

## Electronic supplementary information (ESI)

### Supramolecular Catalysis in the Methylation of *meta*-Phenylene Ethynylene Foldamer Containing *N,N*-Dimethylaminopyridine

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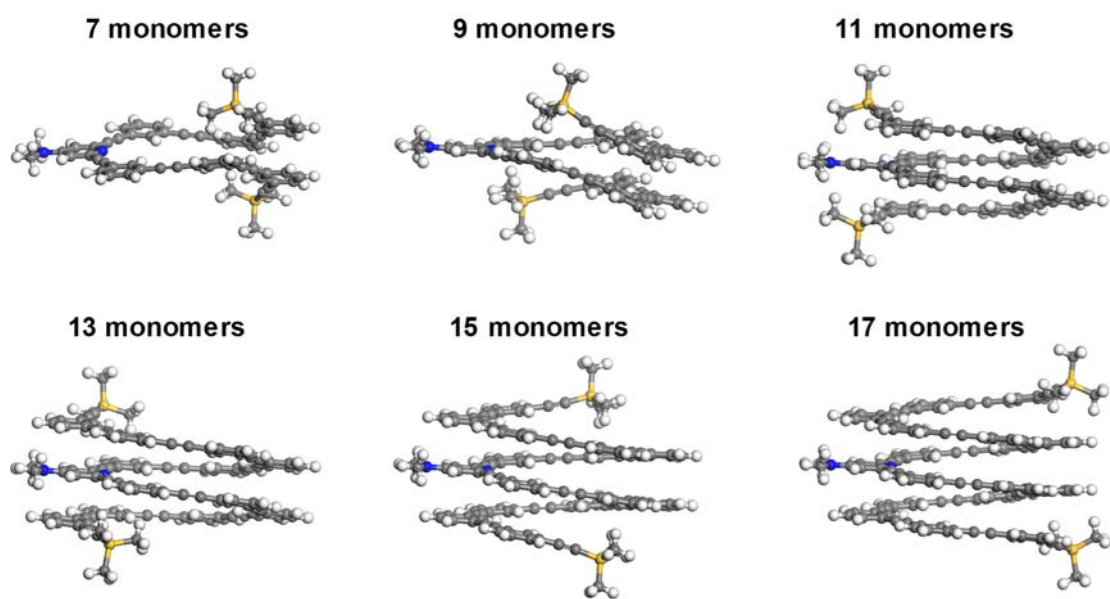
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**Figure S1.** Optimized structures of DMAP-modified *m*PE foldamers with 7-17 monomer

units.....S2

**Table S1.** The absolute free energies of all stationary points in methylation reactions of DMAP-modified foldamer **1** and trimer **1'** with methyl sulfonate esters **2a-2h**.....S3

**Table S2.** The atom coordinates of all stationary points in methylation reactions of DMAP-modified foldamer **1** and trimer **1'** with methyl sulfonate esters **2a-2h**.....S5



**Figure S1.** Optimized structures of DMAP-modified *m*PE foldamers with 7, 9, 11, 13, 15, and 17 monomer units.

**Table S1.** The absolute free energies of all stationary points in methylation reactions of DMAP-modified foldamer **1** and trimer **1'** with methyl sulfonate esters **2a-2h**.

Structure	G (Hartree)	Structure	G(Hartree)
2a	-703.402014	1 (13 monomer)	-5035.392477
3a	-5738.789734		
TS-a	-5738.751932		
4a	-5738.806610		
5a	-663.712884	6	-5075.099942
2b	-781.941030	1 (13 monomer)	-5035.392477
3b	-5817.326831		
TS-b	-5817.291206		
4b	-5817.347909		
5b	-742.252393	6	-5075.099942
2c	-860.478431	1 (13 monomer)	-5035.392477
3c	-5895.862795		
TS-c	-5895.828611		
4c	-5895.888045		
5c	-820.788992	6	-5075.099942
2d	-939.014976	1 (13 monomer)	-5035.392477
3d	-5974.402161		
TS-d	-5974.369665		
4d	-5974.423484		
5d	-899.325441	6	-5075.099942
2e	-781.944623	1 (13 monomer)	-5035.392477
3e	-5817.331348		
TS-e	-5817.294885		
4e	-5817.353127		
5e	-742.255719	6	-5075.099942
2f	-860.478505	1 (13 monomer)	-5035.392477
3f	-5895.868733		
TS-f	-5895.831861		
4f	-5895.887966		
5f	-820.788651	6	-5075.099942
2g	-939.015298	1 (13 monomer)	-5035.392477
3g	-5974.408741		
TS-g	-5974.368660		
4g	-5974.423613		
5g	-899.325756	6	-5075.099942
2h	-1017.552222	1 (13 monomer)	-5035.392477
3h	-6052.944188		
TS-h	-6052.905975		
4h	-6052.961137		
5h	-977.862053	6	-5075.099942
2a'	-703.402014	1'(trimer)	-995.997614
3a'	-1699.389359		
TS-a'	-1699.352450		
4a'	-1699.406310		

5a'	-663.712884	6'	-1035.699567
2b'	-781.941030	1'(trimer)	-995.997614
3b'	-1777.925505		
TS-b'	-1777.891435		
4b'	-1777.944038		
5b'	-742.252393	6'	-1035.699567
2c'	-860.478431	1'(trimer)	-995.997614
3c'	-1856.465917		
TS-c'	-1856.425592		
4c'	-1856.483805		
5c'	-820.788992	6'	-1035.699567
2d'	-939.014976	1'(trimer)	-995.997614
3d'	-1935.001073		
TS-d'	-1934.963813		
4d'	-1935.018041		
5d'	-899.325441	6'	-1035.699567
2e'	-781.944623	1'(trimer)	-995.997614
3e'	-1777.930666		
TS-e'	-1777.892074		
4e'	-1777.946061		
5e'	-742.255719	6'	-1035.699567
2f'	-860.478505	1'(trimer)	-995.997614
3f'	-1856.466989		
TS-f'	-1856.428134		
4f'	-1856.480621		
5f'	-820.788651	6'	-1035.699567
2g'	-939.015298	1'(trimer)	-995.997614
3g'	-1935.00336		
TS-g'	-1934.963664		
4g'	-1935.014344		
5g'	-899.325756	6'	-1035.699567
2h'	-1017.552222	1'(trimer)	-995.997614
3h'	-2013.54089		
TS-h'	-2013.502122		
4h'	-2013.556689		
5h'	-977.862053	6'	-1035.699567
2a	-703.402014	1 (15 monomer)	-5649.422914
3a	-6352.823352		
TS-a	-6352.783888		
4a	-6352.845603		
5a	-663.712884	6	-5689.131902
2a	-703.402014	1 (17 monomer)	-6263.454097
3a	-6966.849861		
TS-a	-6966.816914		
4a	-6966.874153		
5a	-663.712884	6	-6303.165033

**Table S2.** The atom coordinates of all stationary points in methylation reactions of DMAP-modified foldamer **1** (13, 15, and 17 monomers) and trimer **1'** with methyl sulfonate esters **2a-2h**.

Structure	Atom	x, y, and z		
3a	O	-0.41828500	-5.33888600	-1.02866800
	C	-0.32153200	-3.93282200	-0.67673100
	H	0.15149600	-3.80857000	0.29981300
	H	0.31197400	-3.49101700	-1.44343700
	H	-1.30860700	-3.46982200	-0.68434200
	N	-0.03682700	-0.97063900	-0.20810400
	S	-1.34399800	-6.28005800	-0.12754400
	O	-1.53956000	-7.48430100	-0.91643100
	O	-2.50449200	-5.52566900	0.32747300
	C	-0.31225700	-6.64963300	1.26636800
	H	-0.07810900	-5.72444700	1.79337200
	H	0.59115000	-7.13712100	0.90180600
	H	-0.88145100	-7.31805400	1.91353500
	C	1.13300300	-0.33189100	-0.04530000
	C	1.29646300	1.04998000	-0.08317900
	H	2.28632100	1.46382500	0.05819300
	C	0.16918800	1.87303900	-0.28057700
	N	0.26734600	3.22850200	-0.31647000
	C	-1.06551000	1.21273800	-0.44174200
	H	-1.98621900	1.75494700	-0.61239900
	C	-1.10220300	-0.17828400	-0.40978000
	C	1.57313100	3.85871800	-0.26593800
	C	-0.93695500	4.03394900	-0.39580200
	H	1.45125600	4.93671800	-0.35994400
	H	2.20990200	3.51135200	-1.08823000
	H	2.08708700	3.64915000	0.68022400
	H	-1.48422700	3.84877900	-1.32809100
	H	-0.66395600	5.08737400	-0.36100600
	H	-1.60814600	3.82190100	0.44521200
	C	-1.46979100	-14.24014500	1.58778800
	C	-2.52307500	-13.33832800	1.68353800
	C	-2.26973200	-11.95715100	1.66883000
	C	0.10452400	-12.40993800	1.44988100
	C	-0.15933300	-13.78672800	1.47444700
	H	-1.67132000	-15.30623700	1.59904200
	C	-3.34535800	-11.01867200	1.78219600
	C	-4.25394500	-10.22242700	1.87860300
	C	-7.71298100	-8.86716300	2.18272800
	C	-7.46974400	-7.49994400	2.22293800
	C	-6.15344900	-7.01685800	2.14716500
C	-5.33923100	-9.29472100	1.98812200	
C	-6.65774400	-9.76582900	2.06960300	
H	-8.73177700	-9.23632600	2.23795900	
C	-5.90867200	-5.60724500	2.20116700	

C	-5.72565000	-4.41033500	2.24881100
C	-6.50837300	-0.76969600	2.33175700
C	-5.24035900	-0.21712300	2.46417700
C	-4.11169500	-1.05057300	2.52305800
C	-5.54956000	-2.99096800	2.31463000
C	-6.66972600	-2.14858600	2.26008000
H	-7.37720300	-0.12176900	2.28375000
C	2.29246900	-1.15540200	0.18214800
C	3.26988600	-1.84226900	0.38411800
C	6.83393600	-2.81425400	0.87953500
C	6.74308300	-4.20029900	0.89927800
C	5.49268700	-4.82587700	0.76729600
C	4.43757800	-2.64955500	0.57464500
C	5.69109000	-2.03613200	0.72256300
H	7.80282200	-2.33641800	0.98445700
C	5.40000800	-6.25358900	0.81917700
C	5.34022800	-7.46249300	0.87886000
C	6.27486000	-11.07429600	1.03186900
C	5.02393100	-11.67373200	1.12269300
C	3.86646100	-10.88025300	1.13829800
C	5.24217100	-8.88881700	0.96000600
C	6.39249200	-9.69042300	0.95241800
H	7.16724400	-11.69106800	1.01873500
C	1.44382500	-11.91771900	1.33357400
C	2.56496300	-11.46733000	1.24136800
C	-0.95510700	-11.49943500	1.54469500
C	-5.09079700	-7.91680100	2.02204100
C	-4.26976600	-2.43751700	2.43884900
C	4.34275300	-4.04654000	0.59760100
C	3.98208300	-9.48976700	1.05129600
H	-3.54506900	-13.69069100	1.77417200
H	0.66395000	-14.48878000	1.39500900
H	-8.28870800	-6.79461300	2.31528000
H	-6.84300800	-10.83408100	2.03348300
H	-5.10939900	0.85796200	2.52608300
H	-7.65680100	-2.58554100	2.15386600
H	7.63119600	-4.81038600	1.02499700
H	5.75590300	-0.95290700	0.69739000
H	4.93126100	-12.75269200	1.18550700
H	7.36771100	-9.22242600	0.87233800
H	-0.75533600	-10.43334300	1.51565500
H	-4.07460200	-7.54346000	1.94302200
H	-3.39991500	-3.08570400	2.46074900
H	3.37567100	-4.52491300	0.47961200
H	3.08944800	-8.87371500	1.05133600
C	0.80378100	2.77724000	2.97171100
C	-1.72295800	0.04806600	2.79812400
C	-2.80979000	-0.47263200	2.66940900
C	1.96932600	2.06187400	3.22663700

C	1.92424000	0.66490700	3.35629900
C	-0.46451000	0.71586300	2.94128700
C	-0.40937800	2.11444900	2.83612900
H	0.84056000	3.85854700	2.88273800
C	0.70570200	-0.00579100	3.20252400
H	2.91775900	2.57571100	3.34431400
H	-1.32372500	2.66617000	2.64199200
H	0.66728100	-1.08648700	3.29023900
C	3.11521300	-0.06137900	3.69511100
C	4.12257800	-0.65534800	4.03705800
Si	5.61092500	-1.55115500	4.67935800
C	7.15133500	-0.77438100	3.93870900
C	5.44308100	-3.36816600	4.25128400
C	5.64459600	-1.33183100	6.54559100
H	7.27575100	0.24828700	4.30649000
H	7.10847900	-0.74366700	2.84807500
H	8.03656600	-1.34905000	4.22951600
H	5.25335600	-3.51299800	3.18465200
H	4.61712800	-3.81618900	4.81234500
H	6.36117300	-3.90527100	4.51132400
H	4.74606900	-1.74818400	7.00941700
H	5.71334700	-0.27472200	6.81701700
H	6.51414200	-1.84705400	6.96655800
C	-0.01907100	-14.25880300	-1.90741700
C	1.16598800	-13.53988200	-2.00555500
C	1.13960600	-12.13633300	-1.98616400
C	-1.27478500	-12.19675200	-1.76080000
C	-1.23745100	-13.59810900	-1.78820800
H	0.00615100	-15.34339100	-1.92082600
C	2.35370300	-11.38524700	-2.09303500
C	3.37595700	-10.74072800	-2.18226800
C	6.97991700	-9.80027300	-2.42476300
C	6.89433400	-8.41413300	-2.47888300
C	5.63929900	-7.78596500	-2.44398100
C	4.57078100	-9.95841200	-2.28436100
C	5.82884300	-10.57565100	-2.32967000
H	7.95219800	-10.28122600	-2.45214500
C	5.53903400	-6.35901000	-2.50850700
C	5.44957300	-5.15181100	-2.56642400
C	6.44439300	-1.56030800	-2.58475800
C	5.21611900	-0.93685700	-2.76224700
C	4.04559700	-1.70438600	-2.88193700
C	5.36361900	-3.72383200	-2.63189700
C	6.52588200	-2.94707800	-2.52126600
H	7.34500400	-0.96228700	-2.49264900
C	-2.36566400	-0.83978600	-0.60753400
C	-3.43825200	-1.38514700	-0.75056700
C	-7.11088500	-1.91147800	-1.14006400
C	-7.18619300	-3.29921500	-1.17186400

