
H	3.39443600	-0.03224600	4.75085500	C	2.74344700	-0.94964600	2.65271500
C	4.25850000	0.87706300	-3.35768000	H	1.81212500	-0.42648100	2.41753600
H	4.98242700	1.68179300	-3.52183900	C	4.31606200	1.13178700	-1.79527400
H	4.30526900	0.21556900	-4.22912600	H	3.44156400	1.75999700	-1.60527800
H	3.26124100	1.32306800	-3.32251300	C	-0.87181200	3.06103200	2.73814100
C	5.97099800	-0.55398800	-2.16062800	H	-0.00970600	2.38605800	2.75432700
H	6.74569600	0.21794000	-2.22152700	C	0.12840500	2.97985300	-2.33314500
H	6.19015600	-1.17284800	-1.28472000	H	1.03240600	2.48564500	-1.96862000
H	6.05524800	-1.18624400	-3.05089200	C	-1.92647600	-1.15201600	0.67960700
C	-0.19747100	-1.82637800	-3.57702000	N	-2.90936900	-1.62701700	-0.30391800
H	0.38779500	-1.47546900	-4.43396300	C	-3.94962100	-0.86125900	-0.80491900
H	-1.10682400	-2.29619700	-3.96549600	C	-4.47831700	-1.13444900	-2.08515100
H	-0.50089400	-0.95568100	-2.98817700	C	-4.54338400	0.17052900	-0.04985800
C	1.11243300	-4.00528700	-3.57655900	C	-5.54959700	-0.40006900	-2.58394200
H	1.73173300	-4.68980500	-2.98776000	H	-4.04272200	-1.93746600	-2.67147200
H	0.26937300	-4.57880600	-3.97557200	C	-5.61697300	0.89826400	-0.56112900
H	1.70688200	-3.65461000	-4.42696000	H	-4.16731400	0.37996800	0.94659200

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C	1.26788300	1.12705100	0.24148900	H	-5.93753400	-0.63291800	-3.57294500
C	1.94723800	3.19887800	0.91078700	H	-6.06162000	1.68285600	0.04704400
C	3.02126900	2.37778800	0.99010000	H	-6.96911300	1.19326100	-2.22326100
N	2.59771900	1.11901200	0.57297900	B	-1.60401300	-2.08757800	-0.73657000
N	0.88294800	2.42540600	0.46131100	C	-0.10055200	-3.66704400	-1.57448200
C	4.34093100	0.01662000	-0.75070700	O	-1.26657700	-3.46751800	-0.77727500
C	3.51328200	0.01208500	0.39281700	C	-0.16587900	-2.46286300	-2.59041100
C	3.58737900	-0.99308300	1.38098200	O	-0.76492600	-1.41468900	-1.77537800
C	4.51647200	-2.02169000	1.18135500	C	1.14036300	-3.61909600	-0.66632400
C	5.34021700	-2.04651900	0.05927100	H	1.01023300	-4.35328800	0.13361200
C	5.25397000	-1.03629200	-0.89249100	H	2.06243800	-3.85439300	-1.20779900
H	4.59717400	-2.81426800	1.91660800	H	1.26126100	-2.63658600	-0.19769500
H	5.90696800	-1.06116000	-1.75926400	C	-0.19504200	-5.04795000	-2.23004900
C	-0.80330300	3.21245900	-1.14640800	H	-1.13596500	-5.16733900	-2.77003400
C	-2.07669200	3.74789600	-1.37628400	H	0.63582300	-5.22030100	-2.92355700
C	-2.93708400	4.04336400	-0.32512900	H	-0.15563400	-5.81978500	-1.45573900
C	-2.53743400	3.81358100	0.98755700	C	1.18025900	-1.98277100	-3.12228900
C	-1.28263300	3.26664000	1.28128800	H	1.67449800	-2.77760200	-3.69127500
				H	1.03363000	-1.13001100	-3.79293700
				H	1.84628900	-1.67358100	-2.31353100

C	-1.13004700	-2.72199700	-3.75546600	H	1.04926400	4.96804600	-2.21478400
H	-2.08751200	-3.10340900	-3.39310100	H	1.26551600	4.15551300	-3.77608800
H	-1.31352000	-1.78262000	-4.28455700	C	-0.49585400	2.05314700	-3.39368300
H	-0.71675300	-3.44412500	-4.46640600	H	-0.78072100	1.08796300	-2.96540000
C	-1.97677000	-1.73217900	2.05285100	H	-1.38860900	2.49768900	-3.84599100
C	-2.74501500	-2.87265600	2.34316600	H	0.22380900	1.87295000	-4.20029200
C	-1.23857900	-1.15752900	3.10280900				
C	-2.77389000	-3.40956500	3.62992300	L₃-16			
H	-3.32288800	-3.32167300	1.54245500				
C	-1.27427600	-1.68891000	4.39253000	Cu	0.37692500	-0.20265800	-0.07665200
H	-0.63192600	-0.27700500	2.90145200	N	-2.49504900	0.11242100	-0.62184000
C	-2.04204100	-2.82356400	4.66570700	N	2.66951000	1.53500100	0.77541500
H	-3.37983700	-4.29075700	3.82659800	N	3.20638100	-0.54659300	0.68606500
H	-0.70614700	-1.21128700	5.18797400	O	-4.90700500	0.68122000	-0.22415200
H	-2.07174500	-3.24072400	5.66842900	O	-3.95543300	-1.00711400	1.01289800
H	-1.85413300	-0.05228500	0.70193700	B	-3.75407700	-0.05071700	0.02722200
H	-3.92171700	4.45306400	-0.52907500	C	2.16540600	0.30757300	0.44369100
H	6.05391500	-2.85515100	-0.07045000	C	3.98523100	1.44244400	1.21735900
C	3.46895000	-0.14550200	3.75344400	C	4.32529800	0.13119600	1.15675300
H	4.41987300	-0.62106500	4.01838100	C	3.16087500	-1.98153500	0.51402600
H	3.68338600	0.88010900	3.43703100	C	3.45084900	-2.52465800	-0.75320100
H	2.85291700	-0.09677800	4.65764300	C	3.43796000	-3.91970100	-0.87533400
C	2.35457400	-2.34278500	3.17512000	H	3.65181900	-4.36999200	-1.83971500
H	1.90181500	-2.95527900	2.39086200	C	3.15106500	-4.73667800	0.21386200
H	3.21639200	-2.88369200	3.58157800	C	2.86288100	-4.17209000	1.45325100
H	1.61885500	-2.24468200	3.97735000	H	2.63353000	-4.81825100	2.29526700
C	-1.97965800	2.41123800	3.58810300	C	2.85890100	-2.78349300	1.63350600
H	-1.59669800	2.18920000	4.58957800	C	2.53094400	-2.20155100	3.00582000
H	-2.83919600	3.07785600	3.71251600	C	3.76981200	-1.66342400	-1.97064100
H	-2.33310700	1.47420100	3.15237600	C	1.95177100	2.78835600	0.69432900
C	-0.43683100	4.39657000	3.37976700	C	2.20192300	3.63497800	-0.40537500
H	-0.11192200	4.23692800	4.41345200	C	3.16661100	3.26360600	-1.52850300
H	0.38806300	4.86809700	2.83697600	C	1.53980800	4.86779900	-0.43525500
H	-1.26973500	5.10791400	3.39522900	H	1.70992400	5.54251100	-1.26811400
C	4.18251500	0.59839600	-3.23357400	C	0.66069600	5.23799000	0.57805700
H	4.10686700	1.43535400	-3.93589100	C	0.42719400	4.37913000	1.64712100
H	5.05133300	0.00210100	-3.53100300	H	-0.26347500	4.67569000	2.43052900
H	3.29149100	-0.02334000	-3.34803500	C	1.06800400	3.13701200	1.73532700
C	5.56718900	2.02630900	-1.66896400	C	0.80021400	2.23832200	2.93858200
H	5.65586100	2.46327900	-0.66946600	C	-1.45032400	-0.90688900	-0.32126000
H	6.48045100	1.45283800	-1.86085900	H	-1.65780100	-1.24194300	0.70150400
H	5.52677200	2.84620000	-2.39394000	C	-2.23005100	1.12985200	-1.56767400
C	0.56137400	4.32401500	-2.95398300	C	-1.26668800	0.94521900	-2.57979900
H	-0.29670300	4.87205300	-3.35753200	H	-0.74178500	0.00093300	-2.65140600

C	3.74029700	-2.42453100	1.30326600	C	-5.60821800	-1.35914900	-1.06724500
C	3.96315500	-2.52170600	-0.03081900	C	-5.96896000	-2.77673800	-1.50895800
C	2.72383400	-1.87290300	-2.09626600	H	-5.58757500	-2.95225700	-2.51914100
C	3.17394900	-0.72161000	-2.77379300	H	-7.05499500	-2.91757200	-1.52856600
C	3.07538200	-0.71722300	-4.17076000	H	-5.53063400	-3.52780500	-0.84920500
H	3.41435300	0.15342500	-4.72269100	C	-6.06703900	-0.34549200	-2.12575200
C	2.54496500	-1.80339600	-4.86089000	H	-5.81258300	0.67638000	-1.83123800
C	2.09292900	-2.92023800	-4.16390300	H	-7.14595600	-0.40042100	-2.30181400
H	1.67028600	-3.75779000	-4.71066900	H	-5.55124800	-0.55948500	-3.06575300
C	2.17187800	-2.98294400	-2.76713700	C	-1.53251900	0.81036900	-1.94712900
C	1.66065000	-4.22209400	-2.03783100	C	-0.81489900	0.49584300	-3.12181500
C	3.75979100	0.48600800	-2.04896900	H	-0.28771800	-0.45466800	-3.17671000
C	1.94495000	-1.47231000	2.75016800	C	-0.76569300	1.36796200	-4.20512200
C	2.44327500	-0.35894500	3.45801700	H	-0.20611700	1.08526400	-5.09380200
C	3.54715000	0.54218000	2.91052100	C	-1.42978200	2.59978300	-4.15713500
C	1.90022300	-0.10270500	4.72224500	H	-1.39007300	3.28277100	-5.00120600
H	2.26018000	0.74786100	5.29232400	C	-2.15046700	2.92717000	-3.00973100
C	0.90214200	-0.91253800	5.25549700	H	-2.68289400	3.87406900	-2.95331600
C	0.42952000	-2.00393600	4.53398100	C	-2.20449200	2.04620900	-1.92376100
H	-0.35013000	-2.62859000	4.95883800	H	-2.78808800	2.31452300	-1.04890800
C	0.94053100	-2.31450600	3.26770900	H	3.71577100	0.27420000	1.86359200
C	0.41445400	-3.53905600	2.52508300	H	0.91189400	-3.58754700	1.55285700
C	-1.55675600	-0.17390900	-0.80718600	H	1.79018100	-4.06300600	-0.96381300
H	-1.87870900	-1.12924900	-1.23656200	H	3.53704300	0.37840600	-0.98395600
C	-2.19812000	0.98857100	1.32461200	C	-1.70418800	5.96278400	0.13534200
C	-1.09998000	1.86618700	1.21650100	H	-2.31678000	6.80546100	0.44183300
H	-0.52986700	1.89138200	0.29644000	H	-2.05372700	4.97171000	0.41206900
C	-0.74852900	2.71784800	2.26646400	Br	2.04408300	4.99377100	-0.03062400
H	0.08826200	3.39846500	2.13147800	C	-0.56755300	6.14045500	-0.54255900
C	-1.47162800	2.71628000	3.45896700	H	-0.22445800	7.14353500	-0.78955200
H	-1.20146800	3.38340700	4.27238500	C	0.28165400	5.01623000	-1.01286400
C	-2.55181700	1.83954000	3.58256500	H	-0.16111100	4.04002200	-0.83065600
H	-3.12586000	1.81122300	4.50570300	H	0.58021300	5.10439500	-2.05655300
C	-2.91178400	0.98770400	2.54078200	H	2.47774200	-1.77688200	-5.94482400
H	-3.75764000	0.32438800	2.66042300	H	0.48958100	-0.69040800	6.23539200
C	-6.05774900	-0.97515400	0.39454600	H	4.32592700	-2.74757800	2.14855600
C	-7.38487900	-0.22496800	0.49391800	H	4.78254200	-2.94708300	-0.58740100
H	-7.59118800	0.02084900	1.53988300	C	4.87246200	0.31397600	3.66599000
H	-8.21105500	-0.84028400	0.12169700	H	4.77172400	0.57169000	4.72592200
H	-7.36156100	0.70832500	-0.07115200	H	5.19757300	-0.73028800	3.60944200
C	-6.05531200	-2.17045900	1.35873700	H	5.66684100	0.93877400	3.24369400
H	-5.11076600	-2.71921800	1.30415500	C	3.15342600	2.03028900	2.93485800
H	-6.87364000	-2.86520900	1.14610000	H	3.03987000	2.40452200	3.95796600
H	-6.17535100	-1.80182200	2.38146800	H	3.92993000	2.63159800	2.45059900

H	2.21186800	2.20183900	2.40843600	H	-0.55449400	5.12056300	-1.96747900
C	3.11553900	1.80646400	-2.51157900	C	0.62746400	3.33431400	-1.77347400
H	3.42770600	2.62944300	-1.86142400	C	-0.14054400	2.59877900	-2.86972900
H	3.40986500	2.06428200	-3.53516400	C	3.72514500	2.90759800	0.52499900
H	2.02393300	1.74606100	-2.48222600	C	2.12087100	-2.14233900	-1.63374300
C	5.29361100	0.53273800	-2.20075200	C	3.13701900	-2.94601800	-1.07411500
H	5.76623800	-0.37365600	-1.80756200	C	4.44606300	-2.37499600	-0.53454600
H	5.58270700	0.62967900	-3.25314500	C	2.93926400	-4.33374700	-1.08462700
H	5.70493100	1.39147600	-1.65958600	H	3.69924000	-4.97979800	-0.65826400
C	-1.09863900	-3.43393400	2.25306700	C	1.79371100	-4.89869200	-1.63457100
H	-1.43887800	-4.29993500	1.67458600	C	0.81863800	-4.08449000	-2.20304900
H	-1.67363000	-3.41083400	3.18502600	H	-0.06522300	-4.53700500	-2.63885600
H	-1.33683200	-2.52855100	1.68679200	C	0.96052700	-2.69221700	-2.22491400
C	0.75641400	-4.83818100	3.28165400	C	-0.07997300	-1.82961900	-2.93573300
H	1.83547300	-4.93813900	3.43910800	C	-1.34351500	0.35606300	0.73314100
H	0.27293100	-4.86885000	4.26389300	H	-1.21948600	0.75825300	-0.27669200
H	0.41352100	-5.71088500	2.71532100	C	-2.06070600	-2.02510500	1.28293100
C	2.47269900	-5.47597100	-2.41694700	C	-0.85661300	-2.71307000	1.06508700
H	2.11825300	-6.34547500	-1.85308700	H	-0.11004700	-2.28126900	0.40666200
H	2.37561700	-5.70909100	-3.48259800	C	-0.61383100	-3.94604800	1.66974100
H	3.53825100	-5.34402500	-2.20193600	H	0.32585900	-4.45528300	1.47496900
C	0.15476100	-4.43787000	-2.28427400	C	-1.57579300	-4.52955300	2.49779400
H	-0.05575500	-4.63506300	-3.34085200	H	-1.38919600	-5.49198700	2.96575300
H	-0.20419000	-5.29797900	-1.70861100	C	-2.78306800	-3.86178400	2.70889500
H	-0.42394700	-3.55939800	-1.98371800	H	-3.54384200	-4.30062300	3.34914000
L₃-TS18				C	-3.02394200	-2.62252200	2.11353300
Cu	0.68330700	-0.02532000	0.91547600	H	-3.96733300	-2.11586600	2.27983800
N	-2.31049800	-0.76769100	0.65797700	C	-5.62783200	-0.86066300	-0.91307500
N	2.30742000	-0.70661500	-1.70204100	C	-7.01647100	-1.08052800	-0.31216200
N	2.13488100	1.42352600	-1.45627400	H	-7.20428000	-2.15350200	-0.21145900
O	-4.64501400	-1.37181500	0.02011500	H	-7.79502900	-0.66022200	-0.95770200
O	-3.77625100	0.60160100	-0.78224700	H	-7.10358100	-0.62997200	0.67813700
B	-3.54591100	-0.52833400	-0.01320200	C	-5.49010800	-1.67321300	-2.20790000
C	1.72553400	0.23977300	-0.89439600	H	-4.50295200	-1.54098800	-2.65757800
C	3.05478500	-0.12428800	-2.72296500	H	-6.24886600	-1.39437300	-2.94571400
C	2.95075100	1.21420000	-2.56585100	H	-5.61159700	-2.73422300	-1.97260000
C	1.72109200	2.76216400	-1.08559800	C	-5.19604900	0.65226700	-1.06802300
C	2.47631200	3.48163000	-0.13574600	C	-5.39047800	1.23886900	-2.46569900
C	2.07981400	4.79674100	0.14149900	H	-5.03879300	2.27442500	-2.48056600
H	2.63646200	5.37518900	0.87107100	H	-6.44920200	1.23773200	-2.74630800
C	0.99606500	5.37868400	-0.50868400	H	-4.82998500	0.68138300	-3.21853700
C	0.28346200	4.65485500	-1.45943200	C	-5.83201700	1.57747700	-0.02097300
				H	-5.69696800	1.18603500	0.99050300
				H	-6.90171800	1.72118200	-0.20218100

H	-5.33842200	2.55187700	-0.06482800
C	-1.80085200	1.47089200	1.62367800
C	-1.19102600	2.74025400	1.52324600
H	-0.40274200	2.89076300	0.79248700
C	-1.57378700	3.80103300	2.33774700
H	-1.08182200	4.76370300	2.22271900
C	-2.58521100	3.63784100	3.29162100
H	-2.88482600	4.46590100	3.92771000
C	-3.20203200	2.39337100	3.40693500
H	-3.99186700	2.24365200	4.13934400
C	-2.81762400	1.32797400	2.58784900
H	-3.32135800	0.37241600	2.69059300
H	4.28508400	-1.31703900	-0.31262300
H	-0.04143400	-0.82954300	-2.49562500
H	0.10324800	1.53509900	-2.79834700
H	3.67328400	1.81873300	0.46046100
C	-0.26421200	-0.34737700	3.61189800
H	-1.23797100	-0.72624200	3.34295000
H	-0.13027200	0.72789800	3.58399500
Br	2.82611500	-0.34310400	2.10117500
C	0.68744500	-1.16685900	4.17640700
H	0.51527300	-2.24041900	4.18969000
C	1.95223700	-0.68507300	4.51391300
H	2.11106500	0.37585200	4.66390600
H	2.71968800	-1.34420000	4.90474700
H	3.36724600	2.03223900	-3.13033800
H	3.57629600	-0.71469100	-3.45788600
C	3.82559600	3.24955300	2.02098300
H	3.99340200	4.31877700	2.19254000
H	2.92089800	2.94860600	2.55510300
H	4.66821700	2.70999700	2.46381200
C	4.99147700	3.37222300	-0.22506500
H	5.88612000	2.93599500	0.23218700
H	4.97279500	3.07183400	-1.27764900
H	5.09228100	4.46306500	-0.19135400
C	5.56544300	-2.48765200	-1.59232300
H	5.76790700	-3.53666900	-1.83643800
H	5.30861400	-1.97508900	-2.52410700
H	6.49319400	-2.04587200	-1.21288000
C	4.89738200	-3.04082000	0.77741000
H	4.10988500	-2.99600700	1.53203700
H	5.18950000	-4.08628900	0.62877500
H	5.77083400	-2.51349900	1.17449000
C	-1.52145900	-2.33512400	-2.76216400

H	-1.69889700	-3.27078700	-3.30356000
H	-1.77090500	-2.49339100	-1.71047400
H	-2.21473100	-1.59183500	-3.16819500
C	0.26096400	-1.70178700	-4.43636500
H	1.25429800	-1.27223600	-4.59473900
H	0.23749000	-2.68343500	-4.92289100
H	-0.46833200	-1.05849700	-4.94112400
C	-1.66840100	2.72540000	-2.72872700
H	-2.15866000	2.11904400	-3.49768100
H	-2.02739700	2.37878500	-1.75719600
H	-2.00428900	3.75842200	-2.87104700
C	0.30947100	3.08721400	-4.26349500
H	0.08789000	4.15218900	-4.39386800
H	1.38421500	2.94964900	-4.41638900
H	-0.21613800	2.53561600	-5.05049100
H	1.66313000	-5.97723800	-1.62821200
H	0.71042800	6.40149800	-0.27923000

L₃-19

Cu	0.65614700	0.01636000	1.13355500
N	-2.22298200	-1.10995100	0.60553200
N	2.67027100	-0.33171900	-1.28944800
N	1.71615800	1.59324400	-1.43885600
O	-4.50892500	-1.92420400	0.03671100
O	-4.01235100	0.28115100	-0.38554900
B	-3.55263900	-0.92835600	0.10520200
C	1.63250900	0.40050700	-0.75669700
C	3.38761300	0.40053400	-2.23126300
C	2.78867300	1.60664100	-2.32566600
C	0.78075300	2.70326500	-1.43663400
C	1.11746000	3.89199400	-0.75487800
C	0.21944900	4.96564300	-0.84859000
H	0.44952000	5.89027600	-0.32971300
C	-0.95213700	4.87015000	-1.59002200
C	-1.24241500	3.69895100	-2.28429800
H	-2.14808100	3.64270700	-2.87776600
C	-0.37922100	2.59843300	-2.24220800
C	-0.65826300	1.38188600	-3.12399600
C	2.42047000	4.07415900	0.01639700
C	2.97872100	-1.73795500	-1.09659200
C	3.99635100	-2.10534300	-0.19096800
C	4.81542700	-1.08336500	0.58977500
C	4.31335000	-3.46791600	-0.09350800