C	-6.01494700	-4.06742600	-1.07861600
C	-4.70547300	-2.03340300	-0.90900300
C	-5.88023500	-1.27397500	-1.01275900
H	-8.01888900	-1.32098100	-1.21086100
C	-6.06571300	-5.49706200	-1.13134900
C	-6.07133900	-6.70761400	-1.18524500
C	-7.23398600	-10.25299300	-1.27618700
C	-6.02475400	-10.93024400	-1.37561700
C	-4.81805600	-10.21291900	-1.41942700
C	-6.05936800	-8.13799400	-1.25054100
C	-7.25939500	-8.86327100	-1.21654700
H	-8.16396600	-10.81164500	-1.24168500
C	-2.52154800	-11.50398300	-1.63733600
C	-3.57124300	-10.90748900	-1.53360700
C	-0.08247500	-11.46962100	-1.85761700
C	4.48156500	-8.56262600	-2.34181500
C	4.12307500	-3.09806500	-2.80971900
C	-4.77649200	-3.43087600	-0.93840900
C	-4.83769400	-8.81618800	-1.34924100
H	2.11746100	-14.05224100	-2.10043900
H	-2.16372600	-14.15657300	-1.70603000
H	7.79095700	-7.80786900	-2.55121100
H	5.89360600	-11.65728800	-2.27831100
H	5.14755000	0.14451600	-2.81467000
H	7.48182900	-3.43880200	-2.37680100
H	-8.14408000	-3.79752700	-1.27618800
H	-5.81753100	-0.19092300	-0.97739300
H	-6.00074700	-12.01389400	-1.42372600
H	-8.20118500	-8.33108400	-1.13284400
H	-0.10928100	-10.38531100	-1.82788000
H	3.50986000	-8.08172900	-2.30103800
H	3.22160700	-3.69669300	-2.88862900
H	-3.87459800	-4.02680900	-0.83673800
H	-3.90499900	-8.25857700	-1.36369700
C	-0.27822600	2.67612900	-3.57981600
C	1.77120800	-0.40673600	-3.24113400
C	2.79289600	-1.03768000	-3.07567200
C	-1.54653000	2.15174200	-3.80477500
C	-1.73543000	0.76193900	-3.85638500
C	0.62858600	0.43583900	-3.43022800
C	0.80658200	1.82810200	-3.40038700
H	-0.13375400	3.75147500	-3.54822100
C	-0.64579300	-0.09463000	-3.65941500
H	-2.39633600	2.80917800	-3.95662900
H	1.80096300	2.22922200	-3.23202900
H	-0.79040300	-1.16956900	-3.68615000
C	-3.03704100	0.23571000	-4.15531800
C	-4.13803900	-0.18641000	-4.46141500
Si	-5.77352700	-0.83518900	-5.03796800



	C	-7.14150000	0.17893400	-4.24905700
	C	-5.88251600	-2.64857700	-4.58083200
	C	-5.84357800	-0.62814400	-6.90418500
	H	-7.08158800	1.22281600	-4.56971700
	H	-7.08832800	0.15007000	-3.15870400
	H	-8.11732000	-0.21344900	-4.55278700
	H	-5.67637700	-2.79970100	-3.51828600
	H	-5.16073600	-3.23307100	-5.15857800
	H	-6.88375900	-3.03663600	-4.79358400
	H	-5.03371600	-1.17507400	-7.39453000
	H	-5.76710300	0.42517700	-7.18762400
	H	-6.79403600	-1.01381500	-7.28668100
	O	0.06306000	-4.75294300	-0.65302900
	C	-0.01141200	-2.90635000	-0.39879100
	H	0.46534300	-2.95639000	0.56874800
	H	0.60377500	-2.77931500	-1.27814900
	H	-1.08794100	-2.88044300	-0.46763200
	N	-0.00622400	-0.87510900	-0.22197900
	S	-0.95411600	-5.62389000	0.08210600
	O	-1.23045700	-6.84129800	-0.68824400
	O	-2.13106400	-4.83541800	0.48681000
	C	-0.11928900	-6.11443600	1.57559400
	H	0.13168800	-5.21867000	2.14445300
	H	0.78410200	-6.66004900	1.30383700
	H	-0.79251800	-6.75111300	2.15001300
	C	1.16756300	-0.24225500	-0.03677400
	C	1.30346200	1.13718100	-0.04982700
	H	2.28567700	1.56152000	0.10800800
	C	0.16025400	1.94661800	-0.23623500
	N	0.24177700	3.29674700	-0.25365100
TS-a	C	-1.07071600	1.27457700	-0.40530800
	H	-1.99801900	1.80856200	-0.56193200
	C	-1.09936500	-0.11264700	-0.40939300
	C	1.54162800	3.94392200	-0.18866100
	C	-0.97145800	4.09295400	-0.33737900
	H	1.40578800	5.02047500	-0.27300100
	H	2.18539800	3.61141700	-1.01081300
	H	2.04889200	3.73084400	0.75968900
	H	-1.50874900	3.90412500	-1.27397100
	H	-0.70685700	5.14786300	-0.29836100
	H	-1.64338000	3.87251400	0.49978300
	C	-1.49871100	-14.35557100	1.63546100
	C	-2.59189200	-13.49779600	1.67552400
	C	-2.39615900	-12.10877800	1.62787400
	C	0.00062900	-12.46343400	1.48881000
	C	-0.20634900	-13.84901700	1.54532600
	H	-1.65489200	-15.42850400	1.67252400
	C	-3.50555500	-11.20540200	1.68542900
	C	-4.42002100	-10.41222100	1.74070200

C	-7.84131500	-8.92685400	1.88027900
C	-7.54367200	-7.57235000	1.96093800
C	-6.20603900	-7.14494200	1.97013300
C	-5.48188900	-9.45433900	1.81223800
C	-6.82082700	-9.86952600	1.80803100
H	-8.87638800	-9.25186000	1.87047600
C	-5.90515000	-5.74827700	2.06019700
C	-5.67907400	-4.56047700	2.13856100
C	-6.39544300	-0.91533000	2.36869400
C	-5.11689700	-0.38897500	2.50122100
C	-4.00035900	-1.24150900	2.50250500
C	-5.47030700	-3.14829700	2.24688200
C	-6.57799600	-2.28794500	2.24649700
H	-7.25501300	-0.25360100	2.36176100
C	2.32026000	-1.06873100	0.19015100
C	3.28992100	-1.77332400	0.36344200
C	6.83844800	-2.83357400	0.77157500
C	6.70606700	-4.21547500	0.82183800
C	5.43448800	-4.80746000	0.74326400
C	4.44244900	-2.60449800	0.53945900
C	5.71505900	-2.02354900	0.63604200
H	7.82405200	-2.38409700	0.83634300
C	5.30351400	-6.23042200	0.83128300
C	5.21796100	-7.43563300	0.92509700
C	6.14353000	-11.03885800	1.21181400
C	4.89118900	-11.63702300	1.28480600
C	3.73240500	-10.84586600	1.24245800
C	5.10989900	-8.85871700	1.04386700
C	6.26098700	-9.65797300	1.09302600
H	7.03676600	-11.65386700	1.24113000
C	1.32373300	-11.92353400	1.39853100
C	2.43347100	-11.44216100	1.32586400
C	-1.09832200	-11.59763800	1.52808900
C	-5.17877300	-8.08891000	1.88950300
C	-4.17783800	-2.62133700	2.36112100
C	4.30393100	-3.99709300	0.59242300
C	3.84760700	-9.45828300	1.11675800
H	-3.60001400	-13.89135200	1.74918200
H	0.64806200	-14.51626400	1.50966500
H	-8.33682700	-6.83461300	2.02004500
H	-7.04934900	-10.92769300	1.73908000
H	-4.96694200	0.68026000	2.60653200
H	-7.57329600	-2.70690200	2.14376900
H	7.57929900	-4.84970000	0.93124700
H	5.81029400	-0.94353000	0.58696200
H	4.79723600	-12.71375500	1.37739400
H	7.23726300	-9.19004600	1.02544500
H	-0.94332000	-10.52501200	1.47583600
H	-4.14397700	-7.76218000	1.87849300

H	-3.31855700	-3.28309000	2.31964700
H	3.31892400	-4.44556000	0.50740700
H	2.95413400	-8.84474900	1.07392800
C	0.79347200	2.68275400	3.04574700
C	-1.61414500	-0.14220500	2.79202700
C	-2.69264400	-0.67692500	2.65048200
C	1.99195200	2.01213600	3.26751600
C	2.01030900	0.61092400	3.34845200
C	-0.38139600	0.56774000	2.95262200
C	-0.38946400	1.97050100	2.89519100
H	0.78052100	3.76695200	2.99527000
C	0.82168500	-0.10904000	3.18132100
H	2.91756200	2.56343500	3.39649300
H	-1.32973400	2.48573000	2.72702100
H	0.83336200	-1.19289000	3.23261700
C	3.23447500	-0.07343000	3.65300300
C	4.26986900	-0.63482500	3.96370700
Si	5.79980200	-1.48485400	4.56884300
C	7.29787500	-0.70023100	3.75356100
C	5.63904200	-3.31385100	4.19101900
C	5.90140400	-1.21915300	6.42610600
H	7.41679300	0.33260500	4.09390100
H	7.21745700	-0.69489100	2.66479600
H	8.20265300	-1.25280800	4.02615100
H	5.35765400	-3.48289600	3.14881100
H	4.87508900	-3.76532200	4.83102000
H	6.58685300	-3.82865500	4.37754600
H	5.02899200	-1.63934600	6.93392100
H	5.96237700	-0.15500500	6.67031300
H	6.79530500	-1.70999300	6.82434700
C	-0.02302700	-14.41037900	-1.81739200
C	1.16719700	-13.69785000	-1.90311100
C	1.14454100	-12.29460300	-1.92470000
C	-1.27609700	-12.34289100	-1.76675400
C	-1.24255700	-13.74437800	-1.75089800
H	-0.00079400	-15.49491300	-1.79747500
C	2.35861600	-11.54139400	-2.01575600
C	3.36999800	-10.87840400	-2.09287300
C	6.95588000	-9.85220100	-2.23739600
C	6.83750000	-8.47156800	-2.34058800
C	5.56659900	-7.87574500	-2.37331200
C	4.54796600	-10.06938700	-2.18145200
C	5.82181400	-10.65396000	-2.15856500
H	7.94024300	-10.30772000	-2.21057300
C	5.43557600	-6.45385600	-2.48198000
C	5.32529600	-5.25008900	-2.56868100
C	6.31171500	-1.66038400	-2.71250300
C	5.07778300	-1.04127200	-2.86029200
C	3.90415700	-1.81170000	-2.91829900

C	5.22995500	-3.82476300	-2.66833900
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C	-2.34608800	-0.79233100	-0.62588200
C	-3.40611900	-1.35637600	-0.78706500
C	-7.06501600	-1.97874000	-1.14341400
C	-7.09839600	-3.36690300	-1.20424400
C	-5.90421700	-4.10369800	-1.14704000
C	-4.65624900	-2.03620800	-0.95074100
C	-5.85166500	-1.30736700	-1.02397700
H	-7.99134600	-1.41499600	-1.18719200
C	-5.92840400	-5.53273900	-1.23526000
C	-5.94301700	-6.74129200	-1.32254000
C	-7.20643300	-10.24013100	-1.58510200
C	-6.01742100	-10.95720500	-1.63360000
C	-4.78719100	-10.28309600	-1.58309900
C	-5.96536100	-8.16942800	-1.42620600
C	-7.18830000	-8.85304300	-1.48499400
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C	-2.52005800	-11.63755400	-1.69834500
C	-3.55922200	-11.01684100	-1.64287500
C	-0.07899500	-11.62250000	-1.85092400
C	4.42563900	-8.67893900	-2.28976200
C	3.98268800	-3.20330800	-2.81468500
C	-4.68276000	-3.43531900	-1.00709500
C	-4.76489100	-8.88894900	-1.47222900
H	2.11879400	-14.21594700	-1.95616400
H	-2.17192900	-14.29877200	-1.67642900
H	7.72057800	-7.84426500	-2.39823800
H	5.91171800	-11.73117400	-2.06757100
H	5.00589400	0.03847100	-2.93610300
H	7.35538500	-3.53409700	-2.49683700
H	-8.04295300	-3.89107300	-1.30412700
H	-5.81934200	-0.22382900	-0.96868200
H	-6.02720200	-12.03895100	-1.71345500
H	-8.11437500	-8.28977000	-1.44194000
H	-0.10167100	-10.53783000	-1.85488100
H	3.44123100	-8.22323600	-2.30279300
H	3.07898000	-3.80331700	-2.84371100
H	-3.75886400	-3.99828300	-0.91102800
H	-3.81695800	-8.36359800	-1.41215700
C	-0.35700800	2.63616700	-3.53365900
C	1.63950700	-0.48629700	-3.22947600
C	2.64911200	-1.14098100	-3.08131000
C	-1.63642800	2.13472900	-3.74910600
C	-1.84929200	0.74849600	-3.80547700
C	0.51273000	0.38032700	-3.40290500
C	0.71537600	1.76925900	-3.36678600
H	-0.19357900	3.70879200	-3.50093800

	C	-0.77237200	-0.12698200	-3.62359800
	H	-2.47579700	2.80752000	-3.89094100
	H	1.71754200	2.15330000	-3.20485300
	H	-0.93498500	-1.19932600	-3.65674200
	C	-3.15822300	0.23975900	-4.10038100
	C	-4.26523300	-0.16880200	-4.40225900
	Si	-5.90261500	-0.79941700	-4.99347500
	C	-7.26997900	0.18292400	-4.16355600
	C	-5.99213400	-2.63037100	-4.60521500
	C	-5.98216000	-0.52219300	-6.85032300
	H	-7.22249600	1.23353400	-4.46418700
	H	-7.20301400	0.13367400	-3.07483400
	H	-8.24610800	-0.21136300	-4.46350900
	H	-5.73561000	-2.82393400	-3.56061400
	H	-5.29585700	-3.18773700	-5.23867800
	H	-7.00071400	-3.01464900	-4.78714900
	H	-5.17374400	-1.04933800	-7.36416200
	H	-5.90851900	0.54124900	-7.09422500
	H	-6.93379500	-0.89487100	-7.24268000
	O	-0.14519400	-5.27228900	-0.51965600
	C	-0.06081500	-2.34536600	-0.22588400
	H	0.48507300	-2.72897000	0.63508600
	H	0.40691500	-2.71405100	-1.14050200
	H	-1.09288100	-2.68186500	-0.17164900
	N	-0.00580900	-0.87110200	-0.21078800
	S	-1.31935500	-5.78342800	0.22616600
	O	-1.96638400	-6.95556400	-0.41396200
	O	-2.28612700	-4.70907000	0.58319600
	C	-0.67392700	-6.37613400	1.78454700
	H	-0.20398000	-5.54050500	2.30657300
	H	0.06315700	-7.15660300	1.58769700
	H	-1.49646400	-6.77736800	2.37786800
	C	1.19989200	-0.24762200	-0.03880600
	C	1.31873700	1.12322500	-0.06012000
	H	2.30454800	1.54180700	0.08450100
	C	0.17308900	1.94061900	-0.23116900
	N	0.25776800	3.27866600	-0.23944900
	C	-1.06422200	1.27023400	-0.39420700
	H	-1.98899500	1.80722000	-0.54940000
	C	-1.12390400	-0.10664900	-0.40192700
	C	1.56133800	3.92731300	-0.16950000
	C	-0.95531000	4.08335200	-0.31527600
	H	1.42257700	5.00397700	-0.23546200
	H	2.19761300	3.60705700	-1.00073900
	H	2.06645700	3.69672900	0.77468000
	H	-1.48954900	3.90096800	-1.25360800
	H	-0.68429400	5.13553800	-0.26892800
	H	-1.62220300	3.85658700	0.52271400
	C	-1.48444100	-14.32262000	1.64561800

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C	-2.58734000	-13.47676900	1.67449300
C	-2.40738300	-12.08605500	1.61725500
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C	-5.48659900	-3.17643200	2.23527700
C	-6.56950500	-2.28550100	2.24545800
H	-7.18868100	-0.23280200	2.37432800
C	2.34697200	-1.06535500	0.17587600
C	3.32037100	-1.76494900	0.34823200
C	6.87407200	-2.80891700	0.71852000
C	6.74448300	-4.19086900	0.77793100
C	5.47362000	-4.78737400	0.72279000
C	4.47652600	-2.58943000	0.51972400
C	5.74741600	-2.00165400	0.59491000
H	7.85978900	-2.35767000	0.76579100
C	5.34385600	-6.20902000	0.82139900
C	5.25359500	-7.41328700	0.91927100
C	6.13835300	-11.02473700	1.22200200
C	4.87881500	-11.60744400	1.29539800
C	3.72889500	-10.80325000	1.24801600
C	5.13019000	-8.83430200	1.04383500
C	6.27211100	-9.64576000	1.09802800
H	7.02415600	-11.65020300	1.25527600
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C	-4.17702400	-2.68811200	2.33891400
C	4.33883100	-3.98141800	0.58401700
C	3.86011700	-9.41781500	1.11676200
H	-3.59128100	-13.88105300	1.74733800
H	0.66463100	-14.45886200	1.53171800
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H	-7.08268300	-10.95336600	1.70012200
H	-4.87372200	0.63363200	2.61570800

H	-7.57699300	-2.67583700	2.14727900
H	7.62102500	-4.82225300	0.87701500
H	5.83875300	-0.92174700	0.53794100
H	4.77188200	-12.68264200	1.39197500
H	7.25369600	-9.18909100	1.03020100
H	-0.97311000	-10.48630800	1.45723200
H	-4.20077800	-7.76813500	1.82776900
H	-3.33871700	-3.37492100	2.26952200
H	3.35362300	-4.43237100	0.51912100
H	2.97448500	-8.79285600	1.07030700
C	0.79352100	2.61929100	3.04557600
C	-1.56346500	-0.24553600	2.78380400
C	-2.64266400	-0.77812400	2.63672500
C	2.00716000	1.97082400	3.25241500
C	2.05280600	0.56991700	3.32870200
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C	-0.37661300	1.88484300	2.89947900
H	0.75854600	3.70354200	3.00360900
C	0.87625600	-0.17264300	3.17103500
H	2.92313500	2.53938000	3.37528100
H	-1.32839400	2.38270300	2.74287200
H	0.90909000	-1.25600900	3.22631000
C	3.29262100	-0.09151700	3.61945800
C	4.34135700	-0.63366900	3.91906000
Si	5.88955100	-1.45539500	4.51986600
C	7.36867300	-0.66057600	3.67999300
C	5.74414100	-3.29026300	4.16562900
C	6.00324600	-1.16411400	6.37226400
H	7.47945400	0.37620800	4.01094100
H	7.27613800	-0.66424500	2.59216600
H	8.28285300	-1.20045900	3.94653700
H	5.44286400	-3.47366700	3.13144200
H	4.99778300	-3.74281500	4.82542500
H	6.70110200	-3.79279800	4.33830100
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H	6.05184200	-0.09620400	6.60244100
H	6.90701300	-1.63783300	6.76899700
C	0.01297400	-14.38453700	-1.79993400
C	1.20990900	-13.68311100	-1.88640400
C	1.19916800	-12.28001400	-1.91758700
C	-1.22234700	-12.30601800	-1.76727300
C	-1.20099600	-13.70767700	-1.74198500
H	0.02570200	-15.46908400	-1.77248000
C	2.41760400	-11.53415000	-2.00931100
C	3.42759000	-10.86914900	-2.08712500
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C	6.88126600	-8.44299900	-2.33668500
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C	4.60132300	-10.05419600	-2.17634500

C	5.87857600	-10.63112300	-2.15145700
H	7.99496400	-10.27217600	-2.20225000
C	5.46759000	-6.43388800	-2.48618000
C	5.35092400	-5.23105500	-2.57806900
C	6.32908800	-1.63945300	-2.74344900
C	5.09322200	-1.02268100	-2.88469600
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H	7.23165700	-1.03873900	-2.70673300
C	-2.36861800	-0.76291200	-0.62333700
C	-3.43282700	-1.31481100	-0.79657800
C	-7.08911800	-1.94484200	-1.16073700
C	-7.11135700	-3.33400500	-1.21570200
C	-5.91337100	-4.06387900	-1.14813700
C	-4.68475500	-1.98740200	-0.95837800
C	-5.88167500	-1.26284100	-1.04191700
H	-8.01974400	-1.38902300	-1.21153400
C	-5.92156400	-5.49270400	-1.23647400
C	-5.91518700	-6.70088200	-1.32791500
C	-7.14240400	-10.20603400	-1.64193000
C	-5.94583700	-10.91036300	-1.68307500
C	-4.72238500	-10.22590000	-1.60376200
C	-5.92026400	-8.12806500	-1.44276600
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H	-8.08559600	-10.73935400	-1.69922300
C	-2.45950800	-11.58866500	-1.70434900
C	-3.49242800	-10.95721400	-1.65381300
C	-0.01883200	-11.59702600	-1.85249200
C	4.47061700	-8.66463100	-2.28769700
C	4.00196400	-3.18735700	-2.82501800
C	-4.69800400	-3.38691300	-1.00180300
C	-4.71003200	-8.83289200	-1.47324300
H	2.15701500	-14.21002400	-1.93263300
H	-2.13529900	-14.25356800	-1.66602100
H	7.76063400	-7.81057200	-2.39511700
H	5.97480700	-11.70763900	-2.05875200
H	5.01892000	0.05661700	-2.96409800
H	7.37697600	-3.51051200	-2.52776800
H	-8.05231200	-3.86414400	-1.31874900
H	-5.85638600	-0.17875100	-0.99598200
H	-5.94365600	-11.99115700	-1.77690800
H	-8.06793000	-8.26409100	-1.49199000
H	-0.03225500	-10.51234600	-1.86338400
H	3.48342300	-8.21508400	-2.30247300
H	3.09887200	-3.78820000	-2.84789600
H	-3.77079900	-3.93960600	-0.87779600
H	-3.77000200	-8.29566800	-1.37572700
C	-0.36308700	2.63285600	-3.52884100



	C	1.65003200	-0.47960800	-3.23564600
	C	2.66369800	-1.12868100	-3.09119500
	C	-1.64244500	2.12534400	-3.73210600
	C	-1.84937300	0.73812500	-3.78891900
	C	0.51780600	0.38074900	-3.40475600
	C	0.71489300	1.77093200	-3.37108100
	H	-0.20366600	3.70630500	-3.50140400
	C	-0.76679400	-0.13285200	-3.61702900
	H	-2.48597700	2.79427800	-3.86682100
	H	1.71743800	2.15940400	-3.22209400
	H	-0.92399500	-1.20595800	-3.65467700
	C	-3.15804200	0.22658100	-4.07919300
	C	-4.26433600	-0.18031500	-4.38550600
	Si	-5.89366400	-0.80916100	-5.00297500
	C	-7.27369200	0.18034400	-4.20365300
	C	-5.99206200	-2.63872500	-4.61233900
	C	-5.93610300	-0.53440200	-6.86128900
	H	-7.21516400	1.22980800	-4.50642900
	H	-7.23194500	0.13426000	-3.11359800
	H	-8.24442800	-0.21071900	-4.52466500
	H	-5.74260400	-2.83179500	-3.56611600
	H	-5.29271400	-3.19855100	-5.24016700
	H	-7.00032400	-3.02068600	-4.80057900
	H	-5.12065800	-1.06589100	-7.35929000
	H	-5.85327400	0.52839500	-7.10500500
	H	-6.88203000	-0.90340400	-7.27054700
3b	N	0.01498400	-0.88887800	-0.21083200
	C	-0.26414900	-3.80409700	-0.36457200
	H	0.01933700	-3.59997100	0.66916700
	H	0.54202600	-3.51092700	-1.03380100
	H	-1.17896100	-3.26798400	-0.61272000
	O	-0.43471200	-5.23204500	-0.58500400
	S	-1.48187700	-6.01784900	0.33823500
	O	-2.17489800	-6.96047400	-0.52833800
	O	-2.26908600	-5.05801500	1.10285200
	C	-0.39553900	-6.91574400	1.43080400
	H	0.20903100	-6.16397500	1.94820200
	H	0.25019500	-7.51371600	0.78138800
	C	-1.19442900	-7.78019300	2.40355900
	H	-1.86274100	-7.13940000	2.98865500
	C	-0.26088400	-8.54871800	3.33717000
	H	-1.82562900	-8.47356500	1.83351600
	H	0.45333700	-9.15978100	2.77359100
	H	-0.83611900	-9.21405800	3.98694300
	H	0.31001200	-7.86102300	3.96873200
	C	1.18254500	-0.24998800	-0.03858500
	C	1.34053600	1.13232100	-0.05611200
	H	2.32805400	1.54921400	0.09199000
	C	0.20798800	1.95187600	-0.24051600