H	5.08436400	-3.78070800	0.60248300	C	-3.20525200	1.78357700	3.61089300
C	3.67823300	-4.41902700	-0.88346100	H	-3.84277700	1.50518500	4.44593400
C	2.71514700	-4.02429500	-1.80860100	C	-2.74615500	0.79732800	2.73877200
H	2.24868800	-4.76999000	-2.44378900	H	-3.04458800	-0.23410400	2.89398100
C	2.34872500	-2.67971100	-1.94594200	H	4.25320100	-0.14821200	0.62452300
C	1.38101300	-2.27489200	-3.05882000	H	0.96696600	-1.29558800	-2.80437600
C	-1.38188100	0.09077500	0.71250900	H	-0.18042800	0.51512600	-2.65901600
H	-1.18029500	0.52223100	-0.26947500	H	2.84854700	3.08653000	0.19953300
C	-1.75465400	-2.43253400	0.87389700	C	0.08069100	-0.74811000	2.94200700
C	-0.54017000	-2.90039600	0.35705400	H	-0.94805700	-1.06839800	2.84295200
H	0.07032700	-2.23872100	-0.24675900	H	0.18162200	0.15459000	3.53957400
C	-0.10924400	-4.20355500	0.61821100	Br	2.52460100	1.21813600	2.22238900
H	0.83872200	-4.53801300	0.20901900	C	0.96758200	-1.85513100	3.30956300
C	-0.89005500	-5.06646100	1.38800600	H	0.72899900	-2.82430800	2.87710200
H	-0.55566200	-6.08043500	1.58709600	C	1.98914500	-1.76935800	4.18155600
C	-2.10499800	-4.60822300	1.90160900	H	2.28129000	-0.82120900	4.62157700
H	-2.72223400	-5.26349500	2.51019800	H	2.55610700	-2.64980200	4.47147400
C	-2.53162900	-3.30463500	1.65432900	H	4.24313900	-0.01096900	-2.74021000
H	-3.47418800	-2.95581100	2.05931200	H	3.01084300	2.46685900	-2.93486200
C	-5.61993700	-1.40378800	-0.73997500	H	-1.63555300	5.71326000	-1.63919900
C	-6.91453200	-1.98664700	-0.17625600	H	3.94649900	-5.46810500	-0.79349300
H	-6.91895400	-3.07150100	-0.31591000	C	2.20225400	4.71300400	1.39966000
H	-7.78697200	-1.57545900	-0.69509000	H	3.14552900	4.71397500	1.95420000
H	-7.01655600	-1.78438200	0.89147600	H	1.86156600	5.75255900	1.32649500
C	-5.41550300	-1.87363300	-2.18656300	H	1.47890800	4.14122500	1.98448500
H	-4.49401200	-1.46358200	-2.60940900	C	3.42744900	4.90637000	-0.80546600
H	-6.25221400	-1.58383700	-2.82949400	H	3.04399200	5.91456300	-1.00019000
H	-5.33499200	-2.96405000	-2.19569300	H	4.36998500	5.00601500	-0.25669100
C	-5.44945400	0.15389800	-0.56063400	H	3.65271200	4.44667300	-1.77340300
C	-5.87254500	0.99790200	-1.76095600	C	5.05923400	-1.49457900	2.05080300
H	-5.67336600	2.05326200	-1.55356600	H	5.72004700	-2.36567000	2.13359200
H	-6.94502800	0.88808900	-1.95356500	H	5.53511400	-0.66746600	2.58594200
H	-5.32668000	0.72185400	-2.66465100	H	4.11765600	-1.71544500	2.55792000
C	-6.10719600	0.69207500	0.71724100	C	6.15912600	-0.81933800	-0.12346600
H	-5.82753300	0.09482600	1.58908100	H	6.76685700	-1.73026200	-0.17502600
H	-7.19838200	0.70134900	0.63610100	H	6.01944900	-0.45592800	-1.14675400
H	-5.76193800	1.71453300	0.89012100	H	6.73199700	-0.06260800	0.42301000
C	-1.91964600	1.12130400	1.64441800	C	-2.15255600	1.04848300	-3.26895200
C	-1.58281600	2.47643000	1.45828200	H	-2.26129800	0.09208100	-3.79243600
H	-0.95957900	2.75806900	0.61841800	H	-2.65365600	0.96906900	-2.30143100
C	-2.04003800	3.45963000	2.33068800	H	-2.68007300	1.79882800	-3.86850000
H	-1.76422500	4.49604500	2.15712800	C	-0.02658000	1.57678800	-4.52028400
C	-2.85264100	3.12033300	3.41601400	H	-0.46921500	2.44335700	-5.02397600
H	-3.21098900	3.88781200	4.09611400	H	1.05348800	1.73488000	-4.46339500

H	-0.20505900	0.69574800	-5.14677900	C	1.94663700	-1.87199000	-1.72307200
C	0.19416200	-3.23933100	-3.23744800	C	0.78044000	-2.60602700	-1.46681000
H	0.51301400	-4.21050600	-3.63097300	H	0.07039300	-2.22466300	-0.73981500
H	-0.34068100	-3.41224500	-2.30113000	C	0.53924100	-3.80750100	-2.13566500
H	-0.51261700	-2.82005700	-3.96149600	H	-0.36562000	-4.36619000	-1.92156300
C	2.13587100	-2.12931900	-4.39885900	C	1.46027700	-4.30510700	-3.05903600
H	1.44844700	-1.81570500	-5.19220400	H	1.27037000	-5.24363100	-3.57160000
H	2.93782300	-1.38912000	-4.33808500	C	2.62948800	-3.58697000	-3.30935400
H	2.58108400	-3.08495600	-4.69699900	H	3.35965900	-3.96132700	-4.02145100

L₃-TS20

Cu	-0.75665000	0.44772900	-0.83368900	C	5.53536900	-1.04648300	0.54392400
N	2.23410200	-0.66249500	-1.01169500	C	6.87732500	-1.47040100	-0.05076300
N	-3.11288300	-0.44652700	0.96629000	H	6.94084300	-2.56227400	-0.07252100
N	-1.34304700	-0.13832600	2.15173000	H	7.70895300	-1.09495900	0.55490500
O	4.48056900	-1.49980700	-0.34673500	H	6.99793200	-1.10535800	-1.07205100
O	3.85887500	0.60487000	0.34977500	C	5.31457400	-1.74037200	1.89345200
B	3.49605200	-0.53028100	-0.34441800	H	4.35745200	-1.44792100	2.33144700
C	-1.76421800	-0.18089100	0.84419400	H	6.11252100	-1.50509100	2.60460100
C	-3.49663700	-0.55909600	2.29907300	H	5.30172000	-2.82254400	1.73572700
C	-2.38826000	-0.36238500	3.04348400	C	5.28739600	0.51344100	0.59344300
C	-0.00579200	0.03924300	2.68429700	C	5.59674600	1.17663900	1.93352600
C	0.42680100	1.33903900	3.02692600	H	5.37531400	2.24601100	1.87192200
C	1.63991300	1.45023200	3.71893800	H	6.65582600	1.06416100	2.18889900
H	2.00118000	2.43441100	3.99618200	H	4.99251700	0.75428000	2.73725700
C	2.37683600	0.32546700	4.07469200	C	5.98427400	1.27610900	-0.54238300
C	1.93100300	-0.94347800	3.71746000	H	5.77800300	0.82146500	-1.51502300
H	2.51085100	-1.81501500	4.00376000	H	7.06836800	1.31493900	-0.39762600
C	0.73476800	-1.11787200	3.01051800	H	5.59944500	2.29877600	-0.56844400
C	0.25495100	-2.52988000	2.68083100	C	2.04458500	1.63932300	-1.92815700
C	-0.39943300	2.58642600	2.72738800	C	1.86117000	2.99147900	-1.58729500
C	-4.10577800	-0.65849100	-0.07137800	H	1.22385300	3.24478200	-0.74887300
C	-4.97603600	0.40005000	-0.41349400	C	2.45406900	4.00421700	-2.33814300
C	-4.89870200	1.78638300	0.22276000	H	2.29727300	5.04071600	-2.05290300
C	-5.98835000	0.12403500	-1.34378100	C	3.24121900	3.69466800	-3.44974600
H	-6.66831300	0.91735400	-1.63387500	H	3.70386900	4.48622800	-4.03264400
C	-6.14232400	-1.14155300	-1.89783200	C	3.42666100	2.35710000	-3.80570700
C	-5.28767500	-2.17415600	-1.52215300	H	4.03414600	2.10156100	-4.66990200
H	-5.43116400	-3.16176700	-1.94691600	C	2.83505100	1.34219000	-3.05477500
C	-4.25985400	-1.96189600	-0.59509800	H	2.99662300	0.30817400	-3.33973700
C	-3.40608900	-3.13898900	-0.12719600	H	-3.87935600	1.93385500	0.58779500
C	1.43271000	0.56634200	-1.09325000	H	-2.44671600	-2.74081300	0.21693700
H	1.22473600	0.94256900	-0.08657700	H	-0.54118600	-2.44709200	1.93488900
				H	-1.04188700	2.37627200	1.86837500

H	-1.79373600	4.30761500	0.33173500	C	-1.96173200	3.85327000	-0.13063900
C	2.34843300	3.37380900	0.47439600	C	-3.10045600	3.38549400	0.51701200
H	1.85493500	2.79839900	1.26315100	C	-3.02159400	2.28963400	1.37253000
H	3.35201600	3.63482700	0.82695200	C	-1.80569000	1.63630700	1.60464200
H	1.79343900	4.30746200	0.33221200	C	-0.66923400	2.13538200	0.93311400
C	3.05795400	3.40855400	-1.96879900	H	-2.03776500	4.70425700	-0.80057200
H	4.09622300	3.66030700	-1.72801600	H	-3.92143900	1.92537400	1.85455800
H	3.05989400	2.86552000	-2.91977600	Cu	0.24936100	-0.41138900	-1.04891900
H	2.51479100	4.34819500	-2.11554600	H	3.49260700	0.96105600	2.60016300
C	3.05964000	-3.39844700	-1.98486300	H	1.30885200	2.66814800	2.82870600
H	3.06403200	-2.85138500	-2.93352000	C	2.00428300	-2.51197200	2.12842900
H	4.09718600	-3.65206700	-1.74293800	H	1.43522100	-1.60541200	2.35331000
H	2.51611100	-4.33705400	-2.13677100	C	4.31335600	0.82898700	-1.05126000
C	2.34538200	-3.37336300	0.45706800	H	3.56272200	1.48058400	-0.59493000
H	3.34824100	-3.63577200	0.81064700	C	-1.73343400	0.45950700	2.57461500
H	1.85030500	-2.80106700	1.24709700	H	-0.85501000	-0.13803400	2.30805200
H	1.79063900	-4.30640700	0.30997800	C	0.50750300	3.77139600	-0.67852100
C	-2.34527500	-3.37332000	0.45739700	H	1.36550600	3.14587900	-0.41511300
H	-1.85031300	-2.80093900	1.24743700	O	-4.33881500	-1.43826800	-0.75402900
H	-3.34814200	-3.63581900	0.81090000	C	-5.67558400	-1.61336600	-0.45189000
H	-1.79042700	-4.30631600	0.31041800	C	-5.83353800	-2.68652000	0.65230500
C	-3.05947500	-3.39862600	-1.98454000	H	-5.30201500	-2.37558200	1.55838800
H	-4.09704000	-3.65221400	-1.74266000	H	-6.88336000	-2.86943900	0.91559500
H	-3.06378500	-2.85167900	-2.93326200	H	-5.39285900	-3.63047800	0.31282300
H	-2.51593900	-4.33725800	-2.13629100	C	-6.28600000	-0.27985400	0.04388700
H	-6.15293300	-0.00032900	0.24393300	H	-6.16710900	0.48836700	-0.72838700
H	6.15293300	-0.00021200	0.24392000	H	-7.35324600	-0.36736700	0.28468600
L₃-22				H	-5.75898800	0.06104900	0.94194300
C	1.08801500	0.44628700	0.42195800	C	-6.44930100	-2.07595600	-1.71010400
C	1.50873000	1.85621900	2.14867500	H	-6.02706900	-3.01862300	-2.07704400
C	2.57649100	1.02487100	2.03554100	H	-7.51957100	-2.22989400	-1.51965100
N	2.30268300	0.16878400	0.97606600	H	-6.34641500	-1.32658000	-2.50360200
N	0.60805700	1.48857800	1.15787900	Li	-2.94894200	-1.39927500	-1.64445700
C	4.16454900	-0.56410700	-0.44753600	Br	-0.78486800	-1.41372200	-2.81275000
C	3.19266000	-0.87821400	0.52344700	H	-4.05763700	3.87017400	0.34890000
C	3.05614000	-2.16638000	1.07837800	H	5.57388300	-3.66364600	-0.67299200
C	3.93513200	-3.15754100	0.62436600	C	-1.53398000	0.96065600	4.02170600
C	4.90428700	-2.87820200	-0.33469800	H	-2.38280900	1.57750100	4.33631400
C	5.01604400	-1.59517200	-0.86268100	H	-1.46084500	0.11317500	4.71175800
H	3.85502700	-4.16258800	1.02688300	H	-0.62578000	1.56233800	4.12983900
H	5.77381200	-1.38868000	-1.61219700	C	-2.95844200	-0.46972900	2.49452600
C	-0.71785200	3.23789600	0.05796600	H	-3.84861600	0.00395200	2.92360300
				H	-3.20357400	-0.76796700	1.46933700
				H	-2.76777800	-1.37406400	3.08241600

C	1.00356100	-3.55774700	1.59903600	C	-2.82607100	0.88672200	-1.70075100
H	0.51265100	-3.21132500	0.68453200	C	-2.40578800	-0.37670600	-1.23956200
H	1.49834000	-4.50838100	1.37365900	H	-5.27763400	-1.51892300	0.15333600
H	0.22884000	-3.75446000	2.34742400	H	-4.51600300	2.21253300	-1.80335600
C	2.65520600	-2.97897500	3.44509400	Cu	-0.21000500	0.12854400	1.14596100
H	3.34061500	-2.22371200	3.84350500	H	1.39921100	-2.25579700	-3.07927600
H	1.88661400	-3.17275300	4.20050600	H	-1.30686300	-1.72121200	-3.41421000
H	3.22401800	-3.90444400	3.30673600	C	3.13895000	0.62696100	-2.22528300
C	5.69498900	1.43580700	-0.73724800	H	2.05879700	0.79886100	-2.26831900
H	5.87771100	1.47969200	0.34138500	C	1.59763600	-3.29809900	0.75091700
H	6.50335900	0.85012500	-1.18742900	H	0.63432000	-2.99716000	0.33180200
H	5.76278000	2.45402700	-1.13468200	C	-1.91231700	1.83776500	-2.46654900
C	4.04116400	0.81706100	-2.56828600	H	-0.89644800	1.43319000	-2.43335200
H	4.77137300	0.20018500	-3.10264400	C	-2.83129500	-2.65639300	-0.10259200
H	3.04460400	0.42272700	-2.78954900	H	-1.75293800	-2.74546000	-0.26037600
H	4.10440400	1.83264700	-2.97333700	O	-0.13143300	3.19519200	1.29721000
C	0.33214900	3.67830700	-2.20692100	C	0.98398200	4.02351500	1.20863900
H	0.12209000	2.65119500	-2.52072000	C	1.21247300	4.46912200	-0.25364800
H	-0.49222900	4.30879500	-2.55604800	H	0.35122400	5.04329900	-0.61044900
H	1.24322300	4.01272200	-2.71501600	H	2.10932100	5.09164600	-0.36451500
C	0.84317600	5.21170300	-0.24396500	H	1.31943900	3.59054900	-0.89855000
H	0.03224300	5.90410500	-0.49308700	C	0.77252800	5.28664100	2.07844700
H	1.01337800	5.27519000	0.83584400	H	0.63850100	4.99939500	3.12936500
H	1.74775000	5.56286900	-0.75186300	H	1.61656000	5.98648000	2.02639500
L₃-TS23				H	-0.13126600	5.81266200	1.75150200
C	-0.00317900	-0.59761200	-0.60939400	C	2.23998000	3.27520000	1.71457000
C	-0.62768200	-1.48041800	-2.61247700	H	2.38303200	2.35713400	1.13330900
C	0.69416400	-1.73726100	-2.45091100	H	3.15380300	3.87961800	1.64345500
N	1.06394600	-1.18780100	-1.22718500	H	2.10607400	2.98236800	2.76267400
N	-1.03836100	-0.78655400	-1.48151900	Li	-1.02275600	2.47688500	2.54318800
C	2.65494000	-2.30459200	0.27757300	Br	-0.95528600	0.22470300	3.36135000
C	2.39902300	-1.29971000	-0.67826600	C	1.44029200	-3.29656200	2.28299800
C	3.40276400	-0.42856700	-1.15396500	H	0.64033000	-3.98387000	2.57816800
C	4.69176300	-0.58565800	-0.63057700	H	2.35666000	-3.62378300	2.78558600
C	4.96988400	-1.55868200	0.32507000	H	1.18376400	-2.30117500	2.65661100
C	3.96182900	-2.40634700	0.77153400	C	1.90556800	-4.71504500	0.22514800
H	5.48768400	0.06752700	-0.97225200	H	1.97057600	-4.73298500	-0.86780500
H	4.19087900	-3.16635800	1.51209700	H	2.85610100	-5.08930100	0.62056500
C	-3.26764800	-1.27120400	-0.57059000	H	1.11924800	-5.41398500	0.52987500
C	-4.58832000	-0.85661100	-0.36094200	C	-3.50906100	-3.75897800	-0.94142900
C	-5.03073100	0.38833400	-0.79863700	H	-3.28962200	-3.64583100	-2.00829100
C	-4.15908700	1.24590300	-1.46262700	H	-3.15988200	-4.74825000	-0.62635600
				H	-4.59767300	-3.73561800	-0.82230900
				C	-3.08700600	-2.86818400	1.40184600

H	-4.15696500	-2.85357800	1.63596300	H	-7.42106300	3.41132700	0.28004400
H	-2.69823000	-3.84370300	1.71412400	H	-7.10430100	1.66322900	0.25421200
H	-2.59891700	-2.09532800	2.00221500	C	-4.94611600	4.14150100	-0.85771700
C	-1.86127500	3.23765900	-1.82780000	H	-3.87679700	4.35318800	-0.76836200
H	-1.47118300	3.20138000	-0.80502900	H	-5.50355700	5.02657800	-0.53586800
H	-1.19897500	3.88410100	-2.41356400	H	-5.16953200	3.96089800	-1.91310700
H	-2.84933800	3.71145500	-1.81621400	C	-4.79653100	2.93153700	1.43591500
C	-2.33104500	1.91103000	-3.94996300	C	-4.69272500	4.32402300	2.05636600
H	-2.32359600	0.92295600	-4.42337500	H	-4.28803700	4.24411700	3.06957800
H	-3.34077800	2.32204400	-4.05783800	H	-5.67792200	4.79804100	2.12205400
H	-1.64596200	2.55898200	-4.50695000	H	-4.03038700	4.97272600	1.48003900
C	3.59606200	0.12876600	-3.61320300	C	-5.56093000	1.98986700	2.37769000
H	3.38034400	0.88111300	-4.37934800	H	-5.64219700	0.98610800	1.95150300
H	4.67516400	-0.06011500	-3.62119400	H	-6.56756300	2.35996200	2.59602300
H	3.09571000	-0.79976000	-3.90426000	H	-5.00992000	1.90889100	3.31852600
C	3.80095600	1.97999800	-1.90765600	C	-1.62922800	-0.53347200	1.89596800
H	4.89295300	1.92468300	-1.97213400	C	-0.85995700	-0.62947300	3.07579900
H	3.47251000	2.73266600	-2.63143200	H	-0.06266100	0.09198400	3.24378000
H	3.53509600	2.33457000	-0.90961800	C	-1.09142200	-1.62264400	4.02214600
H	-6.05958500	0.69006300	-0.62361100	H	-0.47732800	-1.66012300	4.91892900
H	5.97663600	-1.65708300	0.72096100	C	-2.10357600	-2.56968600	3.82549900
L₃-17₂				H	-2.28362600	-3.34799700	4.56195300
N	-2.37016500	0.72317900	-0.15349300	C	-2.88200700	-2.48767200	2.67164200
O	-4.60517500	1.77709300	-0.60871000	H	-3.68130300	-3.20577900	2.50160800
O	-3.46246100	2.39314400	1.28776100	C	-2.65156600	-1.48411700	1.72418400
B	-3.45481200	1.60054700	0.14825300	H	-3.28022400	-1.43140000	0.84119500
C	-1.33311200	0.56276100	0.90518000	C	-1.85501700	-4.85002400	0.03122000
H	-1.34986600	1.49919700	1.47357400	C	-3.00527300	-5.78817500	0.09609000
C	-2.27440500	-0.03146700	-1.34562000	C	-4.17983100	-5.54677000	-0.49075700
C	-1.50349700	-1.21137200	-1.39629300	H	-5.01364700	-6.23584700	-0.39638200
H	-0.98713000	-1.54851900	-0.50656100	H	-4.34705500	-4.65009300	-1.08215000
C	-1.41999300	-1.97027500	-2.56666400	H	-2.85742900	-6.69760100	0.67550900
H	-0.83622800	-2.88785400	-2.55743800	H	-1.44647200	-4.60020600	1.00933200
C	-2.09148900	-1.57584800	-3.72405300	H	-2.07526100	-3.94194400	-0.52644000
H	-2.03012200	-2.17041600	-4.63086900	Cu	0.53926400	0.60354200	0.27797200
C	-2.84497200	-0.40052100	-3.68895000	N	3.03027600	1.29240800	-1.24958800
H	-3.36960500	-0.06431200	-4.58006300	N	3.44823300	0.66576800	0.76598500
C	-2.93635300	0.36246000	-2.52700000	C	2.41582700	0.83952800	-0.11454400
H	-3.53301500	1.26450100	-2.52590300	C	4.40607500	1.39978400	-1.07495200
C	-5.33373200	2.89635200	-0.04680100	C	4.67015400	1.00034300	0.19360500
C	-6.82902900	2.62009300	-0.19227400	C	3.31038200	0.23239600	2.13886100
H	-7.09538900	2.58589700	-1.25286400	C	3.27810600	-1.14787700	2.41953200
				C	3.19408500	-1.52961100	3.76469900
				H	3.16288600	-2.58554600	4.01446200