N	0.30034500	3.30808300	-0.25419800
C	-1.02506700	1.28962100	-0.41140000
H	-1.94794200	1.83132800	-0.57154100
C	-1.05513000	-0.10146900	-0.40088600
C	1.60337400	3.94265200	-0.18727900
C	-0.90696300	4.11003300	-0.32280800
H	1.47790000	5.02132500	-0.26705200
H	2.24595800	3.60905800	-1.01080600
H	2.11279000	3.72191000	0.75901200
H	-1.45574400	3.93082600	-1.25530800
H	-0.63737100	5.16402900	-0.27995100
H	-1.57505100	3.88865400	0.51834500
C	-1.43843700	-14.22300600	1.79350000
C	-2.51922700	-13.34816800	1.80223000
C	-2.30679200	-11.96898400	1.65133500
C	0.08227100	-12.36891400	1.48490100
C	-0.14092600	-13.74401500	1.64340200
H	-1.60858500	-15.28828500	1.90910300
C	-3.39986100	-11.04485200	1.69197100
C	-4.30920600	-10.24451400	1.73887000
C	-7.77123000	-8.87223800	1.92582400
C	-7.52084400	-7.50773900	2.00155300
C	-6.19970400	-7.03284600	1.98408000
C	-5.39561800	-9.31448200	1.81579000
C	-6.71898500	-9.77750900	1.83747100
H	-8.79391600	-9.23438600	1.93496500
C	-5.94168100	-5.62790100	2.07341500
C	-5.73751800	-4.43630100	2.15298800
C	-6.47819000	-0.79309000	2.34925000
C	-5.20309200	-0.25832200	2.48467600
C	-4.08191800	-1.10432700	2.50777900
C	-5.54057900	-3.02207400	2.25832500
C	-6.65286400	-2.16766900	2.23929400
H	-7.34091400	-0.13572900	2.32840200
C	2.33753500	-1.08194600	0.18049900
C	3.31850400	-1.77223400	0.35021000
C	6.88801800	-2.76045600	0.78367900
C	6.78834800	-4.14591600	0.81516300
C	5.53152300	-4.76334200	0.70983100
C	4.48837300	-2.58031400	0.52202700
C	5.74825600	-1.97477400	0.64074200
H	7.86162700	-2.28841100	0.86832700
C	5.42246700	-6.18936700	0.77196400
C	5.34139300	-7.39670400	0.83681200
C	6.22709000	-11.01933100	0.99309100
C	4.96968100	-11.60141700	1.10180100
C	3.82251300	-10.79262900	1.12604600
C	5.22164400	-8.82096500	0.92279800
C	6.36112700	-9.63751800	0.90508200

H	7.11126000	-11.64759300	0.97243200
C	1.40771900	-11.84539600	1.34853900
C	2.51870400	-11.37159000	1.24594500
C	-1.00551000	-11.48978200	1.47815300
C	-5.14054900	-7.93917600	1.87992500
C	-4.25247400	-2.48713600	2.38475000
C	4.38487200	-3.97620100	0.55711500
C	3.95412600	-9.40440900	1.03140500
H	-3.52946700	-13.72119600	1.93216700
H	0.70365100	-14.42452800	1.64146500
H	-8.33842700	-6.79871000	2.07716000
H	-6.91013500	-10.84351900	1.77617900
H	-5.05993900	0.81316000	2.57599600
H	-7.64499100	-2.59261600	2.13037500
H	7.67451600	-4.76112700	0.92904400
H	5.82084700	-0.89245700	0.60423100
H	4.86291500	-12.67868100	1.17083000
H	7.34111300	-9.18210200	0.81155900
H	-0.83583000	-10.42911900	1.32901100
H	-4.11983500	-7.57193700	1.83951500
H	-3.39069400	-3.14677800	2.37028200
H	3.41230400	-4.44815800	0.46109600
H	3.06944100	-8.77645900	1.04079100
C	0.76185400	2.77875800	3.03899700
C	-1.69347800	-0.00720300	2.79395400
C	-2.77617900	-0.53384600	2.65381700
C	1.94690200	2.08864700	3.27168000
C	1.94023000	0.68795800	3.36136200
C	-0.45004100	0.68450300	2.95463100
C	-0.43268300	2.08657800	2.88793500
H	0.76880000	3.86252400	2.97847400
C	0.74002400	-0.01185000	3.19248200
H	2.88160600	2.62437000	3.40096300
H	-1.36242800	2.61763100	2.71059900
H	0.73218400	-1.09526800	3.24826100
C	3.15288100	-0.01431500	3.67232500
C	4.17809300	-0.59180200	3.98802900
Si	5.69820500	-1.45775100	4.59510900
C	7.20731400	-0.65538600	3.81852900
C	5.55368100	-3.27794100	4.17107000
C	5.77208800	-1.23640900	6.45974700
H	7.32024200	0.37132000	4.17864500
H	7.14169000	-0.63167000	2.72890300
H	8.10876200	-1.21215800	4.09376300
H	5.33667400	-3.42544800	3.11024500
H	4.75236500	-3.74133100	4.75426200
H	6.48818800	-3.79829500	4.40396900
H	4.89353500	-1.67031400	6.94495600
H	5.82649000	-0.17814400	6.72994900

H	6.66144500	-1.73447300	6.85926600
C	0.01347700	-14.34966200	-1.71544100
C	1.18410600	-13.61410400	-1.85701800
C	1.12670800	-12.21424800	-1.94857800
C	-1.29009700	-12.31358900	-1.75262500
C	-1.22152700	-13.71081000	-1.66311500
H	0.06331400	-15.43084900	-1.63853300
C	2.32431500	-11.44057200	-2.08147500
C	3.32722500	-10.76862100	-2.18803400
C	6.91405900	-9.78278300	-2.47341100
C	6.81166800	-8.39843400	-2.53375700
C	5.55012600	-7.78364100	-2.48931800
C	4.50807300	-9.96721500	-2.30802200
C	5.77276600	-10.57004300	-2.36236300
H	7.89138300	-10.25261500	-2.50818300
C	5.44245200	-6.35721200	-2.56002000
C	5.36439700	-5.14924600	-2.62037200
C	6.44073700	-1.58257500	-2.67810300
C	5.22470600	-0.93005700	-2.83385300
C	4.03387300	-1.66950400	-2.92561700
C	5.30699500	-3.71990100	-2.69333500
C	6.48954400	-2.97055800	-2.60849900
H	7.35729200	-1.00642100	-2.60651200
C	-2.31131300	-0.77567600	-0.60617600
C	-3.36754400	-1.34729900	-0.76695500
C	-7.02366200	-1.96447200	-1.16258000
C	-7.06279000	-3.35202600	-1.22680200
C	-5.87248200	-4.09354200	-1.15340100
C	-4.61540400	-2.02928700	-0.93882700
C	-5.80938100	-1.29870300	-1.02349600
H	-7.94672100	-1.39627500	-1.21759500
C	-5.90439600	-5.52239400	-1.23826100
C	-5.93699900	-6.73108100	-1.32058900
C	-7.23779200	-10.21977900	-1.54755900
C	-6.05555800	-10.94856900	-1.60261800
C	-4.81957100	-10.28468800	-1.57071900
C	-5.97667300	-8.15978500	-1.41702800
C	-7.20656200	-8.83206600	-1.45877900
H	-8.19128200	-10.73681900	-1.57214600
C	-2.54784900	-11.63194100	-1.69182500
C	-3.59373100	-11.02246400	-1.63488700
C	-0.11209900	-11.56966500	-1.89221600
C	4.40191900	-8.57261200	-2.37195100
C	4.07890700	-3.06469100	-2.84925600
C	-4.65170600	-3.42783600	-0.99865500
C	-4.78302700	-8.88985100	-1.46976900
H	2.14777600	-14.11076000	-1.89502200
H	-2.13554200	-14.28254100	-1.54333000
H	7.70039300	-7.78212500	-2.61803900

	H	5.84989200	-11.65052800	-2.30560300
	H	5.18121200	0.15243500	-2.88957100
	H	7.43604600	-3.48446000	-2.47961600
	H	-8.00761100	-3.87272000	-1.34038000
	H	-5.77379000	-0.21564500	-0.96275800
	H	-6.07677000	-12.03078800	-1.67431900
	H	-8.12742700	-8.26052800	-1.41109100
	H	-0.16224100	-10.48738100	-1.95074900
	H	3.42517200	-8.10297000	-2.32439400
	H	3.16173400	-3.64127800	-2.90805100
	H	-3.73320200	-3.99841100	-0.90742500
	H	-3.83148500	-8.37069400	-1.41624200
	C	-0.26926700	2.76760700	-3.52599800
	C	1.78186000	-0.32219300	-3.23907700
	C	2.79307800	-0.97413300	-3.09279500
	C	-1.53799000	2.24462300	-3.75287000
	C	-1.72482100	0.85526000	-3.82108100
	C	0.64180000	0.52742900	-3.40925900
	C	0.81803000	1.91927200	-3.36156500
	H	-0.12627700	3.84272600	-3.48119400
	C	-0.63288400	-0.00130200	-3.63965100
	H	-2.38916100	2.90295600	-3.89267600
	H	1.81212800	2.32037000	-3.19154900
	H	-0.77580300	-1.07603600	-3.67939700
	C	-3.02420100	0.32533500	-4.12249200
	C	-4.12428900	-0.10066200	-4.42623200
	Si	-5.75745000	-0.74405900	-5.01439700
	C	-7.13018100	0.23874800	-4.19431800
	C	-5.84999600	-2.57147200	-4.60963000
	C	-5.83464500	-0.48339700	-6.87378900
	H	-7.07070900	1.29318900	-4.47887800
	H	-7.08095600	0.17279700	-3.10541900
	H	-8.10398900	-0.14450100	-4.51546100
	H	-5.62034100	-2.75422900	-3.55674200
	H	-5.13833100	-3.13475200	-5.22020300
	H	-6.85362800	-2.95837200	-4.81256200
	H	-5.02303500	-1.01130300	-7.38173900
	H	-5.76472000	0.57828900	-7.12645800
	H	-6.78391900	-0.86318000	-7.26493600
TS-b	N	-0.00795600	-0.87966100	-0.22783600
	C	-0.09203800	-2.91412400	-0.37795000
	H	0.18606300	-2.97582800	0.66330700
	H	0.67766000	-2.85291000	-1.13334500
	H	-1.13013800	-2.80994500	-0.64414600
	O	-0.13041600	-4.76936300	-0.60110600
	S	-1.22841800	-5.54650400	0.12849100
	O	-1.99295500	-6.38793200	-0.80364000
	O	-2.03817300	-4.64876000	0.97058400
	C	-0.30442100	-6.63056200	1.21175600

H	0.28575900	-5.97183500	1.85620800
H	0.37997400	-7.19262200	0.56911700
C	-1.20481400	-7.55481900	2.02226800
H	-1.95053700	-6.95043900	2.55072100
C	-0.39157400	-8.36943600	3.02642100
H	-1.74963600	-8.21586000	1.33682600
H	0.39883500	-8.94134500	2.52723400
H	-1.03074800	-9.07496100	3.56437700
H	0.08596900	-7.71334800	3.76016100
C	1.17244100	-0.26141400	-0.03848500
C	1.32449700	1.11710700	-0.05292500
H	2.31144000	1.53010700	0.10605600
C	0.19282000	1.94048800	-0.24644100
N	0.29039500	3.28961600	-0.26809800
C	-1.04610100	1.28330900	-0.41602500
H	-1.96724900	1.82796600	-0.57237200
C	-1.09166300	-0.10297900	-0.41418300
C	1.59712200	3.92189300	-0.20145800
C	-0.91404300	4.09893400	-0.34894600
H	1.47404000	4.99952800	-0.29209100
H	2.23959600	3.57777300	-1.01979700
H	2.09891900	3.70779200	0.74963300
H	-1.45668100	3.91410500	-1.28320900
H	-0.63783700	5.15095900	-0.31301700
H	-1.58544500	3.88714000	0.49107100
C	-1.46264800	-14.28561100	1.70315100
C	-2.54654000	-13.41559200	1.74564800
C	-2.33832900	-12.03133500	1.64587000
C	0.05123200	-12.41623200	1.45855400
C	-0.16719400	-13.79681000	1.56750600
H	-1.62857300	-15.35499200	1.77954900
C	-3.43151100	-11.10968500	1.71902800
C	-4.33719600	-10.30781100	1.79709800
C	-7.77442100	-8.88925800	2.09147300
C	-7.50321500	-7.52731000	2.13900900
C	-6.17730300	-7.07103800	2.06836800
C	-5.41051400	-9.36583700	1.90310900
C	-6.73823200	-9.81017700	1.97845900
H	-8.80079700	-9.23707300	2.14230100
C	-5.90041100	-5.66784200	2.13010400
C	-5.69105900	-4.47592100	2.19069000
C	-6.45810800	-0.83744300	2.36547500
C	-5.18665500	-0.29209700	2.49149800
C	-4.05967000	-1.13021200	2.50831600
C	-5.50286400	-3.05946100	2.27950400
C	-6.62216600	-2.21411800	2.26447500
H	-7.32641300	-0.18737100	2.34754900
C	2.31620800	-1.09780300	0.19486400
C	3.29242100	-1.79168900	0.37441900

C	6.85167600	-2.79340800	0.83482800
C	6.74432000	-4.17828900	0.86019500
C	5.48586200	-4.79138200	0.74509700
C	4.45660800	-2.60434400	0.55857000
C	5.71647900	-2.00189300	0.68855400
H	7.82721900	-2.32696500	0.92650300
C	5.37557800	-6.21726700	0.80132000
C	5.29640400	-7.42468700	0.86460100
C	6.19527300	-11.04363700	1.01729700
C	4.93939600	-11.63064800	1.11602700
C	3.78882900	-10.82659500	1.13461400
C	5.18172300	-8.84942700	0.94750600
C	6.32468000	-9.66110900	0.93417000
H	7.08187900	-11.66859600	1.00043700
C	1.37539100	-11.88619600	1.33511300
C	2.48656300	-11.41111200	1.24231200
C	-1.03941300	-11.54080900	1.48734400
C	-5.13504800	-7.99348200	1.94082900
C	-4.21750400	-2.51474100	2.38862200
C	4.34343100	-3.99953300	0.58668300
C	3.91558200	-9.43749700	1.04544600
H	-3.55540800	-13.79642000	1.86270000
H	0.67963700	-14.47395300	1.53825400
H	-8.30799100	-6.80615900	2.23375700
H	-6.94584600	-10.87416200	1.93916400
H	-5.05130000	0.78063400	2.58004700
H	-7.61180200	-2.64747200	2.16625500
H	7.62708900	-4.79785100	0.97679300
H	5.79273100	-0.91968900	0.65792600
H	4.83638600	-12.70853100	1.18101500
H	7.30345200	-9.20169600	0.84791000
H	-0.87744100	-10.47381400	1.38119900
H	-4.11152300	-7.64252700	1.85714900
H	-3.34940100	-3.16585400	2.35535200
H	3.36871900	-4.46476700	0.47822600
H	3.02869200	-8.81253900	1.04917700
C	0.79283100	2.75270700	3.01896000
C	-1.67531300	-0.02368300	2.78690800
C	-2.75704400	-0.55300200	2.65041500
C	1.97412500	2.05748500	3.25673100
C	1.95922700	0.65744900	3.35568700
C	-0.43030800	0.66488200	2.94449900
C	-0.40566900	2.06653800	2.87030400
H	0.80543200	3.83624400	2.95492300
C	0.75543100	-0.03665500	3.18924700
H	2.91132700	2.58896300	3.38491000
H	-1.33276100	2.60175800	2.69130000
H	0.74082700	-1.11961700	3.25538000
C	3.16457400	-0.05150000	3.67776300

C	4.18352900	-0.63390300	4.00379000
Si	5.68984500	-1.50493100	4.63754300
C	7.21232100	-0.71546400	3.87431900
C	5.53327300	-3.32657600	4.22554500
C	5.73746100	-1.26811800	6.50091700
H	7.32764900	0.31114300	4.23403000
H	7.15768700	-0.69209200	2.78411100
H	8.10772600	-1.27694000	4.15922100
H	5.32340500	-3.47990500	3.16424600
H	4.72185200	-3.77717000	4.80479300
H	6.46010900	-3.85479400	4.47075700
H	4.84802700	-1.69143100	6.97553800
H	5.79492500	-0.20785100	6.76238600
H	6.61661800	-1.76872100	6.91916400
C	0.00695000	-14.34858000	-1.80822600
C	1.18589000	-13.62302900	-1.93206900
C	1.14526100	-12.22057700	-1.97742800
C	-1.27082900	-12.29640300	-1.76893800
C	-1.21948400	-13.69664300	-1.72714100
H	0.04365300	-15.43217300	-1.76864400
C	2.35007800	-11.45619600	-2.09580800
C	3.35829600	-10.79033400	-2.18872700
C	6.94967900	-9.81119100	-2.44395100
C	6.85041700	-8.42614100	-2.49720700
C	5.58972700	-7.80953500	-2.45751600
C	4.54218300	-9.99183800	-2.29532700
C	5.80617300	-10.59675800	-2.34496600
H	7.92619900	-10.28289800	-2.47582800
C	5.48195600	-6.38298100	-2.52292200
C	5.39722700	-5.17544500	-2.58083800
C	6.42893900	-1.59450800	-2.62713200
C	5.20524900	-0.95804600	-2.78860400
C	4.02524700	-1.71394100	-2.88691200
C	5.32364300	-3.74700700	-2.65035700
C	6.49551500	-2.98190000	-2.55882900
H	7.33757400	-1.00659800	-2.55056500
C	-2.34637400	-0.77098700	-0.61892800
C	-3.40273200	-1.34523400	-0.76561000
C	-7.05711300	-1.96588500	-1.14109000
C	-7.09405900	-3.35422400	-1.18508800
C	-5.90369700	-4.09489400	-1.10195800
C	-4.65033400	-2.02995600	-0.92178300
C	-5.84261600	-1.29831500	-1.01583400
H	-7.98064200	-1.39931500	-1.20328100
C	-5.93640400	-5.52411000	-1.17161000
C	-5.96192300	-6.73332700	-1.24300400
C	-7.21109200	-10.24401900	-1.39797200
C	-6.01885000	-10.95183600	-1.48633200
C	-4.79343300	-10.26702600	-1.49784900



C	-5.98230700	-8.16238500	-1.32495300
C	-7.20100200	-8.85521100	-1.32112200
H	-8.15553000	-10.77790900	-1.38608900
C	-2.52026900	-11.60378900	-1.67700300
C	-3.56255700	-10.99149500	-1.59409900
C	-0.08499200	-11.56284700	-1.89180700
C	4.43915400	-8.59682000	-2.35195200
C	4.08752900	-3.10822200	-2.81135700
C	-4.68113400	-3.42999800	-0.95562600
C	-4.77751000	-8.87152100	-1.40745300
H	2.14297500	-14.12990200	-1.99389500
H	-2.13997800	-14.26057100	-1.62088700
H	7.74078600	-7.81115100	-2.57294700
H	5.88081400	-11.67777300	-2.29466000
H	5.14763000	0.12376500	-2.84418700
H	7.44818300	-3.48334800	-2.42632800
H	-8.03862800	-3.87708200	-1.29083900
H	-5.80575200	-0.21439600	-0.97471500
H	-6.02255400	-12.03481900	-1.54845100
H	-8.12939400	-8.29888800	-1.24797700
H	-0.12162400	-10.47886300	-1.91501900
H	3.46320500	-8.12511200	-2.30729200
H	3.17824300	-3.69688400	-2.87478800
H	-3.76192100	-3.99910200	-0.84770800
H	-3.83422300	-8.33352700	-1.38961000
C	-0.29212700	2.69178800	-3.54003900
C	1.76046500	-0.39279600	-3.21765500
C	2.77677100	-1.03499800	-3.06267600
C	-1.56061200	2.16562800	-3.76118900
C	-1.74667300	0.77550900	-3.81612700
C	0.61964100	0.45334500	-3.39930200
C	0.79567200	1.84583200	-3.36602800
H	-0.14923200	3.76738200	-3.50869500
C	-0.65436700	-0.07896300	-3.62615500
H	-2.41197900	2.82194500	-3.90867500
H	1.78994800	2.24891500	-3.20146100
H	-0.79602500	-1.15438300	-3.65900900
C	-3.04453600	0.24181800	-4.11593200
C	-4.14310300	-0.18730600	-4.42020100
Si	-5.77048200	-0.83723900	-5.01761800
C	-7.14982900	0.16137500	-4.22925700
C	-5.86919800	-2.65703700	-4.58325000
C	-5.82203200	-0.60675300	-6.88177600
H	-7.08158200	1.21206700	-4.52535100
H	-7.11618700	0.10826500	-3.13897300
H	-8.12078800	-0.22143200	-4.55936700
H	-5.65214000	-2.82103100	-3.52469600
H	-5.14920700	-3.23032100	-5.17451000
H	-6.87001500	-3.04801800	-4.79198100

	H	-5.00585300	-1.14625300	-7.36997600
	H	-5.74430600	0.45022600	-7.15121500
	H	-6.76759500	-0.98942400	-7.27909600
4b	N	0.01929600	-0.85692900	-0.20034100
	C	-0.02076000	-2.33047600	-0.23841800
	H	0.46558400	-2.72283000	0.65603300
	H	0.51125800	-2.68007000	-1.12516000
	H	-1.04994600	-2.67821100	-0.26109000
	O	-0.28396900	-5.12738800	-0.93194800
	S	-1.32778400	-5.74855100	-0.08153800
	O	-2.21797800	-6.67367900	-0.82409400
	O	-2.08046600	-4.75745000	0.73175800
	C	-0.42007000	-6.76544500	1.08934700
	H	0.20974300	-6.07781900	1.66373800
	H	0.23376700	-7.40918900	0.49184800
	C	-1.31940500	-7.58953400	2.00008800
	H	-2.03941700	-6.92120600	2.48672100
	C	-0.51167300	-8.34057400	3.05712100
	H	-1.89666200	-8.29101700	1.38437600
	H	0.26835300	-8.95763500	2.59645000
	H	-1.15347800	-8.99769400	3.65115600
	H	-0.01837100	-7.64027200	3.73782700
	C	1.22135200	-0.22847200	-0.01915000
	C	1.33333600	1.14274000	-0.02959100
	H	2.31610700	1.56598700	0.12201000
	C	0.18311400	1.95428500	-0.20010500
	N	0.26050800	3.29290400	-0.20244700
	C	-1.05064400	1.27791200	-0.36773600
	H	-1.97853800	1.81176300	-0.51518700
	C	-1.10375500	-0.09942300	-0.38458100
	C	1.56042300	3.94836800	-0.12692100
	C	-0.95677100	4.09169400	-0.27344600
	H	1.41598900	5.02447200	-0.18972500
	H	2.20026000	3.63428000	-0.95778400
	H	2.06448800	3.71738200	0.81770400
	H	-1.49232100	3.90847100	-1.21083100
	H	-0.69082500	5.14513000	-0.22579900
	H	-1.62047000	3.86018000	0.56588300
	C	-1.45691100	-14.29693500	1.77313000
C	-2.56660300	-13.45850900	1.76879300	
C	-2.39587700	-12.07124900	1.64523700	
C	0.00824300	-12.38771800	1.53007000	
C	-0.17356700	-13.77219300	1.66094000	
H	-1.59332000	-15.36909700	1.86793600	
C	-3.51558700	-11.17926100	1.67021200	
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C	-7.86857600	-8.92458900	1.84709600	
C	-7.57492700	-7.56915800	1.93315700	
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C	-5.50829300	-9.44523400	1.77572900
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H	-8.90282600	-9.25251000	1.83794300
C	-5.93241500	-5.74361600	2.03898400
C	-5.68769200	-4.56023100	2.12704100
C	-6.32989500	-0.90332300	2.38785300
C	-5.04039800	-0.40530000	2.52100200
C	-3.94192800	-1.28148200	2.50988300
C	-5.45002500	-3.15374600	2.24558200
C	-6.54001400	-2.27126900	2.25559400
H	-7.17575600	-0.22406800	2.38854300
C	2.36666600	-1.04932200	0.19147600
C	3.34440400	-1.74294200	0.36294500
C	6.90539600	-2.76774600	0.73590800
C	6.78097400	-4.15028600	0.80004200
C	5.51200200	-4.75122500	0.74818500
C	4.50763100	-2.55619600	0.53921800
C	5.77640200	-1.96365200	0.61013300
H	7.88980900	-2.31309100	0.78022300
C	5.38083600	-6.17284500	0.84756700
C	5.28085900	-7.37657600	0.94364700
C	6.14321300	-10.99497500	1.22222900
C	4.88064100	-11.57004700	1.30107200
C	3.73515300	-10.75849700	1.26563900
C	5.14740400	-8.79726600	1.06292300
C	6.28447300	-9.61621300	1.10479500
H	7.02535800	-11.62609100	1.24594300
C	1.32302500	-11.82845400	1.43252300
C	2.42951600	-11.33928400	1.35623100
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C	-4.14487700	-2.65641300	2.35604900
C	4.37543400	-3.94849300	0.60870700
C	3.87385500	-9.37310900	1.14175800
H	-3.56683400	-13.86634800	1.86798100
H	0.69332500	-14.42422600	1.66741000
H	-8.37042600	-6.83443300	1.99834100
H	-7.07176300	-10.92367500	1.70368300
H	-4.86755000	0.65967400	2.63464600
H	-7.54390200	-2.66954800	2.15299900
H	7.66020300	-4.77784000	0.89946300
H	5.86478800	-0.88375800	0.54772600
H	4.76756000	-12.64509100	1.39230100
H	7.26833900	-9.16522800	1.03260500
H	-0.97477700	-10.47453900	1.39214700
H	-4.17601300	-7.75014100	1.82810400
H	-3.30018200	-3.33610400	2.29199900
H	3.39163000	-4.40286900	0.54659800
H	2.99172100	-8.74225000	1.10529500

C	0.81163600	2.65614800	3.07861700
C	-1.54538200	-0.20674600	2.80292200
C	-2.62535900	-0.73664700	2.65347200
C	2.02482800	2.00635800	3.28471900
C	2.06982900	0.60511400	3.35556400
C	-0.32349700	0.51920000	2.97433100
C	-0.35862400	1.92264300	2.92886300
H	0.77712500	3.74059600	3.04070500
C	0.89333900	-0.13652000	3.19342500
H	2.94086300	2.57408300	3.41108100
H	-1.31042700	2.42108100	2.77389600
H	0.92569700	-1.22018800	3.24353000
C	3.30901600	-0.05834600	3.64420500
C	4.35706200	-0.60333200	3.94118000
Si	5.90963600	-1.41856700	4.53952600
C	7.38368800	-0.61583100	3.69781800
C	5.77290300	-3.25325000	4.18236300
C	6.02255200	-1.12911500	6.39241400
H	7.49065100	0.42106300	4.02976100
H	7.28809800	-0.61865000	2.61012300
H	8.30101700	-1.15198800	3.96127500
H	5.49697200	-3.43674400	3.14094700
H	5.01071900	-3.70647500	4.82373600
H	6.72583600	-3.75522000	4.37848000
H	5.16275100	-1.56099700	6.91216300
H	6.06408300	-0.06114000	6.62374500
H	6.92949600	-1.59730000	6.78867200
C	0.00669200	-14.34121800	-1.69909500
C	1.19882800	-13.63496100	-1.80894200
C	1.17852700	-12.23354800	-1.88428700
C	-1.24271500	-12.27114400	-1.73453300
C	-1.21189900	-13.67106300	-1.66250100
H	0.02678100	-15.42414400	-1.63518100
C	2.39333700	-11.48397000	-1.99169400
C	3.40437100	-10.82092500	-2.07245200
C	6.98958800	-9.79421200	-2.22819700
C	6.87042900	-8.41347900	-2.33095500
C	5.59915400	-7.81777800	-2.36112200
C	4.58161900	-10.01155400	-2.16568700
C	5.85580300	-10.59607800	-2.14684800
H	7.97425700	-10.24963200	-2.20415700
C	5.46849800	-6.39583200	-2.47243100
C	5.36135300	-5.19199700	-2.56301000
C	6.35776500	-1.60575400	-2.74264200
C	5.12424700	-0.98305000	-2.87910900
C	3.94798900	-1.75062500	-2.91993700
C	5.26894500	-3.76703600	-2.67242900
C	6.43673700	-2.99034400	-2.64066800
H	7.26361600	-1.00950700	-2.71171700