C	3.14251600	-0.58254500	4.78267300	H	1.80648300	3.30902900	4.38348300
C	3.16557000	0.77504500	4.47482400	C	4.47947700	3.41033200	3.48022000
H	3.11449100	1.50642500	5.27583100	H	4.46511300	3.33801900	4.57290500
C	3.24981600	1.21530900	3.14848600	H	5.41859200	2.96862000	3.13106800
C	3.25831000	2.71213400	2.85079200	H	4.48713700	4.47388400	3.21873100
C	3.31392100	-2.21883400	1.33400600	C	0.24300300	4.25125400	-1.05861300
C	2.36213300	1.62721600	-2.48799700	H	-0.30723900	4.72615100	-1.87815000
C	2.41562900	0.70190700	-3.55095800	H	-0.30764200	3.35595000	-0.75477200
C	3.13277000	-0.64120000	-3.44186400	H	0.25063200	4.95086400	-0.21570800
C	1.79463600	1.06237600	-4.75249700	C	2.47862400	5.17022200	-1.85172000
H	1.81429300	0.37138900	-5.58914500	H	2.48815000	5.87873300	-1.01635000
C	1.14392500	2.28482800	-4.88916000	H	3.51643200	4.93172200	-2.10685200
C	1.10798900	3.17859900	-3.82384700	H	2.03292000	5.67845800	-2.71345100
H	0.59861500	4.13018200	-3.94150500				
C	1.71918700	2.87653400	-2.60045000	L₃-TS18₂			
C	1.68590900	3.90353400	-1.47228500	N	2.28330700	-0.35665000	0.70377200
H	3.37971300	-0.80816300	-2.38934600	O	4.73403100	0.04569900	0.38933400
H	2.17170900	3.46498400	-0.59670000	O	3.54895800	-0.89755400	-1.34162600
H	3.33201400	2.84418300	1.76797900	B	3.49340300	-0.38187800	-0.05382500
H	3.34642800	-1.71745600	0.36272600	C	1.17931500	-1.20880200	0.20238800
Br	-0.29860200	-5.69077500	-0.93184200	H	1.12635200	-1.07055400	-0.88042700
H	5.05658800	1.74605400	-1.86151300	C	2.20416600	0.26044800	1.97949800
H	5.59740300	0.92305800	0.73810400	C	1.37657700	-0.25544600	2.99198500
H	3.07860200	-0.90267500	5.81880000	H	0.78398400	-1.14164900	2.80470700
H	0.66238600	2.54060000	-5.82859400	C	1.31216600	0.35682100	4.24532400
C	2.03515100	-3.07856100	1.36142400	H	0.65770000	-0.06563300	5.00252900
H	2.02270400	-3.78177300	0.52282300	C	2.07368600	1.49005600	4.52635500
H	1.96631200	-3.66270700	2.28542600	H	2.02710500	1.96007300	5.50446500
H	1.13945800	-2.45368600	1.29923000	C	2.89432200	2.01293600	3.52302100
C	4.57900000	-3.09229700	1.44182800	H	3.48830400	2.90313300	3.71469700
H	4.60770000	-3.64210500	2.38868000	C	2.95399700	1.41776300	2.26610000
H	4.60138900	-3.82815200	0.63117300	H	3.58702800	1.84468200	1.49918000
H	5.49101900	-2.48905900	1.37913100	C	5.65857800	-0.04160000	-0.72200300
C	2.24265900	-1.81556500	-3.88762400	C	7.01921700	-0.47910900	-0.18074100
H	2.03604200	-1.78359000	-4.96275100	H	7.41316100	0.29206300	0.48764800
H	2.74470100	-2.76658800	-3.68026700	H	7.73734400	-0.62107700	-0.99546800
H	1.28451400	-1.80860300	-3.36265900	H	6.94476100	-1.40825900	0.38658700
C	4.45637300	-0.62727900	-4.23372300	C	5.76568000	1.36291700	-1.33318400
H	4.27326900	-0.46455700	-5.30145000	H	4.79965400	1.70129700	-1.71720400
H	5.12897400	0.16542500	-3.88977100	H	6.49647100	1.39837800	-2.14711400
H	4.97843900	-1.58402400	-4.12499100	H	6.08476300	2.06262400	-0.55543500
C	1.94309200	3.37891900	3.29906600	C	4.94787300	-1.08542900	-1.67058600
H	1.94569300	4.44144100	3.03235100	C	5.13538600	-0.83746700	-3.16628600
H	1.07952500	2.90782000	2.82036300				

H	4.57368800	-1.58514000	-3.73400000	C	-1.57899900	3.58708400	1.66276600
H	6.19065200	-0.92421500	-3.44651000	C	0.73377500	4.46676400	1.09030500
H	4.77638000	0.14994700	-3.46150100	H	0.74681700	4.95853600	2.05648300
C	5.29444200	-2.54315900	-1.33403600	C	1.81051200	4.63250400	0.22466900
H	5.15488900	-2.74881300	-0.26938400	C	1.80491100	4.01745000	-1.02325900
H	6.32548300	-2.78942400	-1.60611100	H	2.64116500	4.16890900	-1.69903800
H	4.62232100	-3.20241100	-1.88989200	C	0.73325400	3.21161100	-1.42645800
C	1.35916100	-2.65485000	0.48399800	C	0.72350500	2.61925000	-2.83404700
C	0.61110300	-3.61952200	-0.23409700	H	-2.11253300	2.66217500	1.43027900
H	-0.08684400	-3.27995700	-0.99568300	H	-0.10214800	1.90604800	-2.89811500
C	0.75129000	-4.98589200	0.00182700	H	-0.93332100	-0.31186300	-2.94837500
H	0.16264800	-5.69215900	-0.57857400	H	-4.54543400	0.63158300	0.21623300
C	1.64216900	-5.44962100	0.97310300	Br	-2.37011200	0.00915600	2.47368600
H	1.75398800	-6.51377500	1.15874600	H	-2.48474500	3.80876600	-2.04440800
C	2.39543600	-4.51714600	1.69306700	H	-4.12737500	1.69120100	-2.75478100
H	3.10377200	-4.85810600	2.44453300	H	-4.65544100	-4.28914500	-2.25641300
C	2.25621000	-3.14897600	1.45909600	H	2.65351100	5.25054000	0.52104800
H	2.86065700	-2.44797100	2.02442400	C	-5.74790500	-0.83098900	1.18921600
C	-1.85082000	-2.49100400	1.70666700	H	-6.24266300	-0.07701600	1.81001100
C	-1.86043600	-3.01338000	3.04137200	H	-6.48555800	-1.61353500	0.98108500
C	-0.80835500	-3.67120900	3.57856300	H	-4.93323900	-1.25348000	1.78027200
H	-0.86475700	-4.08846400	4.57956800	C	-6.39900000	0.45720700	-0.87559400
H	0.11868400	-3.81280800	3.03186300	H	-7.11219500	-0.31419100	-1.18724300
H	-2.76929300	-2.88305700	3.62320000	H	-6.93380400	1.17504200	-0.24460600
H	-2.78712100	-2.36665000	1.17947500	H	-6.06918400	0.98323800	-1.77612500
H	-0.97559900	-2.68728000	1.10097900	C	-1.20364800	3.51464100	3.15186900
Cu	-0.68938900	-0.35814000	0.59607600	H	-0.77617200	4.45637400	3.51543500
N	-1.46429000	2.24418000	-0.94686100	H	-2.10162300	3.31495200	3.74490500
N	-2.74176400	0.60212300	-1.49024900	H	-0.48844700	2.71193500	3.34531500
C	-1.62647000	0.89879500	-0.74569700	C	-2.53842700	4.76866500	1.40348600
C	-2.45394200	2.76520300	-1.77705000	H	-2.05030900	5.72560200	1.62149400
C	-3.25558000	1.73169500	-2.12323300	H	-2.87994500	4.79780500	0.36361700
C	-3.27328100	-0.72746500	-1.69388900	H	-3.42320300	4.68752200	2.04431600
C	-4.43734500	-1.12075900	-0.99860600	C	-0.46639900	-2.15813200	-3.90332300
C	-4.91431800	-2.42021900	-1.22499100	H	0.36990600	-1.69907000	-4.44001300
H	-5.80545900	-2.75669900	-0.70577300	H	-0.05595100	-2.67254100	-3.03125100
C	-4.27086200	-3.28445400	-2.10450300	H	-0.90191700	-2.90975500	-4.57099000
C	-3.14697600	-2.85746600	-2.80712200	C	-2.04533500	-0.40340300	-4.78577000
H	-2.67148000	-3.53202600	-3.51061700	H	-2.61161500	-1.12675800	-5.38304400
C	-2.62969400	-1.56833800	-2.63237400	H	-2.71060400	0.43118200	-4.54856700
C	-1.48144600	-1.07180200	-3.51176000	H	-1.22994500	-0.01745500	-5.40741500
C	-5.22146100	-0.16896600	-0.09591800	C	2.01080700	1.84820200	-3.17336100
C	-0.33362000	3.04211100	-0.51839500	H	2.88242400	2.51165200	-3.20159200
C	-0.36844300	3.67701200	0.73962300	H	2.21263300	1.05059900	-2.45444500

H	1.92161300	1.39355700	-4.16654200	C	-1.04504600	-3.73144400	-0.30817400
C	0.46269700	3.72275000	-3.88125900	H	-0.32293300	-3.64988600	0.49983100
H	0.41334700	3.29407800	-4.88829900	C	-1.52798200	-4.98673200	-0.66914400
H	-0.47884200	4.24759200	-3.69080200	H	-1.18459000	-5.86849100	-0.13472700
H	1.26519900	4.46842200	-3.87224600	C	-2.45395300	-5.11337300	-1.70887700
L₃-19₂							
N	-1.89352000	-0.11439300	-0.79493900	C	-2.88652300	-3.96627300	-2.37577200
O	-4.31370800	0.39892400	-0.48323800	H	-3.60767700	-4.04705500	-3.18478900
O	-3.25376200	-0.83326300	1.14392900	C	-2.40098900	-2.70732000	-2.01516500
B	-3.12458700	-0.15339800	-0.05556400	H	-2.76188500	-1.82924500	-2.53882900
C	-0.97202200	-1.22850200	-0.51420000	C	1.38586000	-2.26539900	-1.97950700
H	-0.79313000	-1.26205500	0.55994700	C	1.25386900	-2.23415100	-3.43113300
C	-1.77999400	0.70525300	-1.95504400	C	0.43461100	-3.03662100	-4.13877700
C	-1.14295000	0.26144200	-3.12323000	H	0.39920900	-2.98517900	-5.22343800
H	-0.71200500	-0.72951200	-3.16908600	H	-0.20493600	-3.77199500	-3.66028400
C	-1.07069500	1.08520800	-4.24900500	H	1.88005500	-1.51317100	-3.95148300
H	-0.56722300	0.71565300	-5.13783200	H	2.41867300	-2.21112900	-1.63540700
C	-1.64167400	2.35634200	-4.24085800	H	0.82329800	-3.05576800	-1.49510100
H	-1.59177400	2.99051800	-5.12103800	Cu	0.95692100	-0.54706600	-0.95490500
C	-2.26873900	2.80602600	-3.07549100	N	1.50811300	1.95752000	1.11824000
H	-2.70381500	3.80116500	-3.04001800	N	2.46434100	0.07568800	1.55334500
C	-2.32583500	2.00103500	-1.94177100	C	1.48357200	0.63055800	0.76443200
H	-2.79206900	2.37391400	-1.03828900	C	2.50298900	2.21455100	2.05918000
C	-5.30755000	0.18539400	0.55096100	C	3.10016000	1.03400500	2.33662800
C	-6.63668200	-0.14446400	-0.12880800	C	2.74077300	-1.34178200	1.67931500
H	-6.97108800	0.71746700	-0.71312200	C	3.91886600	-1.87497800	1.11307500
H	-7.40988300	-0.37168000	0.61282100	C	4.14027300	-3.25217800	1.26340100
H	-6.54268800	-0.99364000	-0.80747400	H	5.03301100	-3.69329800	0.83296700
C	-5.43770200	1.50052500	1.33072800	C	3.24509000	-4.05978400	1.95397200
H	-4.49589000	1.77487500	1.81119400	C	2.11613900	-3.49996400	2.54802700
H	-6.21703500	1.44291100	2.09681400	H	1.44555600	-4.13412500	3.11747000
H	-5.70369900	2.29772100	0.63087600	C	1.84388200	-2.13136200	2.44172000
C	-4.67748300	-0.99695800	1.39269000	C	0.68450100	-1.51781600	3.22912500
C	-4.92301700	-0.92282900	2.89840300	C	4.98263000	-1.01313200	0.43574300
H	-4.41093200	-1.75315500	3.39350900	C	0.50542900	2.97105100	0.83353700
H	-5.99205500	-1.00691100	3.12063300	C	0.66927400	3.84575200	-0.25878800
H	-4.55164900	0.00862000	3.32829000	C	1.91251700	3.83162800	-1.13671500
C	-5.06095300	-2.38843600	0.87074500	C	-0.31905500	4.81962200	-0.45866000
H	-4.87870200	-2.47761900	-0.20298000	H	-0.22588400	5.49817100	-1.29970700
H	-6.11200500	-2.61870100	1.06985500	C	-1.40498900	4.93953500	0.40111700
H	-4.44188600	-3.13645500	1.37320900	C	-1.50782400	4.10551200	1.51082300
C	-1.46992500	-2.55928000	-0.96932400	H	-2.33214900	4.23901000	2.20485400
				C	-0.54919100	3.11730800	1.76424000
				C	-0.60903500	2.34295600	3.08061500

H	2.38579800	2.85352000	-1.03876600	N	2.44512700	-1.10614500	-0.64505400
H	0.12876200	1.53931100	3.04183900	O	4.76082300	-1.72664200	0.01476300
H	0.32570400	-0.64661200	2.67496000	O	4.02418800	0.37647000	0.57446100
H	4.52456500	-0.06000400	0.16171000	B	3.72356000	-0.81820900	-0.04602000
Br	2.83799900	0.52083100	-2.15578400	C	1.49523000	-0.00661900	-0.75559800
H	2.67270300	3.20456300	2.44922500	H	1.01550900	0.21753900	0.20502200
H	3.90085000	0.78512700	3.01297100	C	2.06938100	-2.48567000	-0.72485400
H	3.43587000	-5.12512400	2.04900600	C	0.93976000	-2.98587700	-0.06183200
H	-2.15917900	5.70113300	0.22238400	H	0.31162200	-2.30868000	0.50848300
C	5.52842800	-1.62616300	-0.86571900	C	0.59372300	-4.33330700	-0.17695300
H	6.23277700	-0.92764900	-1.32827800	H	-0.30445900	-4.69525900	0.31295000
H	6.06607300	-2.56449300	-0.68994800	C	1.38775200	-5.20863500	-0.91996800
H	4.72851400	-1.80269700	-1.58695000	H	1.11791600	-6.25734700	-1.00261900
C	6.14696500	-0.74174500	1.41391800	C	2.52795300	-4.72017500	-1.55913400
H	6.65458400	-1.67351900	1.68795500	H	3.15456200	-5.38776500	-2.14407700
H	6.88574700	-0.08017700	0.94933400	C	2.86206900	-3.36911400	-1.47186100
H	5.81023700	-0.26850000	2.34168500	H	3.74160400	-2.98850900	-1.97804700
C	1.60819700	4.02127700	-2.63151200	C	5.74890000	-1.18974600	0.93577700
H	1.24492100	5.03154700	-2.85558800	C	7.13614600	-1.59763200	0.44453000
H	2.52384200	3.86556600	-3.20997700	H	7.23921600	-2.68533200	0.49651400
H	0.86596800	3.30088600	-2.98204800	H	7.91728000	-1.15332700	1.07026800
C	2.91513400	4.89964000	-0.64882500	H	7.30182700	-1.29191100	-0.58982600
H	2.49302800	5.90834300	-0.72941700	C	5.46755000	-1.81745200	2.30773000
H	3.20342700	4.74301600	0.39625800	H	4.48026300	-1.53056800	2.68060100
H	3.82652000	4.86540600	-1.25532900	H	6.21702600	-1.52496600	3.04947400
C	-0.52318400	-2.44945000	3.42471700	H	5.48710500	-2.90612800	2.20809400
H	-1.33769500	-1.89101000	3.89591900	C	5.44521300	0.35817200	0.88180600
H	-0.90339600	-2.84135700	2.47859400	C	5.66410100	1.11188600	2.19148100
H	-0.28982600	-3.29553900	4.08034700	H	5.38920100	2.16215000	2.05824700
C	1.18907600	-1.02904700	4.60588400	H	6.71655100	1.07302100	2.49158100
H	1.56701300	-1.87036300	5.19750700	H	5.05550800	0.70364100	3.00019500
H	1.99498800	-0.29655400	4.50990600	C	6.16667600	1.07701700	-0.26576500
H	0.37381400	-0.56077800	5.16846800	H	6.03376300	0.54760000	-1.21295800
C	-1.97206200	1.68604100	3.34816500	H	7.23882600	1.17291100	-0.06856000
H	-2.77235000	2.42983200	3.42897800	H	5.74215400	2.07729500	-0.38174000
H	-2.23705500	0.97415800	2.56337800	C	2.00728300	1.20767200	-1.40528800
H	-1.94316400	1.14203700	4.29933700	C	1.52013100	2.47006500	-1.00232200
C	-0.21773100	3.26605900	4.25485200	H	0.76611400	2.52887500	-0.22571600
H	-0.19899000	2.70382100	5.19495800	C	2.00562100	3.64065900	-1.56886000
H	0.77096700	3.71115400	4.10759800	H	1.61536200	4.59705300	-1.23394800
H	-0.93585900	4.08551100	4.36699900	C	2.99438800	3.59000200	-2.55830700
				H	3.37742200	4.50741000	-2.99653900
				C	3.48472700	2.35393600	-2.97542600
				H	4.25200100	2.30219800	-3.74324200

L₃-TS20₂

C	2.98934900	1.17421800	-2.41700900	H	-3.96472900	-5.48551100	-0.97205500
H	3.39593300	0.22042300	-2.72969100	C	-2.39071700	4.97041000	-0.55449700
C	0.04745800	-1.03352500	-2.51677900	H	-3.28918500	5.13076000	-1.15867900
C	0.98133600	-0.84642800	-3.60362100	H	-2.06546200	5.95065100	-0.18697800
C	0.89688400	0.15010800	-4.50858600	H	-1.62647800	4.55339900	-1.21218600
H	1.61699500	0.24008700	-5.31629200	C	-3.79202800	4.62313600	1.51197100
H	0.10692800	0.89386500	-4.44579600	H	-4.09865900	3.95221700	2.32024400
H	1.80935100	-1.55187700	-3.66466900	H	-3.42299200	5.54596400	1.97413300
H	0.03955600	-2.01628200	-2.06617600	H	-4.68515700	4.87403100	0.92990800
H	-0.94530900	-0.63705400	-2.74791400	C	-5.76525600	-0.48682200	-1.51398700
C	-2.01542200	0.19734600	0.66900900	H	-6.45775200	-1.30399500	-1.74819000
C	-3.40841300	1.13467500	2.22270000	H	-5.89750900	-0.22620400	-0.45911800
C	-4.00371500	0.00240800	1.78397700	H	-6.05201800	0.38519600	-2.11086900
N	-3.14063800	-0.56841300	0.85213100	C	-4.13799400	-1.13283500	-3.33676400
N	-2.19936800	1.24281500	1.54150100	H	-3.13973500	-1.51331900	-3.57329100
C	-3.08540100	-2.99420100	1.18828200	H	-4.87610800	-1.84225700	-3.72941900
C	-3.35720800	-1.90277400	0.33196800	H	-4.26364900	-0.18784400	-3.87163900
C	-3.88628400	-2.07019600	-0.96531500	C	-1.42083500	-3.68837900	3.01750500
C	-4.08425200	-3.38363900	-1.41259600	H	-1.63871100	-4.75875900	2.93976000
C	-3.79841800	-4.47779600	-0.60153600	H	-0.55520400	-3.47537900	2.38582000
C	-3.31722600	-4.28255900	0.68950800	H	-1.13439900	-3.49285100	4.05660300
H	-4.47752200	-3.54891200	-2.40949800	C	-3.80842600	-3.11336600	3.60281000
H	-3.12530800	-5.14213000	1.32466600	H	-3.50588300	-2.93774100	4.64086900
C	-0.12387600	1.95054400	2.65146200	H	-4.67471600	-2.47937400	3.39199800
C	0.77205100	2.97535700	2.97535200	H	-4.13447100	-4.15578000	3.51932700
C	0.56181600	4.28065900	2.53995200	C	-0.66364700	0.41945500	4.58178300
C	-0.55507900	4.58645200	1.77150000	H	-1.73417500	0.61954100	4.47983900
C	-1.48330800	3.60201100	1.40230200	H	-0.54600900	-0.59180300	4.98743700
C	-1.23884500	2.28391300	1.84520400	H	-0.25786500	1.12552500	5.31495100
H	1.64259900	2.75137300	3.58169500	C	1.55470100	0.15611600	3.40140500
H	-0.71350700	5.60846500	1.44469800	H	2.13607700	0.32577100	2.49063100
Cu	-0.75766900	0.18182600	-0.91140600	H	2.03392300	0.71193300	4.21524500
H	-4.94441200	-0.45275700	2.04633600	H	1.62240100	-0.90634800	3.65892600
H	-3.72134900	1.86327600	2.95143200				
C	-4.30734600	-0.88585900	-1.82890800	L₃CuCl₃			
H	-3.67063200	-0.03092800	-1.58742400	C	0.00000000	-0.00001300	-0.17579200
C	-2.63651800	-2.82250800	2.64049100	C	0.67844500	0.00096100	-2.34872400
H	-2.34276300	-1.78012600	2.78739800	C	-0.67844700	0.00092300	-2.34872300
C	-2.71697700	3.99995000	0.59500700	N	-1.07680500	0.00038100	-1.01686900
H	-3.12134000	3.09591000	0.13225700	N	1.07680400	0.00039200	-1.01687100
C	0.07680500	0.55119600	3.23275100	C	-3.10594400	1.23666000	-0.39615200
H	-0.36899700	-0.16600300	2.53789100	C	-2.45858000	0.00025200	-0.58959600
Br	-1.86136900	1.91605800	-2.39964200	C	-3.10592900	-1.23626500	-0.39679300
H	1.26957100	5.06110300	2.80517200				