C	-2.34706000	-0.76151900	-0.60171400
C	-3.40313500	-1.32999500	-0.77227100
C	-7.05636600	-1.93090300	-1.13985100
C	-7.09803100	-3.31834000	-1.20643500
C	-5.91084300	-4.06679400	-1.15009400
C	-4.64942000	-2.01186600	-0.94490300
C	-5.83793300	-1.27080000	-1.01845800
H	-7.97847300	-1.36033700	-1.18147600
C	-5.95237900	-5.49416000	-1.24745800
C	-5.97384900	-6.70194100	-1.33983100
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C	-4.76039700	-10.21751800	-1.60283500
C	-5.97641000	-8.12943600	-1.45144300
C	-7.18750700	-8.83153200	-1.53137700
H	-8.11969100	-10.75995900	-1.69546700
C	-2.48489000	-11.56086200	-1.68916500
C	-3.52361000	-10.93819200	-1.64674900
C	-0.04397800	-11.55709000	-1.84243000
C	4.45842700	-8.62100200	-2.27393500
C	4.02231900	-3.14223500	-2.80954600
C	-4.68227300	-3.41155100	-1.00198100
C	-4.75960900	-8.82379000	-1.48130200
H	2.14969500	-14.15639900	-1.83623700
H	-2.14252700	-14.22026000	-1.56790000
H	7.75327800	-7.78600500	-2.39073600
H	5.94607600	-11.67339300	-2.05620800
H	5.05524400	0.09644600	-2.96073400
H	7.39722300	-3.48155500	-2.52728800
H	-8.04613000	-3.83524500	-1.31045500
H	-5.79508300	-0.18777700	-0.96108000
H	-5.96770500	-11.99404300	-1.76502500
H	-8.12345400	-8.28378000	-1.49855300
H	-0.06440300	-10.47336000	-1.88832000
H	3.47369400	-8.16546600	-2.28376500
H	3.11596500	-3.73863200	-2.82691800
H	-3.76451700	-3.98461900	-0.89736700
H	-3.82541800	-8.27399900	-1.39528500
C	-0.34834300	2.67607200	-3.48084200
C	1.67708100	-0.43097900	-3.21093600
C	2.69238200	-1.07881100	-3.07263700
C	-1.62516400	2.16487400	-3.69071800
C	-1.82595200	0.77726600	-3.75900500
C	0.54203000	0.42683800	-3.37364900
C	0.73318000	1.81744700	-3.32857700
H	-0.19351200	3.74992400	-3.44420300
C	-0.74005700	-0.09047400	-3.59180800
H	-2.47126200	2.83130500	-3.82190900
H	1.73403000	2.20884200	-3.17587300

	H	-0.89243300	-1.16395400	-3.63871100
	C	-3.13160800	0.26160100	-4.05510500
	C	-4.23661700	-0.14825400	-4.36201500
	Si	-5.87098800	-0.76588100	-4.97744800
	C	-7.24022500	0.22059500	-4.15613100
	C	-5.97424300	-2.59894600	-4.60407000
	C	-5.92436800	-0.47217400	-6.83258000
	H	-7.16993800	1.27626500	-4.43378100
	H	-7.19789700	0.14825300	-3.06744600
	H	-8.21545500	-0.15193700	-4.48533000
	H	-5.72932100	-2.80157700	-3.55835500
	H	-5.27342400	-3.15509500	-5.23381900
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	H	-5.11326300	-1.00079400	-7.34072100
	H	-5.84034300	0.59287400	-7.06627300
	H	-6.87364300	-0.83494200	-7.23968500
	N	-0.00406700	-0.80615000	-0.19085600
	C	-0.19014700	-3.64218200	-0.60944800
	H	0.09234100	-3.46188000	0.42757400
	H	0.60766700	-3.31253100	-1.27048400
	H	-1.11425800	-3.11538600	-0.83610000
	O	-0.34010600	-5.06490800	-0.87031800
	S	-1.40869000	-5.86741500	0.01098700
	O	-2.10808700	-6.76648400	-0.89583300
	O	-2.19028200	-4.92201400	0.80227000
	C	-0.35286300	-6.81676500	1.08721900
	H	0.27527100	-6.09178000	1.61338100
	H	0.27372400	-7.42571900	0.42937600
	C	-1.18207100	-7.66143900	2.04814600
	H	-1.82999400	-7.00255700	2.63852500
	C	-0.29499800	-8.48453700	2.98080400
	H	-1.83402500	-8.33096700	1.47070400
	H	0.33527500	-9.16306500	2.38785300
	C	-1.11650200	-9.29219800	3.98448000
	H	0.39301900	-7.81997900	3.51853000
	H	-1.61574400	-8.60203700	4.67550000
	C	-0.25814000	-10.28736800	4.75917000
	H	-1.91609700	-9.82586900	3.45403900
	H	0.21005500	-11.00210300	4.07326300
	H	-0.85208500	-10.85127500	5.48284500
	H	0.54112500	-9.77452600	5.30350400
	C	1.16647400	-0.17402400	-0.01900300
	C	1.33125200	1.20722100	-0.03929300
	H	2.32016700	1.62085400	0.10857300
	C	0.20095300	2.03046000	-0.22329400
	N	0.29964300	3.38583100	-0.24484400
	C	-1.03694000	1.37408300	-0.38722900
	H	-1.95691900	1.92074400	-0.54659300
	C	-1.07273800	-0.01632800	-0.37822100

3c

C	1.60555100	4.01535400	-0.17781500
C	-0.90365900	4.19406400	-0.31867700
H	1.48457800	5.09426800	-0.26049900
H	2.24795000	3.67712500	-0.99954900
H	2.11273900	3.79504900	0.76969200
H	-1.45369600	4.01079000	-1.24962300
H	-0.62814900	5.24675400	-0.28423000
H	-1.57295100	3.98358500	0.52409900
C	-1.49955200	-14.37356300	1.71371100
C	-2.60674100	-13.53133400	1.70603700
C	-2.43031200	-12.14525800	1.58144900
C	-0.02573000	-12.47143300	1.47581700
C	-0.21295600	-13.85473200	1.60891900
H	-1.64068000	-15.44496100	1.80930500
C	-3.53862800	-11.23925400	1.61492200
C	-4.43458000	-10.42446600	1.67284600
C	-7.83251200	-8.88571000	1.79653700
C	-7.51354300	-7.53798600	1.90526600
C	-6.16939100	-7.13254300	1.94181900
C	-5.48229500	-9.45112300	1.74847300
C	-6.82732400	-9.84456800	1.72048500
H	-8.87271500	-9.19267500	1.76745200
C	-5.84779700	-5.74264100	2.06322600
C	-5.61335000	-4.55795100	2.16432800
C	-6.35353000	-0.92135700	2.42439000
C	-5.07917200	-0.38481800	2.55694100
C	-3.95497900	-1.22706400	2.55490200
C	-5.40928400	-3.14588200	2.29036200
C	-6.52437700	-2.29442700	2.29457400
H	-7.21853600	-0.26666800	2.41949200
C	2.31310800	-1.01689000	0.20375800
C	3.27911700	-1.72748000	0.37548600
C	6.83149200	-2.79617300	0.75245100
C	6.69750100	-4.17708200	0.82151400
C	5.42269500	-4.76414100	0.76726300
C	4.43146900	-2.56017200	0.54760100
C	5.70837200	-1.98488800	0.62000100
H	7.81886000	-2.34784000	0.79829600
C	5.28366500	-6.18545500	0.86881400
C	5.18535800	-7.38896700	0.97208600
C	6.09494300	-10.99222700	1.29045900
C	4.84053900	-11.58744400	1.34402500
C	3.68389700	-10.79417800	1.27971000
C	5.06821800	-8.81066800	1.09695300
C	6.21652900	-9.61209100	1.16828000
H	6.98640900	-11.60871700	1.33698500
C	1.28707700	-11.90499400	1.39431400
C	2.38622100	-11.39604200	1.34190900
C	-1.13914300	-11.62589200	1.44861700

C	-5.15835700	-8.09305300	1.85722000
C	-4.12146600	-2.60868200	2.41106600
C	4.29298200	-3.95179100	0.62294000
C	3.80307200	-9.40713700	1.15258200
H	-3.60820100	-13.93596800	1.80496600
H	0.65104700	-14.51023500	1.62406900
H	-8.29529800	-6.78840000	1.96683700
H	-7.07209600	-10.89737400	1.62921300
H	-4.93817800	0.68561400	2.66282800
H	-7.51587700	-2.72108000	2.18680900
H	7.57016900	-4.81292900	0.92634300
H	5.80729400	-0.90602000	0.55418300
H	4.74243700	-12.66364400	1.43819300
H	7.19453400	-9.14590500	1.11470200
H	-1.00080300	-10.55772200	1.31797800
H	-4.11831500	-7.78470800	1.87137100
H	-3.25716800	-3.26352700	2.37312000
H	3.30631800	-4.40013200	0.56421700
H	2.91188700	-8.79060600	1.09630800
C	0.80045800	2.75433700	3.05352100
C	-1.58066000	-0.09652500	2.82557600
C	-2.65260000	-0.64697000	2.69433500
C	2.00629000	2.09705500	3.27452900
C	2.03894400	0.69658200	3.36109200
C	-0.35432200	0.62744800	2.97691000
C	-0.37582100	2.02957100	2.91090000
H	0.77703000	3.83794600	2.99437000
C	0.85662700	-0.03567300	3.20323400
H	2.92711100	2.65822800	3.39557400
H	-1.32081300	2.53497200	2.73984700
H	0.88008500	-1.11895900	3.25582800
C	3.27197800	0.02409400	3.65735200
C	4.31424200	-0.53009500	3.95826600
Si	5.85380800	-1.37336500	4.54695600
C	7.34022300	-0.59849800	3.70100700
C	5.69008400	-3.20676800	4.19129300
C	5.98515100	-1.09051400	6.39997900
H	7.46440200	0.43843200	4.02672600
H	7.24452200	-0.60701600	2.61337400
H	8.24864300	-1.14804500	3.96776800
H	5.39300100	-3.38735400	3.15530600
H	4.93746200	-3.65266600	4.84837600
H	6.64192800	-3.71756000	4.36841500
H	5.12079000	-1.50624300	6.92504800
H	6.04959800	-0.02425100	6.63381500
H	6.88518900	-1.57772200	6.78880900
C	0.01470100	-14.38774500	-1.76491400
C	1.20664000	-13.67858000	-1.85802400
C	1.18470200	-12.27657600	-1.92081600



C	-1.23855300	-12.32016300	-1.79306200
C	-1.20570500	-13.72051500	-1.73203500
H	0.03649900	-15.47113000	-1.71050600
C	2.39858600	-11.52192600	-2.00445200
C	3.40465000	-10.84932900	-2.06860900
C	6.98332800	-9.79219200	-2.14748000
C	6.85521400	-8.41354900	-2.26366700
C	5.58024200	-7.82842600	-2.32836400
C	4.57699800	-10.03022200	-2.14091100
C	5.85489600	-10.60356300	-2.08704300
H	7.97080700	-10.23876800	-2.09634400
C	5.44256100	-6.40790700	-2.45160600
C	5.33282200	-5.20478000	-2.55032900
C	6.34631300	-1.62443200	-2.72357400
C	5.11679900	-0.99581500	-2.86870800
C	3.93606700	-1.75564100	-2.91986300
C	5.24705000	-3.77918700	-2.66227000
C	6.41862700	-3.00922200	-2.62098200
H	7.25446800	-1.03213200	-2.68577900
C	-2.32785400	-0.69332000	-0.58440600
C	-3.37982300	-1.27495000	-0.73864100
C	-7.03485800	-1.94635200	-1.07387400
C	-7.05182800	-3.33357500	-1.15470100
C	-5.84740300	-4.05462300	-1.11942700
C	-4.62167600	-1.97104500	-0.90043900
C	-5.82939200	-1.26093000	-0.95316300
H	-7.96835900	-1.39341800	-1.10180900
C	-5.85581700	-5.48242200	-1.23134200
C	-5.86924300	-6.68953400	-1.33884200
C	-7.15599200	-10.17330700	-1.67320500
C	-5.97231800	-10.89958500	-1.72007200
C	-4.73779700	-10.23579700	-1.64528400
C	-5.89936200	-8.11604600	-1.46662600
C	-7.12729800	-8.78817100	-1.54987000
H	-8.10849300	-10.68969800	-1.73016900
C	-2.48073900	-11.60945200	-1.74659500
C	-3.51459700	-10.97891900	-1.69927500
C	-0.03985900	-11.60337100	-1.88496600
C	4.44500300	-8.64141500	-2.26272400
C	4.00525200	-3.14780200	-2.81195100
C	-4.63532000	-3.36934800	-0.98135600
C	-4.70352000	-8.84358500	-1.51183200
H	2.15840400	-14.19849100	-1.88121700
H	-2.13562800	-14.27265300	-1.64839200
H	7.73401000	-7.77921800	-2.30775300
H	5.95224600	-11.67926100	-1.98655700
H	5.05392300	0.08422800	-2.94850400
H	7.37560000	-3.50517200	-2.49943400
H	-7.99005200	-3.86912800	-1.25382500