C	-4.44949900	-1.20587500	-0.00411700	H	-3.05065800	2.85420900	-2.66329600
C	-5.11660800	0.00003700	0.18990300	H	-4.09344900	3.65324400	-1.48005000
C	-4.44951800	1.20605500	-0.00349500	H	-2.51035400	4.34035900	-1.86229200
H	-4.97650700	-2.14121800	0.15750800	C	-2.35708600	3.37646600	0.73240500
H	-4.97653300	2.14131200	0.15860800	H	-3.36256700	3.63888600	1.07843800
C	3.10589600	1.23671300	-0.39607100	H	-1.86786200	2.80408800	1.52602200
C	4.44947100	1.20613400	-0.00343500	H	-1.80143000	4.30960400	0.58951000
C	5.11660900	0.00012700	0.18989700	C	2.35709900	3.37655500	0.73247800
C	4.44954600	-1.20579500	-0.00418800	H	1.86804000	2.80418400	1.52620200
C	3.10597700	-1.23621300	-0.39688200	H	3.36260800	3.63910300	1.07834100
C	2.45858000	0.00028900	-0.58959900	H	1.80133400	4.30963200	0.58962000
H	4.97645900	2.14139900	0.15871400	C	3.05363400	3.40107300	-1.71450000
H	4.97658200	-2.14113100	0.15739100	H	4.09328100	3.65323300	-1.48015600
Cu	0.00000100	-0.00087700	1.71508300	H	3.05032500	2.85421100	-2.66327100
H	-1.39033100	0.00133800	-3.15837900	H	2.51015100	4.34037900	-1.86221100
H	1.39032700	0.00123400	-3.15838100				
C	-2.40423300	-2.57730200	-0.58643300	L₃CuOtBu₃			
H	-1.36947500	-2.38099600	-0.88111900	O	-0.03548600	2.79610800	-1.27837500
C	-2.40425600	2.57780300	-0.58507000	C	1.00052800	3.65186200	-1.67699600
H	-1.36942800	2.38166500	-0.87962400	C	1.95304300	3.95074600	-0.49906200
C	2.40432100	-2.57726800	-0.58654300	H	1.38339900	4.36193900	0.34128000
H	1.36958500	-2.38098900	-0.88132200	H	2.43719200	3.02573000	-0.16364300
C	2.40416700	2.57783600	-0.58496700	H	2.73790700	4.66855100	-0.76978200
H	1.36932000	2.38167200	-0.87943300	C	0.34953800	4.96767500	-2.15238400
Cl	0.00000200	-0.00190400	3.84042600	H	1.09372300	5.70109500	-2.48597400
H	6.15822600	0.00006700	0.49792200	H	-0.33480900	4.76356700	-2.98211700
H	-6.15822500	-0.00005400	0.49792800	H	-0.23273600	5.40875400	-1.33688600
C	3.05419200	-3.40011400	-1.71612400	C	1.80357300	3.03010800	-2.84012800
H	3.05132800	-2.85288200	-2.66468400	H	2.27049100	2.09348900	-2.51299100
H	4.09371900	-3.65246500	-1.48145300	H	1.13174600	2.80298500	-3.67459600
H	2.51069500	-4.33931600	-1.86442800	H	2.59467500	3.69800200	-3.20467300
C	2.35678000	-3.37642400	0.73062100	C	-0.16941400	-0.53885500	0.24765400
H	3.36217300	-3.63893500	1.07684100	C	0.25210400	-2.56165200	1.21219000
H	1.86731700	-2.80435000	1.52431200	C	-1.09513200	-2.41842600	1.14799500
H	1.80118900	-4.30952400	0.58722300	N	-1.33680700	-1.18243400	0.55832300
C	-2.35680000	-3.37651900	0.73069800	N	0.80258300	-1.40961100	0.65968100
H	-1.86750800	-2.80445600	1.52450000	C	-3.28101700	-0.94437500	-0.92300100
H	-3.36222400	-3.63916100	1.07673900	C	-2.65924600	-0.65481600	0.30807600
H	-1.80109900	-4.30955700	0.58733400	C	-3.27958900	0.11796800	1.30986100
C	-3.05398800	-3.40011700	-1.71610500	C	-4.56972000	0.59571200	1.04956800
H	-4.09355000	-3.65244600	-1.48156600	C	-5.21131300	0.31947800	-0.15409500
H	-3.05098400	-2.85287500	-2.66465800	C	-4.57069100	-0.43979600	-1.12872100
H	-2.51049100	-4.33933100	-1.86434800	H	-5.07430500	1.19877300	1.79830500
C	-3.05383500	3.40106400	-1.71451900				

H	-5.07577300	-0.63952700	-2.06879900	C	-3.39037600	-0.07376300	3.83789500
C	2.88246200	-1.60936000	-0.62834100	H	-4.38102300	0.38789000	3.90759900
C	4.26186100	-1.38335400	-0.71257800	H	-3.53261300	-1.15777000	3.77514900
C	4.95349300	-0.75609600	0.31950400	H	-2.85794000	0.14524200	4.76962800
C	4.27653100	-0.34112700	1.46268000	C	-2.35551300	1.98080200	2.74828100
C	2.89718600	-0.53957100	1.60096400	H	-1.76067100	2.35198800	1.90836800
C	2.22304900	-1.17488000	0.53890700	H	-3.29996100	2.53527900	2.76321800
H	4.79931700	-1.70148800	-1.60078500	H	-1.82087000	2.20858900	3.67704700
H	4.82585700	0.14803400	2.26127600	H	6.02333400	-0.58920300	0.23237600
Cu	0.00943200	1.15367000	-0.54108800	H	-6.21128800	0.70284900	-0.33598600
H	-1.89599600	-3.06867000	1.46119800				
H	0.86558800	-3.36234300	1.59252700	L₃-4₃			
C	-2.59819900	0.46298200	2.63019900	C	-2.01371300	-0.13360000	0.49968300
H	-1.61828100	-0.02225800	2.64338200	C	-3.83588600	-0.97254400	1.59281800
C	-2.59864800	-1.74937500	-2.02451300	C	-3.73842300	0.33883200	1.91745200
H	-1.62716900	-2.08294800	-1.64887200	N	-2.63041400	0.83827600	1.24273400
C	2.19029400	-0.08147600	2.87321000	N	-2.78315500	-1.24598900	0.72922700
H	1.11902000	-0.26277900	2.75017200	C	-2.95285800	3.16144400	0.52876800
C	2.15880700	-2.30556100	-1.77669000	C	-2.26328800	2.23468500	1.33843700
H	1.09748400	-2.36815100	-1.52122000	C	-1.30960400	2.62338200	2.29904900
C	-2.32973000	-0.87257300	-3.26389100	C	-1.06294100	3.99499900	2.43989800
H	-1.79500900	-1.44857200	-4.02727400	C	-1.73156600	4.93378100	1.65998400
H	-3.26444300	-0.51555700	-3.70961500	C	-2.66208000	4.51874500	0.71157400
H	-1.72502800	0.00189000	-3.00546400	H	-0.33433900	4.32893800	3.17158300
C	-3.40265100	-3.01024900	-2.39483600	H	-3.17467000	5.25927600	0.10530500
H	-3.57099000	-3.65005100	-1.52225700	C	-3.26131500	-2.87279900	-1.04372300
H	-4.38150700	-2.75605400	-2.81511000	C	-3.09388100	-4.16480700	-1.55631000
H	-2.86386500	-3.59648100	-3.14687700	C	-2.28688100	-5.09688400	-0.90989500
C	2.66887800	-3.74747400	-1.96903800	C	-1.63404900	-4.75683500	0.27101300
H	3.72654100	-3.76500000	-2.25283400	C	-1.76782100	-3.48089900	0.83315300
H	2.56123400	-4.33613800	-1.05201300	C	-2.58086500	-2.55507700	0.15001600
H	2.10439300	-4.24881700	-2.76250600	H	-3.60255000	-4.44383000	-2.47386800
C	2.26254000	-1.49776800	-3.08455300	H	-1.01395600	-5.49466400	0.77034700
H	1.86211400	-0.48783400	-2.95803000	Cu	-0.41603700	-0.09441100	-0.52990000
H	3.30097100	-1.40989000	-3.42175100	H	-4.34340400	0.96270200	2.55495700
H	1.69661500	-1.99292500	-3.88115700	H	-4.54339800	-1.73017900	1.88796000
C	2.36748600	1.42966000	3.11401900	C	-0.57662900	1.62732400	3.19127500
H	1.80138900	1.73930200	3.99922000	H	-0.81211200	0.61983900	2.83756400
H	3.41708500	1.69108500	3.28615500	C	-4.00813600	2.74611400	-0.49412100
H	2.01041200	2.01110000	2.25943700	H	-4.01810900	1.65380000	-0.54834400
C	2.65755500	-0.89847000	4.09438600	C	-1.08932900	-3.16224000	2.16177100
H	2.49075200	-1.97082300	3.94798600	H	-1.21775800	-2.09490700	2.36156700
H	3.72562800	-0.75195200	4.28793500	C	-4.18287200	-1.88627400	-1.75672600
H	2.11122300	-0.58975200	4.99211700				

H	-4.05754600	-0.90649700	-1.28728200	H	5.84293200	0.44647700	2.53187600
O	1.14077700	-0.40931900	-1.60617700	C	6.24408900	-1.67432200	-0.18371300
C	1.26244400	-1.32042600	-2.72845000	H	6.88994000	-0.97172900	-0.71757800
C	0.35123300	-2.52076000	-2.45618400	H	6.87405700	-2.44289000	0.27580000
H	0.65964400	-3.03854800	-1.54346800	H	5.59181500	-2.15131600	-0.92022300
H	-0.68916500	-2.20399500	-2.33486900	C	4.50924600	-3.25056100	1.55629700
H	0.39071900	-3.23202400	-3.28880300	H	5.38147500	-3.48805600	2.17553100
C	2.71214300	-1.81132000	-2.88024400	H	3.63996100	-3.75105000	1.99363500
H	2.77384900	-2.50882300	-3.72316000	H	4.66841300	-3.66487300	0.55900600
H	3.38863400	-0.97616500	-3.07070100	C	3.85199200	-1.23426100	2.89529100
H	3.03337600	-2.33621700	-1.97661800	H	2.92916800	-1.73749100	3.19697700
C	0.81825900	-0.58396600	-4.00242500	H	4.61824200	-1.44026000	3.64969600
H	0.87119900	-1.24347800	-4.87689200	H	3.65962000	-0.15839000	2.87679200
H	-0.21610300	-0.23549600	-3.89895100	H	-2.16963500	-6.09327600	-1.32637900
H	1.46453800	0.27988700	-4.16615800	H	-1.52334500	5.99211400	1.78823000
B	2.29831600	0.55414900	-1.13198100	C	-1.06533100	1.73278300	4.65027400
O	1.60228800	1.63548600	-0.38976000	H	-0.85149000	2.72225000	5.06900600
O	2.88831500	1.20219400	-2.30285100	H	-2.14482400	1.56412600	4.72975400
C	2.90713300	2.61021500	-2.10342300	H	-0.55924900	0.98985900	5.27609400
C	1.66455200	2.85043400	-1.16087900	C	0.95224600	1.78965900	3.09640900
C	0.34985800	3.00877300	-1.94509300	H	1.44360800	1.00182500	3.67753800
H	-0.48255800	2.98386600	-1.23545400	H	1.29221400	1.72432400	2.05861000
H	0.30341500	3.96084600	-2.48606600	H	1.28089400	2.75068500	3.50800300
H	0.22088900	2.19325600	-2.66044000	C	0.42516900	-3.43679200	2.13196600
C	1.82333900	4.03641400	-0.20478000	H	0.86212200	-3.18943900	3.10566900
H	1.97746400	4.96963200	-0.75945400	H	0.64094900	-4.49335900	1.93888900
H	0.92109600	4.15242500	0.40209800	H	0.93711300	-2.83722000	1.37427000
H	2.67036800	3.89002700	0.46819400	C	-1.76967500	-3.93238000	3.31280200
C	2.81113200	3.30227900	-3.46895100	H	-2.84010800	-3.70833400	3.37111900
H	1.93773700	2.96704800	-4.03232000	H	-1.66402900	-5.01493500	3.18244500
H	2.76081500	4.39217900	-3.36210900	H	-1.31488100	-3.66509900	4.27255000
H	3.70172500	3.06363500	-4.05902600	C	-5.41505200	3.19874900	-0.05418900
C	4.24498300	3.00311800	-1.44461200	H	-5.67846000	2.79711400	0.92975900
H	4.35396400	4.08887800	-1.34416200	H	-5.47970000	4.29044900	0.00532600
H	4.35874000	2.53845200	-0.46368900	H	-6.16916000	2.85824900	-0.77190100
H	5.05878300	2.63348900	-2.07558400	C	-3.68323200	3.26280200	-1.90857500
B	3.40622700	-0.30190200	-0.09994500	H	-3.68911300	4.35697000	-1.95230300
C	5.42839700	-0.89709700	0.86126800	H	-2.70007100	2.92007900	-2.24173000
O	4.70331100	0.12938100	0.14808600	H	-4.43237100	2.90185000	-2.62164300
C	4.26567500	-1.74183800	1.50600200	C	-3.82792000	-1.71944700	-3.24597000
O	3.15615900	-1.47951100	0.60852900	H	-2.78868500	-1.40475200	-3.37602900
C	6.37642100	-0.22297600	1.85439900	H	-3.96985200	-2.64966600	-3.80600100
H	6.92029700	-0.96438000	2.45050500	H	-4.47256800	-0.96083800	-3.70239000
H	7.11124700	0.37385600	1.30609200	C	-5.66030100	-2.29549100	-1.58734800

H -5.85516300 -3.27176000 -2.04428400
H -5.94127300 -2.36175700 -0.53122200
H -6.31880300 -1.56347400 -2.06720300

L₃-TS₅

C 1.71817000 0.29936500 0.51675000
C 3.29275600 1.33768700 1.80907900
C 3.78232000 0.11848100 1.48371700
N 2.81986500 -0.49856600 0.69377200
N 2.04450600 1.44136600 1.20649200
C 3.71387300 -1.82004400 -1.16811400
C 3.07673300 -1.78822200 0.09006500
C 2.78864200 -2.95230900 0.82650300
C 3.14775900 -4.18083400 0.25658200
C 3.77236000 -4.24445600 -0.98520600
C 4.05030200 -3.07534800 -1.68813300
H 2.93692300 -5.09800500 0.79772800
H 4.54302200 -3.13646300 -2.65372800
C 1.77440500 3.73320700 0.39541100
C 1.11960000 4.96851100 0.48390400
C 0.05847100 5.15649900 1.36341100
C -0.37352800 4.10895900 2.17309500
C 0.24099900 2.85160000 2.12934600
C 1.31158600 2.69013500 1.22625300
H 1.45103700 5.79255100 -0.14065100
H -1.20348100 4.26998000 2.85140200
Cu -0.02605600 -0.18386500 -0.19932300
H 4.71159100 -0.36776300 1.73203900
H 3.70976800 2.13923100 2.39645200
C 2.13805300 -2.91683900 2.20461400
H 1.89776900 -1.87632200 2.44014900
C 4.08883800 -0.55743100 -1.94016500
H 3.65054800 0.30014100 -1.42298900
C -0.20286000 1.73596800 3.07105400
H 0.01193600 0.78141300 2.58191000
C 2.96808600 3.58612800 -0.54787100
H 3.29761900 2.54433200 -0.52441400
O -1.01851000 -2.11012900 -0.84872100
C -1.08373800 -2.86064900 -2.08104900
C 0.36991200 -3.17125300 -2.45163100
H 0.92128100 -2.24471300 -2.63428200
H 0.86698200 -3.70816500 -1.63959300
H 0.42031500 -3.78484800 -3.35802500

C -1.75382500 -2.07408900 -3.21836400
H -1.72341200 -2.66384100 -4.14241500
H -2.79607500 -1.85746800 -2.97762800
H -1.24111400 -1.12547000 -3.39026800
C -1.84116800 -4.17661100 -1.83896100
H -1.83336300 -4.79792600 -2.74234900
H -1.37080900 -4.74548100 -1.03055800
H -2.87909800 -3.97149400 -1.57251100
B -2.07733100 -1.28639500 -0.21661900
O -2.06757400 -1.40104500 1.23143400
O -3.43237000 -1.56039400 -0.64925800
C -4.27203900 -1.81714800 0.49383000
C -3.23675000 -2.11550300 1.65395700
C -2.89956700 -3.61132400 1.79792800
H -2.09084900 -3.71997300 2.52535300
H -3.75723200 -4.18930400 2.15910500
H -2.56102500 -4.04133100 0.85476300
C -3.65652700 -1.58591000 3.02993200
H -4.57449700 -2.07107500 3.38096900
H -2.86608100 -1.80159800 3.75644500
H -3.81501600 -0.50720300 3.01434200
C -5.19924700 -2.98858400 0.14598600
H -4.64408100 -3.88605800 -0.13065300
H -5.85520500 -3.23453800 0.98892400
H -5.83255100 -2.70975700 -0.70205100
C -5.13933400 -0.57963400 0.76991600
H -5.82126400 -0.74805400 1.60995000
H -4.52308300 0.29586500 0.97682000
H -5.74472600 -0.36703600 -0.11564300
B -1.97553800 0.59914000 -0.81607900
C -2.32711600 2.24917700 -2.42328400
O -1.79954000 0.92443400 -2.15813600
C -3.26176900 2.50119200 -1.17720300
O -2.71894000 1.58710800 -0.18084700
C -3.03713700 2.21721100 -3.77818300
H -3.49409300 3.18617600 -4.00741700
H -2.30913300 1.99364600 -4.56376700
H -3.81048900 1.44846200 -3.81043800
C -1.12844100 3.20232900 -2.49615800
H -0.44681400 2.84936400 -3.27579400
H -1.43549100 4.22282600 -2.74717600
H -0.58294000 3.22563600 -1.55060900
C -3.21315300 3.91774200 -0.60421600
H -3.57167300 4.64888400 -1.33738600

H	-3.86428700	3.97596800	0.27335300	C	3.42830400	0.83449000	0.17209400
H	-2.20565300	4.19626600	-0.29306900	C	3.49486200	-0.52047600	0.14392800
C	-4.72089000	2.10241500	-1.43261600	N	2.18406900	-0.97916400	0.05989900
H	-5.28297700	2.17362900	-0.49820200	N	2.07893000	1.16577600	0.10443900
H	-5.19135900	2.76652300	-2.16466800	C	1.74155200	-2.99815600	-1.26426600
H	-4.79267900	1.07334100	-1.79045400	C	1.82248900	-2.37720300	-0.00200700
H	4.04457400	-5.20791000	-1.40678700	C	1.57324500	-3.06643900	1.20115500
H	-0.43403500	6.12319500	1.42062000	C	1.23796500	-4.42304300	1.11047000
C	4.15370200	4.45313200	-0.07705000	C	1.15254800	-5.06319200	-0.12225400
H	3.90052900	5.51844000	-0.10013500	C	1.40055000	-4.35581700	-1.29501300
H	4.45299700	4.20750500	0.94693000	H	1.03447700	-4.98181700	2.01892800
H	5.02129500	4.30207800	-0.72834500	H	1.32120900	-4.86263000	-2.25184900
C	2.60677300	3.90671800	-2.00994600	C	1.41007500	3.17797100	-1.13321400
H	2.28158900	4.94537700	-2.13114200	C	0.93275200	4.49400800	-1.10550400
H	3.48075500	3.75887200	-2.65374000	C	0.63981900	5.12872200	0.09803900
H	1.80420000	3.25917100	-2.37064400	C	0.81717900	4.45611700	1.30366400
C	3.52015900	-0.55134000	-3.37124300	C	1.29104700	3.13896600	1.33578600
H	3.78008400	0.38621000	-3.87443400	C	1.58122200	2.52291700	0.10238100
H	3.92379900	-1.37121800	-3.97456500	H	0.78295300	5.02487600	-2.04076900
H	2.43061700	-0.64277500	-3.36590900	H	0.57690400	4.95737400	2.23644100
C	5.61814700	-0.35763300	-1.95462900	Cu	-0.67693700	-0.03830800	-0.04170900
H	6.02657700	-0.30892100	-0.93998100	H	4.33728600	-1.19283400	0.17417700
H	6.12069600	-1.17963400	-2.47564600	H	4.20089800	1.58428800	0.23173300
H	5.87891200	0.57342500	-2.46960700	C	1.63398900	-2.39165200	2.56760900
C	0.81301000	-3.69845200	2.22117800	H	1.94565300	-1.35389000	2.41968100
H	0.34922600	-3.62372600	3.21065700	C	1.97704700	-2.24701100	-2.57104100
H	0.11274100	-3.29671100	1.48547000	H	2.30285000	-1.23230400	-2.32548500
H	0.97037900	-4.76227100	2.00998300	C	1.44748600	2.42212900	2.67309600
C	3.10728200	-3.42459400	3.29079700	H	1.88392200	1.43788500	2.48149100
H	3.37588200	-4.47411400	3.12840000	C	1.69463500	2.50304700	-2.47147400
H	4.03575500	-2.84350900	3.30929700	H	2.12107500	1.51655300	-2.26907200
H	2.64190100	-3.35008600	4.27935400	B	-2.66944700	-0.11905100	-0.08455000
C	-1.71276400	1.75136200	3.35417400	C	-4.85052300	-0.60915400	0.55166800
H	-2.01091300	2.62007700	3.95279800	O	-3.48309300	-0.44420300	1.00451400
H	-2.28402100	1.74624500	2.42266100	C	-4.85944500	0.21300800	-0.78762400
H	-1.98334900	0.85798700	3.92304900	O	-3.47034100	0.14722000	-1.19814900
C	0.60179900	1.78961100	4.38746700	C	-5.79018200	-0.09589600	1.64344400
H	0.30264300	0.96912200	5.04847000	H	-6.83771900	-0.15660000	1.32647500
H	1.67934000	1.70431400	4.21385600	H	-5.67422100	-0.70869700	2.54271700
H	0.42114700	2.73214800	4.91710100	H	-5.56664500	0.93798600	1.91289400
				C	-5.07322000	-2.11523700	0.34160600
				H	-4.84819600	-2.63833100	1.27561000
				H	-6.10686200	-2.34238900	0.05960900
				H	-4.40552300	-2.50525300	-0.43135900
L₃-6₃							
C	1.28821800	0.05300000	0.03446100				

C	-5.72588100	-0.36539600	-1.90706000				
H	-6.78373500	-0.38487100	-1.62069600	C	1.67279400	1.16855300	0.22490100
H	-5.63028800	0.25750700	-2.80173500	C	2.51946100	3.19894900	0.82944900
H	-5.41763000	-1.37865900	-2.17120600	C	3.49906100	2.28006500	1.02257800
C	-5.19571900	1.69904700	-0.58628600	N	2.96601700	1.04971600	0.65404100
H	-4.97944000	2.23786300	-1.51337100	N	1.41538300	2.50577700	0.34584700
H	-6.25127600	1.85181000	-0.33715500	C	4.33982200	-0.68725900	-0.41768500
H	-4.58202200	2.13503500	0.20654300	C	3.69445900	-0.19671300	0.73574100
H	0.88709000	-6.11554900	-0.16957500	C	3.74898800	-0.86089100	1.97804200
H	0.26806900	6.14948100	0.09624100	C	4.48845100	-2.04816100	2.04425200
C	0.66923200	-2.12248600	-3.37781700	C	5.13867100	-2.55441300	0.92281800
H	0.28867300	-3.10679100	-3.67186000	C	5.06161100	-1.88063200	-0.29252500
H	-0.10857200	-1.62126000	-2.79369800	H	4.55138300	-2.58359600	2.98680000
H	0.83947700	-1.54317400	-4.29203600	H	5.57029000	-2.28585700	-1.16147500
C	3.09505400	-2.89172400	-3.41256200	C	-0.06800400	3.55357500	-1.30761500
H	4.03416800	-2.95360800	-2.85276000	C	-1.30160900	4.15095000	-1.59536800
H	2.83002300	-3.90552100	-3.73083100	C	-2.26977600	4.31473300	-0.61002200
H	3.27705200	-2.30089000	-4.31661400	C	-2.02037600	3.89303200	0.69292400
C	0.39168300	2.28249900	-3.26516500	C	-0.80541500	3.29100900	1.03945000
H	0.60116700	1.75429700	-4.20193200	C	0.15211500	3.12769700	0.01679500
H	-0.32608700	1.69021400	-2.68954400	H	-1.50672400	4.48496600	-2.60801100
H	-0.08490400	3.23577300	-3.51850600	H	-2.78719100	4.02082700	1.44946800
C	2.73145100	3.28503900	-3.30024800	Cu	0.58348600	-0.23713500	-0.62139300
H	2.36387400	4.27921800	-3.57540800	H	4.50943900	2.38196100	1.38470800
H	3.66861300	3.41750300	-2.74949900	H	2.50444100	4.26559000	0.98554900
H	2.95623700	2.74935100	-4.22875200	C	3.05294100	-0.33294200	3.22970400
C	2.40924200	3.17070600	3.61556800	H	2.45982500	0.54064200	2.94580100
H	3.39440200	3.30771900	3.15745900	C	4.30961100	0.04270500	-1.75723100
H	2.02589300	4.16135800	3.88189200	H	3.56703000	0.84211100	-1.68917500
H	2.54268200	2.60855400	4.54599000	C	-0.53923200	2.87655100	2.48414600
C	0.07670100	2.18911800	3.33874700	H	0.32551100	2.20638100	2.48667200
H	-0.41615200	3.13801300	3.57743300	C	0.96986100	3.39254800	-2.41414600
H	-0.58814600	1.61859800	2.68287800	H	1.85396100	2.91397700	-1.98373400
H	0.19802100	1.63161700	4.27406500	C	-3.62260700	-0.81520800	0.80895000
C	0.24284600	-2.35703200	3.23085700	N	-3.66366600	-1.03017900	2.07541000
H	-0.48687700	-1.84985200	2.59249000	C	-2.93339200	-2.09613600	2.63713300
H	-0.12885600	-3.36794900	3.43087200	C	-3.42583900	-2.63458800	3.83797800
H	0.29144900	-1.82478100	4.18727800	C	-1.74215700	-2.61947800	2.09652800
C	2.67779300	-3.05579300	3.48599300	C	-2.77346400	-3.69392700	4.46478100
H	2.41646300	-4.09582500	3.70843700	H	-4.33361800	-2.20830000	4.25377400
H	3.67330200	-3.05362200	3.02974500	C	-1.08903000	-3.67261900	2.73607700
H	2.74006900	-2.52045600	4.43947200	H	-1.32291200	-2.19879300	1.18716400
				C	-1.60075800	-4.21907300	3.91656000
				H	-3.17658800	-4.10548100	5.38621200

L₃-7₃

H	-0.17047200	-4.06638600	2.30868600	H	-2.59525400	2.73590100	3.24446700
H	-1.08495600	-5.03887500	4.40848300	H	-2.00452400	1.23992900	2.51258000
B	-0.30615700	-1.66771800	-1.69851200	H	-1.42463300	1.74139700	4.10779000
C	-1.78831000	-3.28465000	-2.49698600	C	-0.17773000	4.10789100	3.34128300
O	-1.65110700	-2.07004800	-1.70598500	H	0.69691000	4.63465400	2.94586300
C	-0.52786900	-3.21208400	-3.43035500	H	-1.00980200	4.82000000	3.37038500
O	0.39938900	-2.43234500	-2.63100700	H	0.04488000	3.80784200	4.37104300
C	-1.75096400	-4.46618700	-1.51628300	C	3.87645000	-0.87430500	-2.91675700
H	-2.53541300	-4.33465600	-0.76587000	H	3.80677400	-0.29100700	-3.84170100
H	-1.91813900	-5.42169800	-2.02415100	H	4.60368400	-1.67460000	-3.09314300
H	-0.79279300	-4.51307500	-0.99206800	H	2.90127900	-1.33257300	-2.72879600
C	-3.13707500	-3.25099200	-3.21503000	C	5.67429600	0.70069800	-2.04753700
H	-3.25092700	-2.34937600	-3.82000900	H	5.96136900	1.39915000	-1.25422400
H	-3.25774300	-4.12400200	-3.86624000	H	6.46665600	-0.05137100	-2.13092300
H	-3.94689000	-3.26755100	-2.47929200	H	5.63912500	1.25569000	-2.99133400
C	0.12123600	-4.55690500	-3.75765500	C	1.41601100	4.75943800	-2.96955700
H	-0.56682500	-5.20345800	-4.31402200	H	0.58471000	5.29227300	-3.44353300
H	1.00704100	-4.39358600	-4.37901800	H	1.81437000	5.40299900	-2.17816000
H	0.43766900	-5.08027000	-2.85393500	H	2.19815300	4.62726200	-3.72494900
C	-0.77316600	-2.42396600	-4.72629800	C	0.45864400	2.47175800	-3.53871000
H	-1.23709000	-1.45665200	-4.51552900	H	0.18810800	1.48687200	-3.14564200
H	0.18883100	-2.23754400	-5.21238300	H	-0.42222800	2.89517500	-4.03353700
H	-1.41123600	-2.97346300	-5.42627900	H	1.23448600	2.33548900	-4.30029100
C	-4.35439000	0.29789800	0.18808700	H	-3.22637900	4.76466500	-0.85770700
C	-5.20345000	1.13529100	0.93352300	H	5.70572600	-3.47823000	0.99548700
C	-4.21212000	0.51677000	-1.19219400				
C	-5.89678100	2.16570100	0.30721700	L₃-TS8₃			
H	-5.30730800	0.94888300	1.99743800	C	0.55928600	-1.44692800	-0.16269000
C	-4.90661900	1.55378200	-1.81581100	C	1.84496400	-3.30840000	-0.47894100
H	-3.54829400	-0.12920000	-1.76065000	C	0.55708900	-3.71687600	-0.41069600
C	-5.75150700	2.37771800	-1.06971000	N	-0.21834500	-2.57476000	-0.22769300
H	-6.55895600	2.80370500	0.88661700	N	1.83574000	-1.92584800	-0.32396500
H	-4.79137900	1.71636800	-2.88386100	C	-2.26668000	-2.80437500	-1.54035100
H	-6.30044900	3.17931800	-1.55688800	C	-1.66238700	-2.63342800	-0.27677300
H	-3.05259000	-1.44491000	0.11517200	C	-2.40020200	-2.60476000	0.92433700
C	2.07754700	-1.36450000	3.82620000	C	-3.78945900	-2.75388600	0.82518100
H	2.60012200	-2.26180900	4.17454100	C	-4.41302300	-2.93095100	-0.40714200
H	1.55408400	-0.93475300	4.68680900	C	-3.65891100	-2.95290700	-1.57592700
H	1.32553200	-1.67388400	3.09551600	H	-4.38973700	-2.73575100	1.72779600
C	4.08014700	0.12986500	4.28246700	H	-4.15622100	-3.08645100	-2.53196700
H	4.70661700	-0.70318400	4.61930100	C	3.43113700	-0.60020400	-1.63931400
H	4.74464500	0.90362900	3.88381200	C	4.67684400	0.03501100	-1.71245900
H	3.57018900	0.54039600	5.16056100	C	5.51158400	0.11469300	-0.60253100
C	-1.71091200	2.10303900	3.11449400				

C	5.10701300	-0.42289200	0.61594700	H	-2.42785900	3.10855500	-4.12232500
C	3.86941300	-1.06406200	0.75075900	H	-2.99621400	1.48290200	-3.72600000
C	3.05514500	-1.15121800	-0.39701400	C	-2.74404800	4.32489800	-1.75884100
H	4.99645800	0.47004200	-2.65411100	H	-2.45075500	4.56409700	-0.73299500
H	5.76210900	-0.34518400	1.47767200	H	-2.02972300	4.80165700	-2.43592500
Cu	0.10798400	0.36453300	0.24589700	H	-3.73017200	4.76195000	-1.94308800
H	0.11441600	-4.69662600	-0.48622700	C	1.22741800	3.03356100	0.05570600
H	2.76076800	-3.85746200	-0.62443000	C	2.54886600	2.69108800	0.37775000
C	-1.72785200	-2.48112800	2.28908700	C	1.01817400	4.06488600	-0.87381100
H	-0.79580700	-1.92438400	2.15368000	C	3.62436400	3.34461900	-0.22659000
C	-1.47370800	-2.84214800	-2.84678800	H	2.71223600	1.92854400	1.12863400
H	-0.40961500	-2.78598400	-2.60520400	C	2.09172900	4.72223600	-1.47246300
C	3.46295800	-1.65941100	2.09564600	H	0.00694500	4.35595000	-1.12975800
H	2.39386800	-1.88702000	2.05247400	C	3.40345200	4.36171700	-1.15533300
C	2.56174200	-0.69890100	-2.88941900	H	4.63836800	3.06139000	0.04104600
H	1.59255100	-1.11121100	-2.59740200	H	1.90254700	5.52387000	-2.18178100
C	0.06101200	2.37052400	0.77145200	H	4.24106000	4.87717900	-1.61773200
N	0.44990100	1.60676000	1.88809000	H	-0.72923800	3.11524900	0.94800900
C	-0.36957600	1.54674400	3.00878100	C	-2.56714500	-1.69933500	3.31202000
C	0.13163100	0.85386800	4.14218800	H	-3.46418600	-2.25167100	3.61512700
C	-1.64034400	2.15992300	3.15845900	H	-1.97431800	-1.51535800	4.21121400
C	-0.56712900	0.80386200	5.34139400	H	-2.86992400	-0.72410500	2.92268800
H	1.10331800	0.37934700	4.05525400	C	-1.36560300	-3.87788000	2.83891700
C	-2.33331700	2.10482800	4.36886100	H	-2.26685000	-4.48397700	2.98615000
H	-2.10497900	2.66403500	2.31924300	H	-0.70049700	-4.42514600	2.16314500
C	-1.81131500	1.43385200	5.47502400	H	-0.86061200	-3.78472000	3.80619600
H	-0.13269000	0.27618200	6.18818400	C	3.66201900	-0.66460300	3.25329900
H	-3.30257400	2.59428900	4.44146600	H	4.71978700	-0.43412300	3.41971800
H	-2.35506100	1.40052000	6.41454700	H	3.12984200	0.27054000	3.06194100
B	-1.31403000	1.75781800	-0.53449700	H	3.27436500	-1.09381400	4.18327800
C	-3.58080900	1.99152300	-0.94948400	C	4.21738200	-2.97632000	2.37140200
O	-2.57012000	1.61202100	0.02835000	H	4.03536500	-3.72134800	1.59025500
C	-2.74307900	2.81102300	-2.01175700	H	5.29844700	-2.80588700	2.42365300
O	-1.37913400	2.33953400	-1.78259600	H	3.89867200	-3.40648600	3.32689900
C	-4.18669400	0.69819700	-1.50037300	C	-1.79126800	-1.63032200	-3.74409900
H	-4.59802800	0.11805200	-0.67110800	H	-1.20475700	-1.67895800	-4.66832000
H	-4.99216400	0.90331500	-2.21287300	H	-2.85009300	-1.60526700	-4.02459300
H	-3.43265900	0.08095600	-1.99022500	H	-1.54749300	-0.69105600	-3.23890500
C	-4.66213700	2.79028600	-0.21892900	C	-1.69383100	-4.16524600	-3.60593700
H	-4.24884000	3.65342700	0.30566100	H	-1.44623200	-5.03094500	-2.98304000
H	-5.43052400	3.14105800	-0.91650500	H	-2.73349000	-4.27809900	-3.93071600
H	-5.14610700	2.14836200	0.52227300	H	-1.06319000	-4.19986300	-4.50067800
C	-3.09904500	2.53915000	-3.47289700	C	3.18437700	-1.66253900	-3.91969400
H	-4.12595300	2.85196200	-3.69018200	H	4.16025200	-1.30195100	-4.26281400

H	3.32891300	-2.66292400	-3.49809600	N	1.05068700	-0.99732900	1.50646900
H	2.53582200	-1.75536500	-4.79770900	C	1.39265100	-0.50666100	2.75236300
C	2.28837600	0.68312700	-3.51218900	C	0.57907800	0.49903000	3.34966900
H	1.83288600	1.36351500	-2.78802200	C	2.50927600	-0.93110500	3.52519700
H	3.20671500	1.15050400	-3.88302700	C	0.84448600	1.02008600	4.60943000
H	1.60507200	0.58077600	-4.36210200	H	-0.29003200	0.84912100	2.79608600
H	6.47864600	0.60293500	-0.68512900	C	2.75829300	-0.40394000	4.79275600
H	-5.49176600	-3.05145000	-0.45541300	H	3.21398000	-1.64498600	3.11938200
L₃-9₃				C	1.93866100	0.57244800	5.35906200
C	-1.57720600	0.93383500	-0.42140800	H	0.18030100	1.78010900	5.01665300
C	-3.57920300	1.80387500	-1.08156100	H	3.62649500	-0.76373200	5.34174200
C	-2.61542700	2.68077200	-1.45705500	H	2.14414000	0.97528100	6.34618300
N	-1.40320300	2.13896000	-1.04691300	B	3.06971400	-1.65432900	0.23055200
N	-2.93288600	0.74520300	-0.45478100	C	5.17496300	-0.76995300	0.07312700
C	0.55109800	2.42807300	-2.49964100	O	4.29583300	-1.61805100	0.85705000
C	-0.12886100	2.76912300	-1.31274200	C	4.52349800	-0.86212900	-1.35700400
C	0.35489000	3.73423100	-0.40622500	O	3.12280100	-1.11688000	-1.04248700
C	1.56499000	4.36379200	-0.72289100	C	5.09772300	0.63526100	0.68635400
C	2.25805100	4.04930600	-1.88834900	H	5.35853300	0.57230700	1.74581400
C	1.75477800	3.09231500	-2.76511300	H	5.78937500	1.32860700	0.19755800
H	1.96755000	5.11229500	-0.04811800	H	4.08511900	1.04194200	0.61865400
H	2.30309300	2.85741900	-3.67199600	C	6.59790500	-1.31535500	0.18050800
C	-3.92662800	-1.45108900	-0.89201500	H	6.65305300	-2.36633100	-0.10989100
C	-4.62907700	-2.56415900	-0.41420200	H	7.28622200	-0.74096900	-0.44888500
C	-5.01679400	-2.65170200	0.91917400	H	6.94107800	-1.23491400	1.21584700
C	-4.71653900	-1.62015000	1.80458800	C	4.62275800	0.41266900	-2.19136200
C	-4.01883900	-0.48161100	1.38337500	H	5.67131400	0.68165200	-2.36000900
C	-3.62823400	-0.42743900	0.02975800	H	4.15537900	0.25415600	-3.16731000
H	-4.87304400	-3.37158600	-1.09729500	H	4.11835600	1.25055700	-1.70789500
H	-5.03265000	-1.69700800	2.83967400	C	5.01904200	-2.06462000	-2.17218100
Cu	-0.24925900	-0.11399500	0.45438300	H	4.96399000	-2.98804900	-1.58902300
H	-2.67452700	3.62579800	-1.97206500	H	4.38355800	-2.18097100	-3.05478400
H	-4.65004300	1.82851000	-1.20182700	H	6.05123700	-1.92775600	-2.50892400
C	-0.40766200	4.13837600	0.85247300	C	0.85850100	-3.14229800	0.24667600
H	-1.19316000	3.39617900	1.02309200	C	-0.32890400	-3.56493500	0.86885100
C	0.00736700	1.40963500	-3.49711500	C	1.19570100	-3.71550200	-0.98631800
H	-0.83937700	0.89976700	-3.03023500	C	-1.13748700	-4.54171100	0.29109300
C	-3.76852000	0.66684100	2.35676900	H	-0.60189700	-3.12115300	1.82164300
H	-2.99777100	1.31204700	1.92521700	C	0.38754400	-4.69749200	-1.56955100
C	-3.55560100	-1.36513900	-2.37029400	H	2.09616500	-3.39164000	-1.49759700
H	-2.89662900	-0.50294200	-2.50510500	C	-0.77772700	-5.11960200	-0.93095400
C	1.78095200	-2.17922600	0.98960600	H	-2.04571300	-4.85828700	0.79716100
				H	0.67383800	-5.13240400	-2.52393500
				H	-1.40168900	-5.88801400	-1.37975600

H	2.14627400	-2.76178500	1.85065800	C	1.47963500	2.85008800	0.89994000
C	0.48130900	4.15108500	2.10913100	C	1.34078500	3.70308500	-0.21365700
H	1.27362000	4.90399500	2.04136000	C	0.39878400	4.73517700	-0.12205400
H	-0.12421400	4.39785900	2.98782000	C	-0.37053400	4.90906000	1.02467100
H	0.94506900	3.17716800	2.28606000	C	-0.21607100	4.04727400	2.10692100
C	-1.09487300	5.50551500	0.65259400	H	0.26471400	5.40734100	-0.96384300
H	-0.35559100	6.29475900	0.47711300	H	-0.82561100	4.18786400	2.99435000
H	-1.77787600	5.49471600	-0.20330200	C	3.44418800	-2.49972300	1.14898200
H	-1.67242700	5.77817000	1.54237800	C	3.70751100	-3.82432500	0.77805800
C	-3.24540200	0.19470500	3.72486300	C	4.13922900	-4.14105300	-0.50666300
H	-3.98663800	-0.40579400	4.26278000	C	4.31714200	-3.13522700	-1.45200200
H	-2.33079800	-0.39520800	3.62445000	C	4.07500300	-1.79283600	-1.13607100
H	-3.01543300	1.06160300	4.35283500	C	3.64114800	-1.50211000	0.17304600
C	-5.04635700	1.51666600	2.52138900	H	3.56557300	-4.61810400	1.50492100
H	-5.39458900	1.91242600	1.56162700	H	4.64419700	-3.39504700	-2.45413900
H	-5.85992900	0.92178700	2.95096200	Cu	0.55227900	-0.15734400	-0.21112600
H	-4.86022400	2.36463000	3.18940100	H	4.17109000	2.86084100	1.62222600
C	1.04094200	0.32442100	-3.85036500	H	5.38968400	0.39417600	1.21809400
H	0.57641000	-0.43943800	-4.48349100	C	2.16422500	3.54284800	-1.48803700
H	1.88554500	0.74034300	-4.41131000	H	2.79963000	2.66027900	-1.37328100
H	1.43532300	-0.16338600	-2.95488900	C	0.85035700	2.07157600	3.27614200
C	-0.51728100	2.11085300	-4.76676300	H	1.58390700	1.29993300	3.02727400
H	-1.29682800	2.84271400	-4.53051800	C	4.26432200	-0.71814400	-2.20197100
H	0.28818400	2.63966500	-5.28809800	H	4.08316000	0.25573900	-1.73846800
H	-0.94054900	1.37759600	-5.46171900	C	2.96281000	-2.19131800	2.56369000
C	-4.80938900	-1.12416700	-3.23608100	H	2.74450200	-1.12138400	2.62138100
H	-5.51337400	-1.95956800	-3.15539000	C	-2.21973200	0.24603400	-0.75146700
H	-5.33998300	-0.21440100	-2.93624400	N	-1.12953000	-0.74220500	-0.75740100
H	-4.53201400	-1.02182800	-4.29080300	C	-1.42617300	-2.05329700	-1.07076700
C	-2.77992500	-2.60159600	-2.85704800	C	-2.67550800	-2.48913300	-1.58736700
H	-1.88250400	-2.77509900	-2.25897600	C	-0.44172800	-3.06228900	-0.88428200
H	-3.39120300	-3.50922000	-2.81138300	C	-2.91557200	-3.83651900	-1.86682300
H	-2.47831600	-2.46447000	-3.90136300	H	-3.45326100	-1.76692800	-1.80908600
H	-5.55981100	-3.52485200	1.26985700	C	-0.69096200	-4.39618000	-1.17387900
H	3.19318500	4.55370400	-2.11507400	H	0.52929800	-2.76824000	-0.49054100
				C	-1.93707800	-4.80887700	-1.66469800
				H	-3.88721300	-4.12088400	-2.26590300
				H	0.09693600	-5.12791200	-1.00703300
				H	-2.13120100	-5.85356700	-1.88831200
				B	-3.42546600	-0.20158000	0.19625100
				C	-4.45980900	-0.73923900	2.16977000
				O	-3.19237400	-0.68148300	1.46469300
				C	-5.51293600	-0.71211000	0.99009100
				O	-4.76509100	-0.06723300	-0.07907900
L₃-10₃							
C	2.20349000	0.52112900	0.39863000				
C	4.37842600	0.72552000	1.04549300				
C	3.78422200	1.92923000	1.24200100				
N	2.45950600	1.78894900	0.84345200				
N	3.40284000	-0.12206300	0.53110400				
C	0.70954200	2.99709400	2.07157500				