	H	-5.81211500	-0.17815500	-0.87959900
	H	-5.98999900	-11.97992300	-1.81691900
	H	-8.04913600	-8.21791200	-1.50688000
	H	-0.06178100	-10.51927400	-1.92219600
	H	3.45697900	-8.19510600	-2.30199000
	H	3.09798400	-3.74180500	-2.84269100
	H	-3.70582000	-3.92434600	-0.91279600
	H	-3.75360900	-8.32371600	-1.43556300
	C	-0.32022600	2.70765500	-3.51892400
	C	1.67887100	-0.41440000	-3.22023600
	C	2.68566400	-1.07474100	-3.07881100
	C	-1.60033600	2.20588900	-3.72774400
	C	-1.81402500	0.81959600	-3.77774800
	C	0.55027800	0.45191900	-3.38611300
	C	0.75243500	1.84084800	-3.35466000
	H	-0.15672100	3.78027600	-3.48778300
	C	-0.73661400	-0.05552900	-3.59679300
	H	-2.44039300	2.87829900	-3.86759800
	H	1.75491900	2.22538200	-3.19592100
	H	-0.90005800	-1.12794700	-3.62128400
	C	-3.12574200	0.31270500	-4.06495400
	C	-4.23563200	-0.09232300	-4.36160900
	Si	-5.88023600	-0.71644000	-4.93834400
	C	-7.23875100	0.25534900	-4.08149800
	C	-5.97117000	-2.55056700	-4.56551200
	C	-5.98284100	-0.42110000	-6.79134000
	H	-7.18467100	1.31332200	-4.35381200
	H	-7.16999600	0.17553600	-2.99460400
	H	-8.21811600	-0.12422200	-4.39003500
	H	-5.71814700	-2.75151300	-3.52146600
	H	-5.27470100	-3.10505100	-5.20126700
	H	-6.98017200	-2.93163400	-4.75243600
	H	-5.17918300	-0.94108800	-7.31982500
	H	-5.91429600	0.64492400	-7.02533600
	H	-6.93811000	-0.79194100	-7.17647900
TS-c	N	-0.00941000	-0.82651600	-0.22204400
	C	-0.07078600	-2.85425800	-0.45178000
	H	0.23124500	-2.95303700	0.57960800
	H	0.68132600	-2.74896700	-1.22064100
	H	-1.11630000	-2.75379500	-0.69022900
	O	-0.09000800	-4.69885800	-0.74744600
	S	-1.17052100	-5.50426600	-0.02217200
	O	-1.92914400	-6.33895200	-0.96476500
	O	-1.98487200	-4.63214400	0.84199000
	C	-0.22971200	-6.59095500	1.04237400
	H	0.40711500	-5.93568600	1.64433800
	H	0.40786900	-7.18864400	0.38413600
	C	-1.12153300	-7.46037300	1.91890800
	H	-1.78843300	-6.81201000	2.50044900

C	-0.29857600	-8.33638700	2.86176400
H	-1.75533100	-8.09026400	1.28032000
H	0.32070400	-9.02987400	2.27355600
C	-1.16606400	-9.12724000	3.83977900
H	0.40346300	-7.70930500	3.42734600
H	-1.67555200	-8.42601500	4.51222800
C	-0.34848900	-10.13018800	4.64788900
H	-1.95836500	-9.65043900	3.28812200
H	0.14353900	-10.84771700	3.98180700
H	-0.97436300	-10.69143800	5.34659100
H	0.43174300	-9.62259600	5.22433200
C	1.17115900	-0.20948800	-0.03035200
C	1.32324300	1.16877500	-0.03292400
H	2.30998800	1.58105200	0.12893200
C	0.18992300	1.99284200	-0.21405900
N	0.28789300	3.34174000	-0.22924700
C	-1.05077900	1.33701600	-0.37787500
H	-1.97335000	1.88314300	-0.51953300
C	-1.09532100	-0.04903100	-0.39261800
C	1.59510300	3.97329700	-0.15888000
C	-0.91622800	4.15234800	-0.30657800
H	1.47244000	5.05140200	-0.24387900
H	2.23775400	3.63308300	-0.97868600
H	2.09623100	3.75405300	0.79140600
H	-1.46223400	3.96570600	-1.23851100
H	-0.63863200	5.20409700	-0.27443500
H	-1.58461700	3.94360000	0.53651500
C	-1.49799900	-14.38791000	1.70553400
C	-2.60431000	-13.54481600	1.70623700
C	-2.42744500	-12.15769000	1.59262700
C	-0.02405600	-12.48450400	1.48003500
C	-0.21151600	-13.86865000	1.60174400
H	-1.63957300	-15.45996900	1.79258500
C	-3.53739000	-11.25415500	1.63005100
C	-4.43527400	-10.44194200	1.69043500
C	-7.83504500	-8.90887100	1.81769500
C	-7.51820200	-7.56082500	1.92735500
C	-6.17469300	-7.15305900	1.96356000
C	-5.48346300	-9.46966900	1.76909400
C	-6.82785800	-9.86539100	1.74018600
H	-8.87468300	-9.21778100	1.78873200
C	-5.85716400	-5.76192200	2.08079400
C	-5.62436100	-4.57646100	2.17588400
C	-6.35889400	-0.93857800	2.44841600
C	-5.08243200	-0.40467100	2.57014700
C	-3.96058400	-1.25001600	2.55135800
C	-5.41952800	-3.16430600	2.29786100
C	-6.53308100	-2.31141900	2.31671500
H	-7.22307700	-0.28285300	2.45613000

C	2.31327900	-1.05000900	0.19647100
C	3.28087800	-1.75626000	0.37402300
C	6.83083400	-2.81685400	0.76767200
C	6.69720300	-4.19801100	0.83283100
C	5.42406300	-4.78824500	0.77119300
C	4.43336500	-2.58657000	0.55235300
C	5.70747200	-2.00653300	0.63292000
H	7.81763400	-2.36820100	0.81906200
C	5.28858800	-6.20950600	0.87210800
C	5.19217900	-7.41309700	0.97402300
C	6.09960300	-11.01711600	1.29062800
C	4.84435900	-11.61051600	1.34595200
C	3.68870900	-10.81571800	1.28284100
C	5.07527400	-8.83466400	1.09871900
C	6.22295800	-9.63708500	1.16848700
H	6.99023800	-11.63496600	1.33530100
C	1.28943800	-11.92015600	1.39876500
C	2.39001800	-11.41467600	1.34596200
C	-1.13640700	-11.63698000	1.46288400
C	-5.16092600	-8.11111800	1.87932200
C	-4.12888900	-2.63024400	2.40176600
C	4.29357500	-3.97796600	0.62144800
C	3.80942600	-9.42904000	1.15515400
H	-3.60606700	-13.94938400	1.80265700
H	0.65238600	-14.52440700	1.60878100
H	-8.30118900	-6.81249500	1.98930200
H	-7.07052500	-10.91854800	1.64722700
H	-4.93825400	0.66478700	2.68161400
H	-7.52664900	-2.73614200	2.22030900
H	7.57045700	-4.83248700	0.94061700
H	5.80397200	-0.92726300	0.57142200
H	4.74482600	-12.68662700	1.43973900
H	7.20140100	-9.17201600	1.11330600
H	-0.99736400	-10.56717700	1.34459000
H	-4.12113000	-7.80019000	1.89210700
H	-3.26539600	-3.28504000	2.34176800
H	3.30722600	-4.42568900	0.55080400
H	2.91913800	-8.81120300	1.09877300
C	0.80376500	2.71332400	3.06605600
C	-1.58012600	-0.13263800	2.81890000
C	-2.65517300	-0.67670600	2.68686600
C	2.00954300	2.05286300	3.27901600
C	2.04106200	0.65160300	3.35398100
C	-0.35256900	0.58799800	2.97226300
C	-0.37356500	1.99092200	2.91965000
H	0.78086600	3.79755600	3.01877100
C	0.85804200	-0.07846700	3.19087200
H	2.93080000	2.61215500	3.40503700
H	-1.31928900	2.49837400	2.75832000

H	0.88006100	-1.16236600	3.23679400
C	3.27252500	-0.02388500	3.64858600
C	4.31316900	-0.57965300	3.95174700
Si	5.84761200	-1.42569300	4.55089100
C	7.33965900	-0.65383400	3.71246300
C	5.67701500	-3.25866700	4.19693300
C	5.96824200	-1.13968400	6.40401700
H	7.46574000	0.38140300	4.04284600
H	7.24794900	-0.65713100	2.62454200
H	8.24538600	-1.20721000	3.98023000
H	5.37820800	-3.43914100	3.16151300
H	4.92220800	-3.70003200	4.85458800
H	6.62628100	-3.77398800	4.37438100
H	5.09958200	-1.55211400	6.92452800
H	6.03439700	-0.07320200	6.63633500
H	6.86456400	-1.62878100	6.79897100
C	0.01056100	-14.41462500	-1.76593700
C	1.20759500	-13.71373700	-1.85732200
C	1.19560100	-12.31154200	-1.91538400
C	-1.22721400	-12.33777100	-1.78467000
C	-1.20477600	-13.73860100	-1.72954500
H	0.02442700	-15.49830800	-1.71550100
C	2.41331500	-11.56357400	-1.99961300
C	3.42077600	-10.89320300	-2.06350800
C	6.99698300	-9.82653800	-2.14173500
C	6.86453500	-8.44801500	-2.25546700
C	5.58768400	-7.86707100	-2.31829200
C	4.59141200	-10.07194600	-2.13433300
C	5.87113000	-10.64143000	-2.08224300
H	7.98585400	-10.27010000	-2.09166900
C	5.44361400	-6.44722800	-2.43940400
C	5.32559200	-5.24496600	-2.53736200
C	6.31455100	-1.65824800	-2.71758200
C	5.08087900	-1.03827300	-2.86363100
C	3.90559300	-1.80694300	-2.91000200
C	5.22908100	-3.82044600	-2.64935900
C	6.39547600	-3.04230900	-2.61210800
H	7.21892200	-1.06011800	-2.68220500
C	-2.35026100	-0.71694100	-0.59835800
C	-3.40430200	-1.29503200	-0.74703600
C	-7.05629400	-1.97040300	-1.06405800
C	-7.06940800	-3.35776500	-1.14125800
C	-5.86402200	-4.07763400	-1.10683300
C	-4.64435200	-1.99462500	-0.89951200
C	-5.85135100	-1.28337000	-0.95019500
H	-7.99090800	-1.41948800	-1.09120800
C	-5.87308300	-5.50481200	-1.21593200
C	-5.88195500	-6.71174300	-1.32221300
C	-7.14058600	-10.20367500	-1.66394200

C	-5.95071100	-10.91921700	-1.70916700
C	-4.72105100	-10.24644300	-1.62849800
C	-5.90087000	-8.13751700	-1.44962300
C	-7.12328200	-8.81873300	-1.53827000
H	-8.08853600	-10.72786900	-1.72521700
C	-2.46433000	-11.61906000	-1.73391600
C	-3.49570200	-10.98500300	-1.68330000
C	-0.02385300	-11.62938000	-1.87535800
C	4.45490800	-8.68348400	-2.25319800
C	3.98226000	-3.19799300	-2.79563800
C	-4.65090200	-3.39353600	-0.97235300
C	-4.69853300	-8.85458400	-1.49048600
H	2.15553000	-14.24043400	-1.88330700
H	-2.13875400	-14.28402300	-1.64710500
H	7.74128200	-7.81079000	-2.29879800
H	5.97172100	-11.71700900	-1.98367900
H	5.01045800	0.04096400	-2.94759800
H	7.35584400	-3.53195100	-2.49171300
H	-8.00674400	-3.89541200	-1.23718300
H	-5.83367800	-0.20029600	-0.88204700
H	-5.95880200	-11.99928600	-1.80959200
H	-8.04938700	-8.25525200	-1.49830300
H	-0.03763000	-10.54511500	-1.90828800
H	3.46555500	-8.23992800	-2.29003800
H	3.07755000	-3.79680100	-2.81706600
H	-3.71964200	-3.94804300	-0.90081200
H	-3.75335900	-8.32593100	-1.40677200
C	-0.33913700	2.65868800	-3.51140900
C	1.64548800	-0.47301300	-3.21829500
C	2.65179500	-1.13328200	-3.07187400
C	-1.62127400	2.16293500	-3.72344900
C	-1.84011800	0.77766900	-3.78115800
C	0.52187100	0.39894000	-3.38751500
C	0.73018300	1.78701400	-3.34892900
H	-0.17100500	3.73054400	-3.47740500
C	-0.76616400	-0.10259300	-3.60493000
H	-2.45834700	2.83944200	-3.86088100
H	1.73418600	2.16683100	-3.18841200
H	-0.93314300	-1.17425600	-3.64039000
C	-3.15254500	0.27447900	-4.06986600
C	-4.26300000	-0.12989700	-4.36450600
Si	-5.90807400	-0.75365100	-4.94160600
C	-7.26408100	0.23000100	-4.09501400
C	-6.00200400	-2.58431300	-4.55365700
C	-6.00336700	-0.47233000	-6.79696100
H	-7.20491700	1.28537100	-4.37621200
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H	-8.24446100	-0.14789300	-4.40203600
H	-5.74706600	-2.77753200	-3.50856700