H	4.35828900	2.84900700	0.19248200	C	-4.85185900	-0.15577300	-1.20831200
C	3.44214600	-1.83659500	2.26807400	C	-4.00936400	2.05509400	-1.65805700
H	3.32928000	-0.75124400	2.19737600	C	-5.96404400	0.11465300	-2.00477900
C	3.04758700	-1.28614100	-2.84416000	H	-4.76041900	-1.11374100	-0.71045900
H	2.84243200	-0.26050700	-2.52496100	C	-5.12591800	2.32984700	-2.44923600
C	1.65609100	2.73153900	2.79544700	H	-3.24525300	2.81798700	-1.52371500
H	2.18358900	1.81567800	2.51366000	C	-6.10845400	1.35567900	-2.62999800
C	1.56718600	3.16899500	-2.34212200	H	-6.72697600	-0.64882400	-2.13391900
H	2.19953900	2.28346400	-2.23411800	H	-5.22619800	3.30246100	-2.92461300
C	-2.65040800	0.59292000	-0.14496500	H	-6.97896000	1.56165600	-3.24707000
N	-1.59345600	-0.49011900	-0.44245300	H	-2.13360300	1.54357300	0.00219500
C	-1.75752600	-1.43576200	-1.48184900	H	3.52655000	-5.43377300	-0.72565500
C	-1.39367000	-2.77899900	-1.24372600	H	-0.70247900	6.08358300	0.53170700
C	-2.19313800	-1.10528200	-2.78413300	C	0.46992200	2.31429100	3.68565900
C	-1.45519000	-3.73907600	-2.25171100	H	0.83950800	1.76791800	4.56075200
H	-1.05882200	-3.05319000	-0.24900000	H	-0.08058800	3.18606600	4.05641200
C	-2.26513200	-2.07454000	-3.78475400	H	-0.23218000	1.66914400	3.14946200
H	-2.46671600	-0.08194100	-3.01083400	C	2.65138800	3.61750100	3.57213300
C	-1.89863000	-3.39846500	-3.53215300	H	3.52335900	3.87660900	2.96200600
H	-1.16527400	-4.76352700	-2.02986800	H	2.18144800	4.55341100	3.89352400
H	-2.60533400	-1.78551800	-4.77641200	H	3.00680700	3.09775200	4.46831900
H	-1.95712400	-4.14803900	-4.31618700	C	4.80099800	-2.11290800	2.94102700
B	-2.65985300	-0.34577900	1.09744100	H	4.83517500	-1.65223800	3.93400700
C	-3.33214400	-1.95840000	2.59756200	H	4.97565200	-3.18670700	3.06703700
O	-3.60347800	-1.36364000	1.31380400	H	5.63053700	-1.70894000	2.35131600
C	-2.61487800	-0.78061900	3.35919500	C	2.27679900	-2.35607700	3.13122300
O	-1.93407100	-0.09056800	2.29034900	H	2.33163500	-3.44095800	3.27117400
C	-4.66168200	-2.41147900	3.20308200	H	2.30103200	-1.89101100	4.12252400
H	-5.08498700	-3.21645400	2.59451400	H	1.31316300	-2.12276200	2.66950500
H	-4.52445900	-2.79373700	4.22072200	C	1.86739700	-1.72733900	-3.72975000
H	-5.38652100	-1.59587200	3.22877700	H	1.76095100	-1.04071600	-4.57645900
C	-2.41778500	-3.17520300	2.38696800	H	2.02189400	-2.73032700	-4.14124000
H	-1.44541700	-2.87048300	1.99215000	H	0.92490100	-1.73503400	-3.17626800
H	-2.25821800	-3.73121900	3.31684200	C	4.36605300	-1.26521300	-3.64429500
H	-2.88419100	-3.84430000	1.65869000	H	5.20130800	-0.90160900	-3.03633200
C	-3.60963700	0.21008600	3.98803700	H	4.62750700	-2.26639100	-4.00399000
H	-4.12133400	-0.21657900	4.85702200	H	4.27220100	-0.61094700	-4.51767400
H	-3.06311900	1.09997900	4.31388400	C	2.40255700	4.23953300	-3.07172400
H	-4.36254800	0.52289900	3.25948600	H	1.82518900	5.15518400	-3.23801100
C	-1.59209500	-1.21697200	4.40822300	H	3.29623300	4.50994600	-2.49958900
H	-0.79212800	-1.81356200	3.96666900	H	2.72528900	3.86867400	-4.05037500
H	-1.13846000	-0.33568200	4.87231500	C	0.34127100	2.75237200	-3.17790000
H	-2.06865500	-1.80513100	5.20044800	H	-0.33075400	3.59922300	-3.35383200
C	-3.84706700	0.81153300	-1.02416600	H	0.65927100	2.37316200	-4.15505800

H	-0.23083400	1.96573400	-2.67703200	H	-1.90401200	0.49357100	-2.97762700
				C	-2.03931900	-2.77237500	-3.93912200
L₃-12₃				H	-1.97441900	-4.44799300	-2.58273100
				H	-2.09640900	-0.90080300	-5.01102900
C	2.05807300	0.44511100	0.05814100	H	-2.12772800	-3.38576600	-4.83129200
C	3.96871100	1.63549900	0.38581300	B	-2.50603200	-0.47841300	0.87466000
C	4.32941500	0.35175100	0.13248700	C	-3.50786300	-2.04045800	2.27928800
N	3.15282900	-0.36121300	-0.06465300	O	-3.57462300	-1.42795300	0.98640100
N	2.58063200	1.67581000	0.33587300	C	-2.69207700	-0.98076000	3.11530000
C	3.13057600	-2.19666500	-1.69767300	O	-1.78333300	-0.46134600	2.13207600
C	3.10256700	-1.77800500	-0.35236800	C	-4.93668700	-2.29173800	2.76880200
C	3.04019900	-2.68086200	0.72755400	H	-5.42321600	-3.02590000	2.11867000
C	2.99139900	-4.04662500	0.42188100	H	-4.94524300	-2.68796900	3.79074900
C	3.01301600	-4.49058700	-0.89692500	H	-5.53118400	-1.37674800	2.74068500
C	3.08573700	-3.57462300	-1.94230800	C	-2.76633800	-3.38275600	2.14994400
H	2.93452400	-4.77002400	1.22940200	H	-1.72733100	-3.22656700	1.84623600
H	3.10287600	-3.93293000	-2.96668800	H	-2.77185100	-3.95141100	3.08624000
C	1.48554800	3.67585600	-0.57423800	H	-3.26189100	-3.98472800	1.38230100
C	0.72601000	4.82983200	-0.34617900	C	-3.57879900	0.17370500	3.61816400
C	0.30030100	5.17034200	0.93468400	H	-4.25485300	-0.14429400	4.41887000
C	0.62801900	4.36106700	2.01853000	H	-2.93628300	0.96858200	4.00922300
C	1.38178400	3.19283500	1.85075400	H	-4.17591900	0.59153300	2.80340500
C	1.79513600	2.87287100	0.54193700	C	-1.89463800	-1.55835300	4.28565400
H	0.46472200	5.46811800	-1.18465000	H	-1.16148400	-2.29424400	3.95039500
H	0.29004700	4.63561700	3.01276300	H	-1.35589300	-0.75616100	4.80040100
Cu	0.22810800	-0.00065800	-0.14632500	H	-2.55868500	-2.03634400	5.01478800
H	5.29795800	-0.11843300	0.07726300	C	-3.73865700	1.13887000	-0.97540500
H	4.55895800	2.51318300	0.59416100	C	-4.74903300	0.22495300	-1.33445100
C	3.01869800	-2.22925100	2.18481300	C	-3.86072600	2.46231600	-1.43817000
H	3.14128900	-1.14255900	2.20767100	C	-5.82192500	0.62423400	-2.13013400
C	3.23051400	-1.22235700	-2.86760200	H	-4.69564200	-0.79236200	-0.96534300
H	3.12909600	-0.20676500	-2.47426600	C	-4.94237300	2.86496800	-2.22184100
C	1.73685000	2.33984900	3.06463800	H	-3.09317500	3.18575200	-1.17024900
H	2.24929100	1.44105700	2.70982800	C	-5.92801900	1.94339600	-2.57816000
C	1.93597400	3.33498900	-1.99170300	H	-6.58782400	-0.10052600	-2.39470800
H	2.53723300	2.42233900	-1.94838300	H	-5.01103100	3.89647000	-2.55889000
C	-2.59809300	0.78716100	-0.08846300	H	-6.76985500	2.24922100	-3.19358800
N	-1.62489700	-0.39466400	-0.44378700	H	-2.00400800	1.66526500	0.16300000
C	-1.81324500	-1.17872900	-1.62172000	H	2.97331700	-5.55475800	-1.11113400
C	-1.84791800	-2.58018500	-1.52933700	H	-0.28979000	6.06921700	1.08851400
C	-1.90769400	-0.58806600	-2.89450800	C	0.48423100	1.87275000	3.83077900
C	-1.95191500	-3.36522400	-2.67761700	H	0.78188600	1.23895400	4.67365500
H	-1.79538600	-3.04030600	-0.55006900	H	-0.07394400	2.72090500	4.24262600
C	-2.02051400	-1.37890400	-4.03771600	H	-0.19099300	1.29414400	3.19349200

C	2.71421600	3.08798100	3.99407300	C	0.56547600	3.16826400	-1.88432100
H	3.62826400	3.38181500	3.46683700	C	-0.20028900	4.33375000	-1.75423700
H	2.25968100	3.99743900	4.40159100	C	-0.05030700	5.17668200	-0.65713400
H	2.99963500	2.45173600	4.83861900	C	0.88055300	4.87601000	0.33334600
C	4.19020800	-2.83399000	2.98302000	C	1.67059300	3.72249800	0.25880200
H	4.19194800	-2.44359900	4.00614300	C	1.48261200	2.87844100	-0.85424000
H	4.11579500	-3.92457000	3.04727600	H	-0.92447100	4.58086600	-2.52431000
H	5.15546100	-2.59308800	2.52550400	H	0.99701500	5.54644000	1.17936400
C	1.66618500	-2.54603000	2.85194500	Cu	0.39351600	0.08108300	0.58592900
H	1.46425100	-3.62283000	2.84947900	H	4.82316100	-0.13521800	-1.91510600
H	1.67226500	-2.21063500	3.89465800	H	3.92783200	2.48942600	-2.10600200
H	0.83913300	-2.04246900	2.34294900	C	4.34498200	-1.16189200	1.63443000
C	2.09828200	-1.42520700	-3.89196000	H	3.89797400	-0.18344500	1.43439400
H	2.16765700	-0.66664300	-4.67917600	C	1.94822300	-2.25348200	-2.78585300
H	2.16114800	-2.40510300	-4.37656900	H	1.63027800	-1.21208000	-2.67717600
H	1.11190700	-1.34507800	-3.42719100	C	2.70194400	3.43937700	1.34672800
C	4.61357400	-1.31767400	-3.54368700	H	3.16529000	2.47232000	1.13211700
H	5.42388600	-1.12156500	-2.83348200	C	0.39322000	2.28464100	-3.11634200
H	4.77885100	-2.31343100	-3.96913700	H	1.07933500	1.43758800	-3.02782500
H	4.69256800	-0.58945400	-4.35805200	C	-2.83305000	0.65766300	0.18193700
C	2.83059300	4.44174000	-2.58326900	N	-2.03318900	-0.59679900	-0.14212200
H	2.28598500	5.38564700	-2.69052800	C	-2.45635000	-1.62678200	-0.98433400
H	3.70427600	4.63196300	-1.95128400	C	-2.21262000	-2.97102100	-0.62947300
H	3.18709800	4.15120400	-3.57719400	C	-3.09023300	-1.37773400	-2.21928500
C	0.73181200	3.04193500	-2.90748900	C	-2.57904900	-4.01460200	-1.47766800
H	0.08204400	3.91768700	-3.00813100	H	-1.74232400	-3.18156000	0.32524600
H	1.07455600	2.76383800	-3.90997700	C	-3.45125100	-2.42817900	-3.06074100
H	0.12843100	2.21930200	-2.51267300	H	-3.31407000	-0.35454900	-2.50013700
L₃-TSI3₃				C	-3.19871200	-3.75535400	-2.70338400
C	1.93842500	0.45722500	-0.44524500	H	-2.38397400	-5.04048800	-1.17341000
C	3.49803200	1.62271800	-1.63052400	H	-3.94312000	-2.20536800	-4.00471800
C	3.93373800	0.34224400	-1.53819800	H	-3.48853200	-4.57015200	-3.36048400
N	2.97400500	-0.35716700	-0.81501700	B	-2.23485400	-0.30683600	1.31386500
N	2.28185000	1.67768300	-0.96101100	C	-2.21292800	-1.31434200	3.43246500
C	2.57158000	-2.69152300	-1.46252800	O	-3.00201400	-1.03731700	2.27679100
C	3.07821400	-1.77042900	-0.52203300	C	-1.13299400	-0.16133200	3.42276100
C	3.72488600	-2.16698300	0.66667600	O	-0.94105900	0.01918800	1.99902200
C	3.83705500	-3.54133100	0.90966400	C	-3.13063400	-1.30128100	4.65821300
C	3.33230900	-4.47418300	0.00810300	H	-3.84435100	-2.12733100	4.58483000
C	2.71139400	-4.05274800	-1.16398500	H	-2.56269300	-1.42618100	5.58720800
H	4.32781500	-3.88520200	1.81427100	H	-3.70234900	-0.37331400	4.71396000
H	2.32671300	-4.79080700	-1.85949000	C	-1.58089300	-2.70996500	3.27859000
				H	-0.86764100	-2.73179200	2.44969300
				H	-1.06614100	-3.03761100	4.18835800

H	-2.37711200	-3.42594500	3.05726300	H	0.10815900	3.89804900	-4.57522400
C	-1.67576800	1.16190900	3.98154700	C	0.70079100	-3.06730000	-3.16771500
H	-1.80354500	1.11967400	5.06758600	H	0.95084400	-4.10434800	-3.41762500
H	-0.96973200	1.96539900	3.75073900	H	-0.04178800	-3.07714600	-2.36723900
H	-2.63608000	1.40945600	3.52329600	H	0.23021900	-2.62864600	-4.05299000
C	0.19552800	-0.51340700	4.08405500	C	2.99622900	-2.30991300	-3.91867800
H	0.66036300	-1.38040000	3.61013900	H	3.86683600	-1.68082600	-3.70746100
H	0.88992100	0.33044600	4.01577100	H	3.35399200	-3.33497200	-4.06579000
H	0.04883900	-0.73844200	5.14590700	H	2.55573100	-1.96941700	-4.86183600
C	-4.28990600	0.76096400	-0.10533000	H	3.42692200	-5.53574000	0.21842600
C	-5.20960900	-0.27085300	0.16782200	H	-0.65746300	6.07362800	-0.57575400
C	-4.79964600	1.96240800	-0.63092400				
C	-6.57065400	-0.10044800	-0.07896300				
H	-4.85391800	-1.20225500	0.59324300	L₃-14₃			
C	-6.16374200	2.13821300	-0.86468800	C	-1.70886200	0.99263200	0.00115500
H	-4.10812500	2.77235600	-0.85498700	C	-3.69165300	2.01686400	0.44446600
C	-7.05958800	1.10289000	-0.59448500	C	-2.75754900	2.98830200	0.29439600
H	-7.25743900	-0.91441400	0.13996400	N	-1.55299300	2.34960100	0.02820600
H	-6.52470600	3.08211500	-1.26649400	N	-3.03908600	0.80547400	0.25694700
H	-8.12238600	1.23063400	-0.78155300	C	0.13596700	3.28091300	-1.49821800
H	-2.29733000	1.56190300	-0.11808400	C	-0.31073000	3.06423500	-0.17941500
C	2.05205300	3.33048700	2.73835600	C	0.37574500	3.55562400	0.95113500
H	1.59208700	4.27550900	3.04588900	C	1.56058200	4.26521700	0.72312000
H	1.27584200	2.56016400	2.74727000	C	2.03875900	4.47675500	-0.56692500
H	2.80508300	3.06991000	3.49015100	C	1.33152600	3.99164500	-1.66278800
C	3.82338600	4.49749600	1.33730600	H	2.11870500	4.65350000	1.56886900
H	4.31776600	4.54837200	0.36166500	H	1.71039700	4.16779000	-2.66466400
H	3.43292000	5.49538100	1.56371500	C	-4.42808800	-0.91690700	-0.80714500
H	4.58216400	4.25778200	2.08998700	C	-5.07630800	-2.15407200	-0.71332000
C	5.86435400	-1.04161400	1.39062500	C	-5.00644000	-2.91798200	0.44902600
H	6.08716600	-0.73664300	0.36344300	C	-4.29338800	-2.45342800	1.54970900
H	6.30485800	-0.29965000	2.06549100	C	-3.62901400	-1.21993800	1.51837600
H	6.36509600	-1.99942400	1.56912000	C	-3.70334100	-0.47820700	0.32202800
C	4.06230400	-1.49109100	3.11059200	H	-5.64489300	-2.52280100	-1.56109200
H	2.99096600	-1.59886300	3.29862200	H	-4.25352200	-3.05297100	2.45345900
H	4.55732800	-2.41486100	3.42780700	Cu	-0.43878400	-0.36645200	-0.34237800
H	4.44041100	-0.68670200	3.75022500	H	-2.83157700	4.06181500	0.35291700
C	-1.03114600	1.70725000	-3.20694700	H	-4.74488800	2.06969900	0.66667300
H	-1.28002800	1.12530800	-2.31637400	C	-0.14475800	3.38611400	2.37650200
H	-1.77943500	2.49981200	-3.31536500	H	-0.97137500	2.66961100	2.35504300
H	-1.11724700	1.04826700	-4.07727900	C	-0.63205400	2.80942900	-2.72983700
C	0.77235200	3.04456500	-4.40328500	H	-1.52394100	2.27375800	-2.39276400
H	1.79848900	3.42514000	-4.36051300	C	-2.90581200	-0.71927700	2.76549600
H	0.69162400	2.38216600	-5.27153100	H	-2.37561200	0.20108600	2.50631300

C	-4.56613500	-0.07927700	-2.07723500	H	7.54371400	-1.16580000	-0.60955900
H	-3.83911800	0.73679500	-2.02617500	H	5.96739900	2.65836200	-1.78290800
C	2.96105300	-0.43804100	-0.01690700	H	7.90181100	1.10151100	-1.57678700
N	2.79443600	-1.60030800	0.86917000	H	2.31022100	0.41717200	0.22574300
C	2.50065600	-1.59664900	2.20965400	H	2.96516300	5.02281800	-0.71796900
C	1.89680100	-2.72533000	2.81473400	H	-5.51514300	-3.87646700	0.49805100
C	2.82966100	-0.50222500	3.04207600	C	0.91690700	2.81724500	3.33383000
C	1.63643300	-2.74871700	4.18127000	H	1.76452500	3.50015100	3.45415000
H	1.66070400	-3.58443100	2.19398300	H	0.47837000	2.66513300	4.32571100
C	2.56278300	-0.54102000	4.40999600	H	1.30176400	1.85539100	2.98707300
H	3.32875000	0.35516400	2.60060200	C	-0.70211400	4.72216200	2.91179500
C	1.96025900	-1.65743900	4.99636100	H	0.08598300	5.48060500	2.96954500
H	1.17963700	-3.63401500	4.61865500	H	-1.49615700	5.12037500	2.27113900
H	2.84121300	0.31025200	5.02763600	H	-1.11378300	4.58921000	3.91784600
H	1.76246700	-1.68485300	6.06393100	C	-1.85016100	-1.71887400	3.27050500
B	2.24342200	-1.82138500	-0.46891800	H	-1.30916100	-1.30240500	4.12515600
C	1.78343200	-3.17758000	-2.32388800	H	-2.30564900	-2.66090900	3.59490600
O	2.73562500	-2.86104800	-1.32268200	H	-1.10902900	-1.94897500	2.50054200
C	0.41514100	-2.95637600	-1.58151300	C	-3.91728400	-0.36760700	3.87576400
O	0.73590700	-1.78868900	-0.76329600	H	-4.64123900	0.38237000	3.53957300
C	1.96772600	-2.22329700	-3.51991400	H	-4.47863200	-1.25127100	4.19784000
H	3.00828100	-2.28560100	-3.84917400	H	-3.39446500	0.03213100	4.75079900
H	1.32109600	-2.48093800	-4.36591200	C	-4.25834400	-0.87701500	-3.35767700
H	1.77472600	-1.18697700	-3.23010900	H	-4.98218000	-1.68182100	-3.52186400
C	2.01685400	-4.62113100	-2.77946700	H	-4.30517000	-0.21550800	-4.22911100
H	2.03108300	-5.30753600	-1.93080500	H	-3.26103700	-1.32291000	-3.32249700
H	1.25009200	-4.94965400	-3.49042600	C	-5.97099900	0.55389100	-2.16062900
H	2.98913700	-4.68755600	-3.27626500	H	-6.74566200	-0.21807300	-2.22150000
C	-0.76945300	-2.64487200	-2.49224400	H	-6.19018500	1.17277100	-1.28474300
H	-0.93718300	-3.47212800	-3.19063900	H	-6.05529400	1.18611600	-3.05091100
H	-1.68475600	-2.52064500	-1.90317800	C	0.19755500	1.82634700	-3.57692100
H	-0.60156300	-1.73592400	-3.07488400	H	-0.38768700	1.47531400	-4.43382900
C	0.06337400	-4.10521900	-0.62839100	H	1.10682100	2.29629000	-3.96545300
H	0.92412900	-4.37059500	-0.01092800	H	0.50113400	0.95572100	-2.98805400
H	-0.75334200	-3.79307400	0.03026300	C	-1.11261800	4.00509400	-3.57650200
H	-0.26157300	-4.99518100	-1.17659700	H	-1.73199300	4.68955900	-2.98772100
C	4.33432900	-0.01505300	-0.40798400	H	-0.26963100	4.57870100	-3.97554100
C	5.43758000	-0.87906800	-0.29483100	H	-1.70703400	3.65432500	-4.42688900
C	4.55566200	1.26322100	-0.94958800				
C	6.70642200	-0.47910500	-0.71092500				
H	5.27972600	-1.86661800	0.12658300				
C	5.82465400	1.66191200	-1.36992200				
H	3.71803000	1.95262500	-1.03565400				
C	6.91129100	0.79245000	-1.25375300				
				L₃-TS15₃			
				C	1.26788300	1.12705100	0.24148900
				C	1.94723800	3.19887800	0.91078700
				C	3.02126900	2.37778800	0.99010000

N	2.59771900	1.11901200	0.57297900	O	-1.26657700	-3.46751800	-0.77727500
N	0.88294800	2.42540600	0.46131100	C	-0.16587900	-2.46286300	-2.59041100
C	4.34093100	0.01662000	-0.75070700	O	-0.76492600	-1.41468900	-1.77537800
C	3.51328200	0.01208500	0.39281700	C	1.14036300	-3.61909600	-0.66632400
C	3.58737900	-0.99308300	1.38098200	H	1.01023300	-4.35328800	0.13361200
C	4.51647200	-2.02169000	1.18135500	H	2.06243800	-3.85439300	-1.20779900
C	5.34021700	-2.04651900	0.05927100	H	1.26126100	-2.63658600	-0.19769500
C	5.25397000	-1.03629200	-0.89249100	C	-0.19504200	-5.04795000	-2.23004900
H	4.59717400	-2.81426800	1.91660800	H	-1.13596500	-5.16733900	-2.77003400
H	5.90696800	-1.06116000	-1.75926400	H	0.63582300	-5.22030100	-2.92355700
C	-0.80330300	3.21245900	-1.14640800	H	-0.15563400	-5.81978500	-1.45573900
C	-2.07669200	3.74789600	-1.37628400	C	1.18025900	-1.98277100	-3.12228900
C	-2.93708400	4.04336400	-0.32512900	H	1.67449800	-2.77760200	-3.69127500
C	-2.53743400	3.81358100	0.98755700	H	1.03363000	-1.13001100	-3.79293700
C	-1.28263300	3.26664000	1.28128800	H	1.84628900	-1.67358100	-2.31353100
C	-0.43403200	2.96500000	0.19313500	C	-1.13004700	-2.72199700	-3.75546600
H	-2.39527600	3.93861000	-2.39601400	H	-2.08751200	-3.10340900	-3.39310100
H	-3.21518200	4.05367200	1.79983800	H	-1.31352000	-1.78262000	-4.28455700
Cu	0.12314400	-0.26841100	-0.35622900	H	-0.71675300	-3.44412500	-4.46640600
H	4.03799800	2.56498200	1.29423800	C	-1.97677000	-1.73217900	2.05285100
H	1.84053700	4.24979400	1.12222400	C	-2.74501500	-2.87265600	2.34316600
C	2.74344700	-0.94964600	2.65271500	C	-1.23857900	-1.15752900	3.10280900
H	1.81212500	-0.42648100	2.41753600	C	-2.77389000	-3.40956500	3.62992300
C	4.31606200	1.13178700	-1.79527400	H	-3.32288800	-3.32167300	1.54245500
H	3.44156400	1.75999700	-1.60527800	C	-1.27427600	-1.68891000	4.39253000
C	-0.87181200	3.06103200	2.73814100	H	-0.63192600	-0.27700500	2.90145200
H	-0.00970600	2.38605800	2.75432700	C	-2.04204100	-2.82356400	4.66570700
C	0.12840500	2.97985300	-2.33314500	H	-3.37983700	-4.29075700	3.82659800
H	1.03240600	2.48564500	-1.96862000	H	-0.70614700	-1.21128700	5.18797400
C	-1.92647600	-1.15201600	0.67960700	H	-2.07174500	-3.24072400	5.66842900
N	-2.90936900	-1.62701700	-0.30391800	H	-1.85413300	-0.05228500	0.70193700
C	-3.94962100	-0.86125900	-0.80491900	H	-3.92171700	4.45306400	-0.52907500
C	-4.47831700	-1.13444900	-2.08515100	H	6.05391500	-2.85515100	-0.07045000
C	-4.54338400	0.17052900	-0.04985800	C	3.46895000	-0.14550200	3.75344400
C	-5.54959700	-0.40006900	-2.58394200	H	4.41987300	-0.62106500	4.01838100
H	-4.04272200	-1.93746600	-2.67147200	H	3.68338600	0.88010900	3.43703100
C	-5.61697300	0.89826400	-0.56112900	H	2.85291700	-0.09677800	4.65764300
H	-4.16731400	0.37996800	0.94659200	C	2.35457400	-2.34278500	3.17512000
C	-6.13077600	0.62535100	-1.83057300	H	1.90181500	-2.95527900	2.39086200
H	-5.93753400	-0.63291800	-3.57294500	H	3.21639200	-2.88369200	3.58157800
H	-6.06162000	1.68285600	0.04704400	H	1.61885500	-2.24468200	3.97735000
H	-6.96911300	1.19326100	-2.22326100	C	-1.97965800	2.41123800	3.58810300
B	-1.60401300	-2.08757800	-0.73657000	H	-1.59669800	2.18920000	4.58957800
C	-0.10055200	-3.66704400	-1.57448200	H	-2.83919600	3.07785600	3.71251600

H	-2.33310700	1.47420100	3.15237600	H	1.11837600	5.81517100	-0.09202100
C	-0.43683100	4.39657000	3.37976700	Cu	0.08622100	0.30860700	0.24261000
H	-0.11192200	4.23692800	4.41345200	H	5.15778600	-0.33907100	-0.43134100
H	0.38806300	4.86809700	2.83697600	H	4.48559300	2.14977600	-1.46272900
H	-1.26973500	5.10791400	3.39522900	C	2.75044900	-0.68667700	2.81007000
C	4.18251500	0.59839600	-3.23357400	H	2.32782500	0.15016500	2.24720500
H	4.10686700	1.43535400	-3.93589100	C	3.37244400	-2.73714000	-1.87854100
H	5.05133300	0.00210100	-3.53100300	H	3.12839200	-1.71146600	-2.17119600
H	3.29149100	-0.02334000	-3.34803500	C	2.52506200	3.75948400	0.97802800
C	5.56718900	2.02630900	-1.66896400	H	2.92322100	2.75199900	1.12645600
H	5.65586100	2.46327900	-0.66946600	C	1.11141200	1.57535300	-3.47674800
H	6.48045100	1.45283800	-1.86085900	H	1.62722600	0.73374300	-3.00630000
H	5.52677200	2.84620000	-2.39394000	C	-1.71648200	0.68476400	0.96527500
C	0.56137400	4.32401500	-2.95398300	N	-2.87116200	0.23445400	0.13750800
H	-0.29670300	4.87205300	-3.35753200	C	-4.00511500	1.09452100	0.08226100
H	1.04926400	4.96804600	-2.21478400	C	-4.75039900	1.22647600	-1.10464000
H	1.26551600	4.15551300	-3.77608800	C	-4.38716100	1.87202200	1.19095200
C	-0.49585400	2.05314700	-3.39368300	C	-5.84635400	2.08419800	-1.16931800
H	-0.78072100	1.08796300	-2.96540000	H	-4.46703200	0.64718800	-1.97497200
H	-1.38860900	2.49768900	-3.84599100	C	-5.47983000	2.73547700	1.11383500
H	0.22380900	1.87295000	-4.20029200	H	-3.83841700	1.78655000	2.12083200
L₃-16₃				C	-6.22110700	2.84879900	-0.06274400
C	1.94574000	0.39188500	-0.30519900	H	-6.40296300	2.16386800	-2.09992600
C	3.87913200	1.37244200	-1.02675900	H	-5.75552200	3.31812600	1.98934900
C	4.20589800	0.15693200	-0.52514200	H	-7.07221400	3.52157400	-0.11799500
N	3.02001500	-0.43406600	-0.09771200	B	-2.87777300	-1.03022100	-0.49941800
N	2.50294400	1.50173600	-0.88441800	C	-2.11715200	-2.99638400	-1.39419000
C	3.13676500	-2.87137900	-0.37510400	O	-1.79372300	-1.90508300	-0.49691400
C	2.97209600	-1.76059500	0.47944200	C	-3.69214700	-2.97081100	-1.39650800
C	2.81668700	-1.89319300	1.87635200	O	-3.96772900	-1.56985800	-1.17549900
C	2.79772500	-3.19175300	2.39962600	C	-1.52426700	-2.64731600	-2.76653100
C	2.94672500	-4.30590400	1.57886400	H	-0.45651900	-2.44630600	-2.65074000
C	3.12249800	-4.14476400	0.20882400	H	-1.64866000	-3.46393700	-3.48462100
H	2.66931400	-3.33158700	3.46703500	H	-1.99066000	-1.74829200	-3.17854600
H	3.24957000	-5.02024400	-0.42009400	C	-1.48641300	-4.27603700	-0.84972900
C	1.12016200	2.74458500	-2.49729100	H	-1.80134300	-4.47100700	0.17699200
C	0.45699900	3.93160300	-2.83302200	H	-1.75512700	-5.13872800	-1.46908300
C	0.45703500	5.02657400	-1.97457900	H	-0.39657700	-4.18185700	-0.85067100
C	1.12493500	4.95594900	-0.75562100	C	-4.35039800	-3.39458000	-2.70951900
C	1.80118500	3.79402700	-0.36538600	H	-4.11139100	-4.43597900	-2.95105200
C	1.78166200	2.69939600	-1.25422400	H	-5.43702700	-3.31054400	-2.61604300
H	-0.06769200	3.99640200	-3.78118200	H	-4.03623400	-2.76160400	-3.54132900
				C	-4.31383800	-3.75041200	-0.22820400
				H	-3.85684600	-3.47077900	0.72507200

H	-5.37881700	-3.50909400	-0.17262700	H	2.91256100	2.21365500	-4.55257900
H	-4.21018900	-4.83210000	-0.35915000	H	1.90042900	1.06279100	-5.44370800
C	-1.78255500	0.27557400	2.41188300	H	-0.06570300	5.93634600	-2.25533800
C	-2.17961000	-1.01075700	2.82845800	H	2.93101800	-5.30270800	2.01044800
C	-1.41994700	1.18713600	3.42617200				
C	-2.21404500	-1.36170600	4.17819000	L₃-17₃			
H	-2.45498000	-1.74533000	2.07914100				
C	-1.44644800	0.83650800	4.77554300	Cu	0.23644100	-0.70160000	-0.17093700
H	-1.13341600	2.19857200	3.14401300	N	-2.55876700	0.14365100	0.25033000
C	-1.84665800	-0.44391300	5.16576500	N	2.51867500	-1.77741800	1.45846300
H	-2.53297600	-2.36251100	4.46091700	N	2.86730900	-1.93973700	-0.65838700
H	-1.17072400	1.57329800	5.52681100	O	-4.99602500	-0.08276500	0.81668200
H	-1.87823500	-0.71835900	6.21638000	O	-4.16834900	-1.25817500	-0.97603900
H	-1.73469900	1.78134300	0.93176700	B	-3.87376200	-0.37441500	0.05303000
C	1.56700000	4.04182700	2.15062700	C	1.95782500	-1.47036600	0.24965500
H	2.10134100	3.95919300	3.10323400	C	3.73983200	-2.42461300	1.30360900
H	1.14428500	5.05056400	2.09510100	C	3.96187800	-2.52320900	-0.03051100
H	0.73867400	3.32833400	2.16131900	C	2.72194200	-1.87550100	-2.09589800
C	3.72036400	4.73317700	0.99361900	C	3.17285000	-0.72516000	-2.77451200
H	4.43095900	4.51133600	0.19051300	C	3.07370200	-0.72177500	-4.17144300
H	3.39175700	5.77038800	0.86770700	H	3.41318300	0.14814600	-4.72420100
H	4.25536000	4.66638200	1.94696100	C	2.54204000	-1.80801700	-4.86050300
C	4.17256300	-0.28416100	3.25820500	C	2.08920700	-2.92387100	-4.16245100
H	4.64508600	-1.09377200	3.82586900	H	1.66562900	-3.76149400	-4.70837900
H	4.81924200	-0.05142700	2.40600500	C	2.16860800	-2.98552100	-2.76566900
H	4.13273100	0.60008100	3.90352600	C	1.65663800	-4.22364100	-2.03513900
C	1.83977000	-0.90354500	4.02877000	C	3.76004600	0.48249800	-2.05084600
H	2.25509100	-1.63898900	4.72718900	C	1.94559900	-1.47043100	2.75061300
H	1.73131300	0.03589300	4.57829300	C	2.44480200	-0.35681700	3.45746700
H	0.83854900	-1.22865500	3.73593100	C	3.54878000	0.54347500	2.90878600
C	2.47358400	-3.67060300	-2.70919400	C	1.90252100	-0.09946800	4.72179000
H	2.60831600	-3.46783100	-3.77702700	H	2.26319200	0.75131100	5.29109800
H	2.71761200	-4.72553300	-2.54624900	C	0.90427600	-0.90843800	5.25607500
H	1.41796700	-3.52962600	-2.46684900	C	0.43075200	-2.00006800	4.53552000
C	4.85482200	-2.98563200	-2.22974600	H	-0.34901200	-2.62406900	4.96112400
H	5.52370100	-2.30372900	-1.69626100	C	0.94104000	-2.31178500	3.26923300
H	5.15165200	-4.00745600	-1.96942100	C	0.41414200	-3.53667400	2.52775900
H	5.02246500	-2.85042500	-3.30373800	C	-1.55701500	-0.17316900	-0.80649300
C	-0.32343600	1.10886300	-3.78788600	H	-1.87916800	-1.12859800	-1.23549200
H	-0.89904900	1.88709100	-4.30031500	C	-2.19812000	0.99061300	1.32467100
H	-0.30187300	0.22940200	-4.44048500	C	-1.09924700	1.86729500	1.21634400
H	-0.85767600	0.84395900	-2.87079300	H	-0.52851100	1.89122700	0.29662500
C	1.87856700	1.92422600	-4.76738600	C	-0.74766000	2.71959500	2.26573600
H	1.40514300	2.75470500	-5.30193500	H	0.08975200	3.39941400	2.13058600

C	-1.47136700	2.71969900	3.45787000	H	-0.21907800	7.14376200	-0.79371000
H	-1.20110600	3.38737000	4.27080900	C	0.28285200	5.01525200	-1.01535800
C	-2.55228900	1.84390300	3.58169200	H	-0.16180000	4.04011600	-0.83201400
H	-3.12683400	1.81684000	4.50455800	H	0.58100000	5.10184500	-2.05929000
C	-2.91239600	0.99140100	2.54050500	H	2.47441800	-1.78230100	-5.94443200
H	-3.75877400	0.32880800	2.66038100	H	0.49230400	-0.68542300	6.23601700
C	-6.05774900	-0.97433500	0.39577600	H	4.32577500	-2.74708000	2.14890400
C	-7.38499000	-0.22433500	0.49515300	H	4.78074900	-2.94949800	-0.58715200
H	-7.59127900	0.02156300	1.54110300	C	4.87417700	0.31576600	3.66423900
H	-8.21109800	-0.83981100	0.12304700	H	4.77385000	0.57487300	4.72387000
H	-7.36184100	0.70890100	-0.07002000	H	5.19887900	-0.72869800	3.60895800
C	-6.05503700	-2.16946100	1.36018700	H	5.66869400	0.93972100	3.24095000
H	-5.11042000	-2.71809900	1.30561900	C	3.15533800	2.03166500	2.93161200
H	-6.87329100	-2.86435800	1.14773900	H	3.04148800	2.40685300	3.95433700
H	-6.17502300	-1.80066500	2.38286600	H	3.93210200	2.63239800	2.44704400
C	-5.60830800	-1.35850900	-1.06596700	H	2.21401300	2.20296000	2.40468500
C	-5.96881300	-2.77624300	-1.50741200	C	3.11722600	1.80325000	-2.51454500
H	-5.58739700	-2.95186200	-2.51756600	H	3.43028300	2.62641000	-1.86505500
H	-7.05482200	-2.91727900	-1.52699100	H	3.41184100	2.05992600	-3.53833300
H	-5.53035100	-3.52712300	-0.84753400	H	2.02555900	1.74406500	-2.48509200
C	-6.06742000	-0.34513500	-2.12463100	C	5.29390600	0.52741000	-2.20284900
H	-5.81310900	0.67684200	-1.83035900	H	5.76559800	-0.37916700	-1.80896500
H	-7.14634600	-0.40029300	-2.30056100	H	5.58297400	0.62316400	-3.25536300
H	-5.55168900	-0.55921700	-3.06464500	H	5.70626300	1.38613700	-1.66244800
C	-1.53267100	0.81065300	-1.94680700	C	-1.09902600	-3.43121600	2.25636700
C	-0.81525400	0.49543600	-3.12143700	H	-1.43983300	-4.29754000	1.67869800
H	-0.28834600	-0.45524800	-3.17596000	H	-1.67362700	-3.40720600	3.18854800
C	-0.76597700	1.36703800	-4.20515700	H	-1.33713200	-2.52618000	1.68950100
H	-0.20659900	1.08378600	-5.09378600	C	0.75603100	-4.83534900	3.28510900
C	-1.42980100	2.59902100	-4.15766000	H	1.83512600	-4.93551800	3.44218000
H	-1.39007200	3.28160500	-5.00205700	H	0.27295800	-4.86518800	4.26758100
C	-2.15028700	2.92708200	-3.01032000	H	0.41263700	-5.70835700	2.71954600
H	-2.68249200	3.87412700	-2.95428300	C	2.46858300	-5.47813600	-2.41241600
C	-2.20436500	2.04665300	-1.92392000	H	2.11357700	-6.34697300	-1.84787600
H	-2.78780000	2.31553400	-1.04913600	H	2.37208400	-5.71230800	-3.47789900
H	3.71715700	0.27430200	1.86212800	H	3.53404700	-5.34626700	-2.19691800
H	0.91110400	-3.58601800	1.55533900	C	0.15082800	-4.43944600	-2.28201700
H	1.78565800	-4.06323900	-0.96126100	H	-0.05924400	-4.63818800	-3.33839200
H	3.53730300	0.37608700	-0.98570900	H	-0.20854000	-5.29865200	-1.70526700
C	-1.70029200	5.96662300	0.13343300	H	-0.42788800	-3.56044900	-1.98301600
H	-2.31110400	6.81069600	0.43962800				
H	-2.05140200	4.97642900	0.41133400				
Br	2.04575600	4.99018600	-0.03399800				
C	-0.56385800	6.14155700	-0.54552100				
				L₃-TS18₃			
				Cu	0.68330700	-0.02532000	0.91547600

N	-2.31049800	-0.76769100	0.65797700	H	-7.20428000	-2.15350300	-0.21145900
N	2.30742000	-0.70661500	-1.70204100	H	-7.79502900	-0.66022300	-0.95770200
N	2.13488100	1.42352600	-1.45627400	H	-7.10358100	-0.62997300	0.67813700
O	-4.64501400	-1.37181500	0.02011500	C	-5.49010800	-1.67321300	-2.20790000
O	-3.77625100	0.60160100	-0.78224700	H	-4.50295200	-1.54098800	-2.65757800
B	-3.54591100	-0.52833400	-0.01320200	H	-6.24886600	-1.39437400	-2.94571400
C	1.72553400	0.23977300	-0.89439600	H	-5.61159700	-2.73422300	-1.97260000
C	3.05478500	-0.12428800	-2.72296500	C	-5.19604900	0.65226700	-1.06802300
C	2.95075100	1.21420000	-2.56585100	C	-5.39047800	1.23886900	-2.46569900
C	1.72109200	2.76216400	-1.08559800	H	-5.03879300	2.27442500	-2.48056600
C	2.47631200	3.48163000	-0.13574600	H	-6.44920200	1.23773100	-2.74630800
C	2.07981400	4.79674100	0.14149900	H	-4.82998500	0.68138300	-3.21853700
H	2.63646200	5.37518900	0.87107100	C	-5.83201700	1.57747700	-0.02097300
C	0.99606500	5.37868400	-0.50868400	H	-5.69696800	1.18603500	0.99050300
C	0.28346200	4.65485500	-1.45943200	H	-6.90171800	1.72118100	-0.20218100
H	-0.55449400	5.12056300	-1.96747900	H	-5.33842200	2.55187700	-0.06482800
C	0.62746400	3.33431400	-1.77347400	C	-1.80085200	1.47089200	1.62367800
C	-0.14054400	2.59877900	-2.86972900	C	-1.19102600	2.74025400	1.52324600
C	3.72514500	2.90759800	0.52499900	H	-0.40274200	2.89076300	0.79248700
C	2.12087100	-2.14233900	-1.63374300	C	-1.57378700	3.80103300	2.33774700
C	3.13701900	-2.94601800	-1.07411500	H	-1.08182200	4.76370300	2.22271900
C	4.44606300	-2.37499600	-0.53454600	C	-2.58521100	3.63784100	3.29162100
C	2.93926400	-4.33374700	-1.08462700	H	-2.88482600	4.46590100	3.92771000
H	3.69924000	-4.97979800	-0.65826400	C	-3.20203200	2.39337100	3.40693500
C	1.79371100	-4.89869200	-1.63457100	H	-3.99186700	2.24365200	4.13934400
C	0.81863800	-4.08449000	-2.20304900	C	-2.81762400	1.32797400	2.58784900
H	-0.06522300	-4.53700500	-2.63885600	H	-3.32135800	0.37241600	2.69059300
C	0.96052700	-2.69221700	-2.22491400	H	4.28508400	-1.31703900	-0.31262300
C	-0.07997300	-1.82961900	-2.93573300	H	-0.04143400	-0.82954300	-2.49562500
C	-1.34351500	0.35606300	0.73314100	H	0.10324800	1.53509900	-2.79834700
H	-1.21948600	0.75825300	-0.27669200	H	3.67328400	1.81873300	0.46046100
C	-2.06070600	-2.02510500	1.28293100	C	-0.26421200	-0.34737700	3.61189800
C	-0.85661300	-2.71307000	1.06508700	H	-1.23797100	-0.72624200	3.34295000
H	-0.11004700	-2.28126900	0.40666200	H	-0.13027200	0.72789800	3.58399500
C	-0.61383100	-3.94604800	1.66974100	Br	2.82611500	-0.34310400	2.10117500
H	0.32585900	-4.45528300	1.47496900	C	0.68744500	-1.16685900	4.17640700
C	-1.57579300	-4.52955300	2.49779400	H	0.51527300	-2.24041900	4.18969000
H	-1.38919600	-5.49198700	2.96575300	C	1.95223700	-0.68507300	4.51391300
C	-2.78306800	-3.86178400	2.70889500	H	2.11106500	0.37585200	4.66390600
H	-3.54384200	-4.30062300	3.34914000	H	2.71968800	-1.34420000	4.90474700
C	-3.02394200	-2.62252200	2.11353300	H	3.36724600	2.03223900	-3.13033800
H	-3.96733300	-2.11586600	2.27983800	H	3.57629600	-0.71469100	-3.45788600
C	-5.62783200	-0.86066300	-0.91307500	C	3.82559600	3.24955300	2.02098300
C	-7.01647100	-1.08052900	-0.31216200	H	3.99340200	4.31877700	2.19254000

H	2.92089800	2.94860600	2.55510300	C	-2.78873200	1.60665500	2.32566700
H	4.66821700	2.70999700	2.46381200	C	-0.78082600	2.70330300	1.43661500
C	4.99147700	3.37222300	-0.22506500	C	-1.11760600	3.89204800	0.75491300
H	5.88612000	2.93599500	0.23218700	C	-0.21966700	4.96574700	0.84866000
H	4.97279500	3.07183400	-1.27764900	H	-0.44977600	5.89038200	0.32979800
H	5.09228100	4.46306500	-0.19135400	C	0.95190900	4.87031500	1.59012200
C	5.56544300	-2.48765200	-1.59232300	C	1.24227500	3.69911000	2.28433600
H	5.76790700	-3.53666900	-1.83643800	H	2.14792400	3.64289900	2.87783400
H	5.30861400	-1.97508900	-2.52410700	C	0.37918100	2.59850400	2.24216100
H	6.49319400	-2.04587200	-1.21288000	C	0.65844100	1.38190300	3.12382300
C	4.89738200	-3.04082000	0.77741000	C	-2.42062100	4.07412600	-0.01636900
H	4.10988500	-2.99600700	1.53203700	C	-2.97868600	-1.73795600	1.09663100
H	5.18950000	-4.08628900	0.62877500	C	-3.99633000	-2.10543200	0.19106800
H	5.77083400	-2.51349900	1.17449000	C	-4.81544500	-1.08353300	-0.58974400
C	-1.52145900	-2.33512400	-2.76216400	C	-4.31324700	-3.46802900	0.09364500
H	-1.69889700	-3.27078700	-3.30356000	H	-5.08427100	-3.78087500	-0.60230700
H	-1.77090500	-2.49339100	-1.71047400	C	-3.67801100	-4.41908800	0.88355100
H	-2.21473100	-1.59183500	-3.16819500	C	-2.71486400	-4.02428000	1.80860900
C	0.26096400	-1.70178700	-4.43636500	H	-2.24828200	-4.76994700	2.44373600
H	1.25429800	-1.27223600	-4.59473900	C	-2.34855100	-2.67966600	1.94593900
H	0.23749000	-2.68343500	-4.92289100	C	-1.38077300	-2.27477400	3.05873300
H	-0.46833200	-1.05849700	-4.94112400	C	1.38176800	0.09061200	-0.71249600
C	-1.66840100	2.72540000	-2.72872700	H	1.18008700	0.52197300	0.26951100
H	-2.15866000	2.11904400	-3.49768100	C	1.75479200	-2.43266700	-0.87400100
H	-2.02739700	2.37878500	-1.75719600	C	0.54026400	-2.90063400	-0.35735100
H	-2.00428900	3.75842200	-2.87104700	H	-0.07038900	-2.23902000	0.24637400
C	0.30947100	3.08721400	-4.26349500	C	0.10947400	-4.20381900	-0.61859200
H	0.08789000	4.15218900	-4.39386800	H	-0.83854100	-4.53834300	-0.20956500
H	1.38421500	2.94964900	-4.41638900	C	0.89046400	-5.06665400	-1.38828400
H	-0.21613800	2.53561600	-5.05049100	H	0.55617000	-6.08064500	-1.58745100
H	1.66313000	-5.97723800	-1.62821200	C	2.10544700	-4.60831200	-1.90170700
H	0.71042800	6.40149800	-0.27923000	H	2.72282100	-5.26353000	-2.51021400
				C	2.53194200	-3.30469500	-1.65434500
				H	3.47453600	-2.95578800	-2.05918300
				C	5.61987900	-1.40354800	0.74010100
				C	6.91460400	-1.98619000	0.17644300
				H	6.91918200	-3.07105000	0.31604000
				H	7.78694500	-1.57489700	0.69536300
				H	7.01667900	-1.78385100	-0.89127000
				C	5.41538600	-1.87353500	2.18663200
				H	4.49378800	-1.46365900	2.60942100
				H	6.25199100	-1.58365000	2.82965800
				H	5.33503900	-2.96396400	2.19567800
				C	5.44920500	0.15414300	0.56086600
L₃-19₃							
Cu	-0.65621500	0.01620900	-1.13365100				
N	2.22295900	-1.11005800	-0.60554900				
N	-2.67033200	-0.33168400	1.28941600				
N	-1.71622600	1.59327400	1.43883900				
O	4.50900000	-1.92404700	-0.03670600				
O	4.01208800	0.28120100	0.38570900				
B	3.55258100	-0.92833000	-0.10516700				
C	-1.63256700	0.40053900	0.75668600				
C	-3.38765900	0.40055400	2.23126000				

C	-0.73476800	1.11787200	3.01051800	C	-2.04458500	-1.63932300	-1.92815700
C	-0.25495100	2.52988000	2.68083100	C	-1.86117000	-2.99147900	-1.58729500
C	0.39943300	-2.58642600	2.72738800	H	-1.22385300	-3.24478200	-0.74887300
C	4.10577800	0.65849100	-0.07137800	C	-2.45406900	-4.00421700	-2.33814300
C	4.97603600	-0.40005000	-0.41349400	H	-2.29727300	-5.04071600	-2.05290300
C	4.89870200	-1.78638300	0.22276000	C	-3.24121900	-3.69466800	-3.44974600
C	5.98835000	-0.12403500	-1.34378100	H	-3.70386900	-4.48622800	-4.03264400
H	6.66831300	-0.91735400	-1.63387500	C	-3.42666100	-2.35710000	-3.80570700
C	6.14232400	1.14155300	-1.89783200	H	-4.03414600	-2.10156100	-4.66990200
C	5.28767500	2.17415600	-1.52215300	C	-2.83505100	-1.34219000	-3.05477500
H	5.43116400	3.16176700	-1.94691600	H	-2.99662300	-0.30817400	-3.33973700
C	4.25985400	1.96189600	-0.59509800	H	3.87935600	-1.93385500	0.58779500
C	3.40608900	3.13898900	-0.12719600	H	2.44671600	2.74081300	0.21693700
C	-1.43271000	-0.56634200	-1.09325000	H	0.54118600	2.44709200	1.93488900
H	-1.22473600	-0.94256900	-0.08657700	H	1.04188700	-2.37627200	1.86837500
C	-1.94663700	1.87199000	-1.72307200	C	0.19796500	-0.25949200	-2.81084900
C	-0.78044000	2.60602700	-1.46681000	H	-0.65330900	0.29242700	-3.18611900
H	-0.07039300	2.22466300	-0.73981500	H	0.20022900	-1.30878900	-3.08933800
C	-0.53924100	3.80750100	-2.13566500	Br	1.57088300	-2.89246900	-0.84089000
H	0.36562000	4.36619000	-1.92156300	C	1.46997700	0.45131200	-2.94272300
C	-1.46027700	4.30510700	-3.05903600	H	1.42292800	1.53828100	-2.95333500
H	-1.27037000	5.24363100	-3.57160000	C	2.66728800	-0.16607800	-3.05625900
C	-2.62948800	3.58697000	-3.30935400	H	2.73893000	-1.24814800	-3.01140800
H	-3.35965900	3.96132700	-4.02145100	H	3.58369900	0.40003200	-3.18353400
C	-2.86927800	2.38128500	-2.65090800	H	4.51445500	0.76895800	2.58128700
H	-3.78804700	1.83681700	-2.83562200	H	2.23668000	0.35823700	4.11002100
C	-5.53536900	1.04648300	0.54392400	H	-3.29975000	-0.43757800	4.63704400
C	-6.87732500	1.47040100	-0.05076300	H	6.93606400	1.32809500	-2.61600800
H	-6.94084300	2.56227400	-0.07252100	C	-0.46572600	-3.79440700	2.32805900
H	-7.70895300	1.09495900	0.55490500	H	0.17711700	-4.58092900	1.92368900
H	-6.99793200	1.10535800	-1.07205100	H	-1.01313200	-4.21356600	3.18059000
C	-5.31457400	1.74037200	1.89345200	H	-1.19032600	-3.52946300	1.55371900
H	-4.35745200	1.44792100	2.33144700	C	1.29782200	-2.95531800	3.92719800
H	-6.11252100	1.50509100	2.60460100	H	0.69548600	-3.17839600	4.81578700
H	-5.30172000	2.82254400	1.73572700	H	1.89290600	-3.84371200	3.69056200
C	-5.28739600	-0.51344100	0.59344300	H	1.99200100	-2.15009700	4.18527100
C	-5.59674600	-1.17663900	1.93352600	C	5.16626500	-2.92398500	-0.77814600
H	-5.37531400	-2.24601100	1.87192200	H	6.20815300	-2.94044200	-1.11891600
H	-6.65582600	-1.06416100	2.18888900	H	4.96445000	-3.88412300	-0.29447900
H	-4.99251700	-0.75428000	2.73725700	H	4.50397600	-2.85446800	-1.64243800
C	-5.98427400	-1.27610900	-0.54238300	C	5.88210600	-1.89903400	1.40827200
H	-5.77800300	-0.82146500	-1.51502300	H	6.91623900	-1.75500900	1.07436900
H	-7.06836800	-1.31493900	-0.39762600	H	5.68020000	-1.16378700	2.19224100
H	-5.59944500	-2.29877600	-0.56844400	H	5.81132700	-2.89373200	1.86111400

C	-1.36598800	3.40296100	2.06848600
H	-0.94993200	4.36157700	1.74096400
H	-1.82880600	2.92358700	1.20294300
H	-2.15424600	3.62524700	2.79558900
C	0.33975900	3.22071300	3.92596900
H	-0.41529800	3.32357400	4.71311400
H	1.18122500	2.65832100	4.34059100
H	0.69829900	4.22430500	3.67217100
C	3.10772700	4.15515700	-1.24220400
H	4.00435400	4.70491200	-1.54689800
H	2.68934300	3.67390200	-2.13064900
H	2.38918500	4.89851100	-0.88189600
C	4.07363600	3.85970500	1.06463000
H	3.45073700	4.69410000	1.40571800
H	4.22732400	3.18848500	1.91326300
H	5.04924100	4.26412500	0.77302200

L₃-2I₃

Cu	0.00000600	-0.00526000	1.44902900
Br	0.00000800	-0.01256600	3.69100800
C	0.00000000	0.00116800	-0.44708400
N	1.07667200	0.00420300	-1.28780800
N	-1.07667500	0.00415600	-1.28780400
C	0.67851800	0.00882400	-2.61970100
C	-0.67852600	0.00873300	-2.61969800
H	1.39034500	0.01155900	-3.42941300
H	-1.39035600	0.01155100	-3.42940800
C	-2.45766900	0.00285100	-0.85800200
C	-3.10406600	-1.23419900	-0.66553600
C	-3.10424300	1.23877400	-0.65894400
C	-4.44610200	-1.20483200	-0.26759400
C	-4.44631000	1.20713000	-0.26129300
C	-5.11253900	0.00057900	-0.06820300
H	-4.97233200	-2.14059900	-0.10587100
H	-4.97270300	2.14196900	-0.09475500
C	2.45766800	0.00291400	-0.85801100
C	3.10412300	-1.23412900	-0.66569200
C	3.10418700	1.23884400	-0.65881400
C	4.44615700	-1.20474300	-0.26773600
C	4.44625700	1.20721800	-0.26117900
C	5.11253900	0.00067400	-0.06821600
H	4.97243000	-2.14050400	-0.10612000
H	4.97260700	2.14206200	-0.09453500

C	-2.40302400	2.58041500	-0.84630600
H	-1.36978700	2.38516500	-1.14698200
C	-2.40262700	-2.57475600	-0.85977800
H	-1.37013500	-2.37777200	-1.16189200
C	2.40291500	2.58047200	-0.84605500
H	1.36970800	2.38521500	-1.14683400
C	2.40273500	-2.57469900	-0.86004600
H	1.37023800	-2.37772300	-1.16214700
C	-3.05805400	3.40830400	-1.96919600
H	-3.05998700	2.86511100	-2.92008300
H	-4.09633200	3.66006500	-1.72845800
H	-2.51491600	4.34793100	-2.11610500
C	-2.34864400	3.37392700	0.47404200
H	-3.35224400	3.63489000	0.82658100
H	-1.85509700	2.79864500	1.26286000
H	-1.79373600	4.30761500	0.33173500
C	2.34843300	3.37380900	0.47439600
H	1.85493500	2.79839900	1.26315100
H	3.35201600	3.63482700	0.82695200
H	1.79343900	4.30746200	0.33221200
C	3.05795400	3.40855400	-1.96879900
H	4.09622300	3.66030700	-1.72801600
H	3.05989400	2.86552000	-2.91977600
H	2.51479100	4.34819500	-2.11554600
C	3.05964000	-3.39844700	-1.98486300
H	3.06403200	-2.85138500	-2.93352000
H	4.09718600	-3.65206700	-1.74293800
H	2.51611100	-4.33705400	-2.13677100
C	2.34538200	-3.37336300	0.45706800
H	3.34824100	-3.63577200	0.81064700
H	1.85030500	-2.80106700	1.24709700
H	1.79063900	-4.30640700	0.30997800
C	-2.34527500	-3.37332000	0.45739700
H	-1.85031300	-2.80093900	1.24743700
H	-3.34814200	-3.63581900	0.81090000
H	-1.79042700	-4.30631600	0.31041800
C	-3.05947500	-3.39862600	-1.98454000
H	-4.09704000	-3.65221400	-1.74266000
H	-3.06378500	-2.85167900	-2.93326200
H	-2.51593900	-4.33725800	-2.13629100
H	-6.15293300	-0.00032900	0.24393300
H	6.15293300	-0.00021200	0.24392000

a-at 298K

C	0.40144000	0.40506700	-0.17067600
N	-0.45621800	-0.50277200	0.11412300
C	-1.83173500	-0.21421000	0.06745800
C	-2.69492200	-1.22832900	-0.37957000
C	-2.38097500	1.00868200	0.49263800
C	-4.06753500	-1.00781900	-0.44692400
H	-2.26236000	-2.17685800	-0.68114700
C	-3.75840000	1.21601700	0.43947500
H	-1.72966900	1.77781300	0.89668600
C	-4.60636500	0.21531000	-0.03831500
H	-4.72125500	-1.79625000	-0.80876900
H	-4.17142500	2.16085300	0.78157400
H	-5.67885800	0.38054000	-0.07631800
C	1.84967900	0.18169700	-0.08297500
C	2.72859000	1.22004100	-0.42687300
C	2.37775600	-1.05126200	0.33858000
C	4.10826000	1.03513700	-0.35195200
H	2.32437700	2.17503300	-0.75391500
C	3.75385400	-1.23420900	0.41081200
H	1.68811200	-1.84626100	0.60132400
C	4.62307400	-0.19243700	0.06683500
H	4.77956700	1.84554900	-0.61993700
H	4.15562600	-2.18929300	0.73655000
H	5.69759500	-0.33953500	0.12566400
H	0.09548800	1.40570600	-0.51167000

b- at 298K

C	2.76408100	-0.33578200	-0.28882300
H	2.86297300	0.03435600	-1.30617400
H	3.56583400	-0.96655200	0.08161800
C	1.71070700	-0.02886900	0.46980000
H	1.62903800	-0.42103900	1.48138900
C	0.60623400	0.85975000	0.02247700
H	0.75255500	1.24406800	-0.98587200
H	0.40948200	1.67722000	0.71600900
Br	-1.13445700	-0.12967600	-0.03450600

LiOtBu- at 298K

O	1.27085700	-0.00031800	-0.00064700
C	-0.11642800	0.00001400	0.00003500

C	-0.63090900	-1.12394400	0.92522200
H	-0.25833500	-0.96687600	1.94337900
H	-1.72614700	-1.16736900	0.96149800
H	-0.25914500	-2.09293400	0.57444200
C	-0.63033500	1.36332900	0.51111700
H	-0.25752000	2.16634000	-0.13411200
H	-1.72556400	1.41707100	0.53100000
H	-0.25813100	1.54393100	1.52551400
C	-0.63199100	-0.23896100	-1.43558200
H	-0.25973900	-1.19923300	-1.80896500
H	-1.72729100	-0.24867000	-1.49033600
H	-0.26067600	0.54931100	-2.09959600
Li	2.87455800	-0.00055300	-0.00080200

B₂(pin)₂- at 298K

B	0.85316000	-0.00022700	-0.00030400
O	1.61574000	-1.08126500	-0.37271300
O	1.61538900	1.08102400	0.37224100
C	3.00462500	0.78754100	0.04605900
C	3.00479200	-0.78750800	-0.04599000
C	3.29226000	-1.47938000	1.29329100
H	3.07495700	-2.54618900	1.19361200
H	4.33916900	-1.36643500	1.59047100
H	2.65953000	-1.08004400	2.09055700
C	3.89178100	-1.37819400	-1.14029100
H	4.94563400	-1.14045600	-0.96069800
H	3.78710500	-2.46673300	-1.14684400
H	3.61451100	-1.00858500	-2.12893000
C	3.89110900	1.37845700	1.14066800
H	3.61355100	1.00886100	2.12922700
H	4.94507700	1.14091400	0.96148700
H	3.78621500	2.46697500	1.14712300
C	3.29243400	1.47940300	-1.29314800
H	4.33949600	1.36675200	-1.58989200
H	2.66015000	1.07977000	-2.09062200
H	3.07475300	2.54615400	-1.19367400
B	-0.85317300	-0.00020600	-0.00031600
C	-3.00462100	0.78754600	0.04638800
O	-1.61541700	1.08085400	0.37275000
C	-3.00480100	-0.78750900	-0.04634800
O	-1.61574200	-1.08108500	-0.37317200
C	-3.29241300	1.48009400	-1.29245400
H	-4.33947500	1.36766300	-1.58926100

H	-3.07465200	2.54677600	-1.19240500	C	2.27577700	1.55961700	1.21959000
H	-2.66011900	1.08088000	-2.09012400	H	2.03812600	1.10689400	2.18367600
C	-3.89111400	1.37793900	1.14129800	H	3.36387700	1.57311900	1.09789700
H	-3.78611700	2.46644400	1.14833000	H	1.92569700	2.59578500	1.23783000
H	-4.94509700	1.14057500	0.96198500	C	1.79989000	1.58591400	-1.24517500
H	-3.61359200	1.00777500	2.12965500	H	2.85876800	1.73067800	-1.47905500
C	-3.29228900	-1.47999300	1.29259200	H	1.32875100	1.06544000	-2.08366700
H	-4.33920400	-1.36724200	1.58979200	H	1.33200700	2.56972000	-1.15021900
H	-3.07490600	-2.54674100	1.19244200				
H	-2.65957900	-1.08099100	2.09003800				
C	-3.89176300	-1.37774400	-1.14095100				
H	-3.78684700	-2.46625700	-1.14810000				
H	-4.94565900	-1.14031900	-0.96120400				
H	-3.61460400	-1.00752600	-2.12938700				

tBuOB(pin)- at 298K

O	-1.56557800	-0.83748400	-0.31031900
C	-2.73239400	-0.03587100	0.00419800
C	-3.92162700	-0.93655200	-0.34320200
H	-3.89668700	-1.20813000	-1.40246000
H	-3.88573400	-1.85757500	0.24572000
H	-4.86753200	-0.42675100	-0.13577300
C	-2.74003900	1.23048700	-0.86138500
H	-3.65305700	1.80773200	-0.68367400
H	-1.87959600	1.86243700	-0.63082300
H	-2.70589900	0.96340000	-1.92228600
C	-2.73085800	0.30561800	1.50013200
H	-3.64379300	0.84677800	1.76896200
H	-2.69022200	-0.61146200	2.09623200
H	-1.87092200	0.92862500	1.75670700
B	-0.27494600	-0.45388900	-0.17735500
O	0.75059600	-1.29857200	-0.54812400
O	0.17777500	0.75702800	0.32142400
C	1.60898700	0.81325100	0.06657600
C	1.98300200	-0.71670400	-0.05441300
C	2.27792000	-1.37300300	1.30140400
H	2.31616300	-2.45719700	1.16675500
H	3.23548200	-1.04181500	1.71434100
H	1.49133200	-1.15061300	2.02799700
C	3.10013000	-1.03519800	-1.04586600
H	4.03919700	-0.55919200	-0.74466500
H	3.26362900	-2.11612500	-1.07671300
H	2.84808400	-0.70543100	-2.05501000