	H	-5.30694200	-3.14452100	-5.18585100
	H	-7.01163700	-2.96575800	-4.73580800
	H	-5.19928000	-0.99866800	-7.31837800
	H	-5.93095700	0.59163900	-7.03890500
	H	-6.95826600	-0.84358000	-7.18256800
4c	N	0.01848400	-0.84672300	-0.19507500
	C	-0.01092400	-2.32019500	-0.23789100
	H	0.39582100	-2.71603600	0.69401200
	H	0.59305800	-2.66337300	-1.07845700
	H	-1.03182600	-2.67082200	-0.35070600
	O	-0.27344500	-5.08209100	-1.07395400
	S	-1.29641800	-5.71158500	-0.20354000
	O	-2.20412600	-6.63025500	-0.93451600
	O	-2.03015700	-4.72671000	0.63498400
	C	-0.36241800	-6.73686900	0.93815400
	H	0.30980600	-6.05869100	1.47446500
	H	0.24750700	-7.40262100	0.31855400
	C	-1.23801500	-7.52549400	1.90016600
	H	-1.89008800	-6.83035200	2.44441700
	C	-0.40933500	-8.34372400	2.88911500
	H	-1.89066100	-8.19352800	1.32112200
	H	0.23791300	-9.04099100	2.33543800
	C	-1.26946300	-9.12672400	3.87954100
	H	0.26884200	-7.67921200	3.44154300
	H	-1.80171500	-8.42054200	4.52917400
	C	-0.44223100	-10.09510700	4.71981200
	H	-2.04410300	-9.67980200	3.33147700
	H	0.06194800	-10.82404600	4.07509100
	H	-1.06307100	-10.64594500	5.43130400
	H	0.32888300	-9.56203600	5.28561000
	C	1.21643500	-0.20986800	-0.01498100
	C	1.32023800	1.16187500	-0.03183800
	H	2.29998400	1.59175500	0.12109900
	C	0.16494600	1.96578700	-0.20440300
	N	0.23473900	3.30467100	-0.21758800
	C	-1.06593800	1.28136600	-0.35911100
	H	-1.99836900	1.80920900	-0.49948000
	C	-1.11090500	-0.09639400	-0.37115700
	C	1.53155000	3.96797400	-0.15601000
	C	-0.98742900	4.09621500	-0.28905300
	H	1.38138000	5.04219700	-0.23579000
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H	2.03981900	3.75465000	0.79046300	
H	-1.52916200	3.89797900	-1.21979400	
H	-0.72672900	5.15156100	-0.25719700	
H	-1.64353500	3.87199500	0.55814800	
C	-1.48168400	-14.36146500	1.70504600	
C	-2.59792600	-13.53158700	1.69686800	
C	-2.43641700	-12.14263000	1.58457400	

C	-0.02857700	-12.43998100	1.49168000
C	-0.20100800	-13.82647100	1.61144000
H	-1.61092500	-15.43523900	1.79050900
C	-3.55716300	-11.25246100	1.61277200
C	-4.46263500	-10.44836400	1.66675600
C	-7.86188700	-8.91211100	1.81142300
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C	-6.27538000	-0.93833500	2.43296300
C	-4.98793400	-0.43438800	2.56491100
C	-3.88521500	-1.30505400	2.54724000
C	-5.38471500	-3.18385200	2.27981400
C	-6.47912400	-2.30671900	2.29580700
H	-7.12455000	-0.26321900	2.43774600
C	2.36528200	-1.02232100	0.20852900
C	3.33645300	-1.72475900	0.38121000
C	6.88658400	-2.78760800	0.74443700
C	6.74689000	-4.16799000	0.81914200
C	5.47090600	-4.75478500	0.77862100
C	4.49044100	-2.55072500	0.55785800
C	5.76589300	-1.97201500	0.61901700
H	7.87619700	-2.34396000	0.78019400
C	5.32596600	-6.17410200	0.88961300
C	5.21782300	-7.37618300	0.99628400
C	6.09253600	-10.98584500	1.32610200
C	4.83212700	-11.56843600	1.37744500
C	3.68274800	-10.76482400	1.30787100
C	5.08642400	-8.79614300	1.12483600
C	6.22742000	-9.60724400	1.20141900
H	6.97782900	-11.61094500	1.37583700
C	1.28091900	-11.86483200	1.41797900
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C	-4.08206000	-2.68022500	2.38846200
C	4.34276400	-3.94064200	0.63835000
C	3.81488100	-9.37933200	1.17739100
H	-3.59569800	-13.94784600	1.78505900
H	0.67060000	-14.47193100	1.62435000
H	-8.32253400	-6.81456600	1.98716700
H	-7.10281600	-10.92415000	1.64283200
H	-4.81974200	0.63097000	2.68195800
H	-7.48123300	-2.70945200	2.19299900
H	7.61915800	-4.80515100	0.91866800



H	5.86553700	-0.89363100	0.54907300
H	4.72335100	-12.64351700	1.47306900
H	7.20972000	-9.15001600	1.14925300
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H	-4.14574700	-7.80944300	1.83415800
H	-3.23396700	-3.35489000	2.31889200
H	3.35364300	-4.38409900	0.58419900
H	2.92969800	-8.75451200	1.11577800
C	0.85376600	2.65695000	3.08147400
C	-1.49406700	-0.21543000	2.82840300
C	-2.57070000	-0.75449800	2.68783100
C	2.07020900	2.01238900	3.28407500
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C	-0.27411800	0.51576300	2.99137900
C	-0.31454800	1.91876600	2.94036300
H	0.81522300	3.74101700	3.03992000
C	0.94617300	-0.13477100	3.20707300
H	2.98470100	2.58397600	3.40357900
H	-1.26858900	2.41335700	2.78763500
H	0.98262400	-1.21808100	3.26060800
C	3.36405600	-0.04525600	3.64712400
C	4.41480900	-0.58481200	3.94427400
Si	5.96515900	-1.40641900	4.53995500
C	7.44030800	-0.62537100	3.68036100
C	5.80927600	-3.24410800	4.20541200
C	6.09583600	-1.09862000	6.38850700
H	7.55755100	0.41408600	4.00061900
H	7.33935600	-0.63889000	2.59332800
H	8.35462900	-1.16607400	3.94478700
H	5.49656400	-3.43711900	3.17644300
H	5.06842400	-3.68688100	4.87779900
H	6.76618900	-3.74835400	4.37328600
H	5.23597200	-1.51585000	6.91967400
H	6.15105500	-0.02898200	6.60881700
H	7.00082100	-1.57283100	6.78187500
C	0.00769600	-14.36191500	-1.76235100
C	1.20418100	-13.65947700	-1.84710200
C	1.19066800	-12.25732500	-1.90474800
C	-1.23272700	-12.28627900	-1.78781000
C	-1.20840300	-13.68719100	-1.73281800
H	0.02253800	-15.44560000	-1.71194100
C	2.40918200	-11.51012700	-1.98377600
C	3.41896000	-10.84293800	-2.04400700
C	6.99947000	-9.78931300	-2.10896200
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C	5.59795000	-7.82571300	-2.29639500
C	4.59283700	-10.02611400	-2.11076300
C	5.87034700	-10.59994200	-2.05222000
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C	5.45801000	-6.40606200	-2.42274800
C	5.33951600	-5.20437100	-2.52599400
C	6.31714500	-1.61496600	-2.73237100
C	5.08037100	-0.99945400	-2.87110800
C	3.90784500	-1.77310500	-2.90510500
C	5.23890800	-3.78085600	-2.64483900
C	6.40294400	-2.99841700	-2.62122700
H	7.21997500	-1.01407100	-2.70708800
C	-2.35351200	-0.76491400	-0.57357300
C	-3.40809300	-1.33901100	-0.73488800
C	-7.05920000	-1.94606700	-1.10522500
C	-7.09897600	-3.33305500	-1.18076600
C	-5.91026000	-4.07948500	-1.13273500
C	-4.65119100	-2.02541500	-0.91308300
C	-5.84112100	-1.28580800	-0.98148800
H	-7.98190100	-1.37610900	-1.14177800
C	-5.94946200	-5.50570100	-1.24402800
C	-5.96225000	-6.71233700	-1.35046000
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C	-7.17314800	-8.84077600	-1.55965200
H	-8.10410800	-10.76838800	-1.73841600
C	-2.47272300	-11.57203800	-1.74359000
C	-3.50883600	-10.94510800	-1.69946000
C	-0.02973000	-11.57614000	-1.87116200
C	4.46181100	-8.63753900	-2.23348300
C	3.98891800	-3.16328000	-2.78430500
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C	-4.74531500	-8.83146000	-1.51708600
H	2.15298900	-14.18482500	-1.86823800
H	-2.14217000	-14.23380300	-1.65581700
H	7.75171800	-7.77662700	-2.26853400
H	5.96665000	-11.67566600	-1.95098200
H	5.00545900	0.07907700	-2.95991700
H	7.36592600	-3.48438600	-2.50672500
H	-8.04641600	-3.85102500	-1.28631300
H	-5.79971000	-0.20307700	-0.91693100
H	-5.95120500	-12.00022800	-1.82267700
H	-8.10923900	-8.29390500	-1.51837300
H	-0.04477900	-10.49182200	-1.90307700
H	3.47430600	-8.19035600	-2.27553400
H	3.08558200	-3.76428100	-2.79611500
H	-3.76378400	-3.99973800	-0.88159100
H	-3.81131200	-8.28119700	-1.43252500
C	-0.37097900	2.66242300	-3.48941600
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	C	-1.65081000	2.15683600	-3.69362000
	C	-1.85916000	0.76997600	-3.75462800
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	C	0.70629900	1.79888100	-3.33518100
	H	-0.21058300	3.73564400	-3.45811600
	C	-0.77763200	-0.10276600	-3.58531200
	H	-2.49372000	2.82703500	-3.82603100
	H	1.70938000	2.18587200	-3.18593600
	H	-0.93581200	-1.17569200	-3.62535500
	C	-3.16831000	0.26050200	-4.04596000
	C	-4.27541000	-0.14485300	-4.35118300
	Si	-5.91065800	-0.76972600	-4.95707500
	C	-7.28015200	0.20623900	-4.12363000
	C	-6.00088300	-2.60396100	-4.58675900
	C	-5.97797000	-0.47134900	-6.81087200
	H	-7.22066300	1.26231000	-4.40218300
	H	-7.22709600	0.13450700	-3.03536700
	H	-8.25549000	-0.17395700	-4.44366100
	H	-5.75086100	-2.80692800	-3.54242200
	H	-5.29939100	-3.15468500	-5.22019500
	H	-7.00769400	-2.98786200	-4.77897000
	H	-5.16566500	-0.99182900	-7.32531800
	H	-5.90370800	0.59494600	-7.04179700
	H	-6.92670800	-0.84034000	-7.21356900
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	C	-0.22677700	-3.69529100	-0.65172100
	H	0.15453000	-3.57723100	0.36520500
	H	0.51652600	-3.34584100	-1.36644000
	H	-1.15855900	-3.14336600	-0.76808400
	O	-0.43168700	-5.10050000	-0.96902900
	S	-1.44583600	-5.92239400	-0.04235200
	O	-2.08636600	-6.89816600	-0.91126400
	O	-2.28044000	-4.99121500	0.70639500
	C	-0.34147200	-6.76772800	1.07330300
	H	0.24871300	-5.99456700	1.57441100
	H	0.31519900	-7.36879800	0.43796200
	C	-1.13153600	-7.62402600	2.05862400
	H	-1.76650000	-6.97743300	2.67510100
	C	-0.20677900	-8.45942400	2.94350600
	H	-1.79530800	-8.29502200	1.49565000
	H	0.42665400	-9.09083900	2.30362800
	C	-0.98815500	-9.35311200	3.90665000
	H	0.47426500	-7.80312500	3.49975300
	H	-1.46382100	-8.73972000	4.68237600
	C	-0.11749500	-10.43531800	4.54449400
	H	-1.80834500	-9.83428600	3.35641400
	H	0.52692700	-10.87472100	3.77037400
	C	-0.92889200	-11.55591700	5.19123300
	H	0.55753500	-9.98578300	5.28548000

H	-1.61704900	-11.96767300	4.43976400
H	-1.55417300	-11.14477500	5.99478400
C	-0.04416900	-12.67545300	5.73293300
H	0.54741200	-13.11904800	4.92371800
H	-0.63658100	-13.47246200	6.19167700
H	0.65340200	-12.29624700	6.48694700
C	1.16823100	-0.21433200	-0.00841400
C	1.34243000	1.16593800	-0.03294400
H	2.33421900	1.57293800	0.11404100
C	0.21886500	1.99659600	-0.22314800
N	0.32685300	3.35132800	-0.24832300
C	-1.02257000	1.34841000	-0.39061000
H	-1.93840200	1.90033100	-0.55576800
C	-1.06835300	-0.04155700	-0.37419900
C	1.63651800	3.97178400	-0.17623900
C	-0.87056700	4.16690900	-0.33056700
H	1.52367300	5.05121500	-0.26409800
H	2.28154300	3.62564200	-0.99261900
H	2.13616700	3.75174400	0.77544400
H	-1.41860000	3.98252500	-1.26249700
H	-0.58823800	5.21793700	-0.30034300
H	-1.54418700	3.96504100	0.51095700
C	-1.54240600	-14.32137000	1.91416300
C	-2.63577500	-13.46334800	1.84937300
C	-2.43901200	-12.09293300	1.62066200
C	-0.04086500	-12.46558200	1.52694100
C	-0.24874000	-13.83238000	1.76406000
H	-1.70023200	-15.37990900	2.09176400
C	-3.53692800	-11.17368600	1.62220600
C	-4.42932500	-10.35356100	1.65557000
C	-7.84485800	-8.85618200	1.74865200
C	-7.54508500	-7.50487200	1.86592100
C	-6.20697800	-7.08137300	1.91276100
C	-5.48680600	-9.38955700	1.71753200
C	-6.82620000	-9.80074600	1.67643200
H	-8.88044500	-9.17734200	1.71089100
C	-5.90502400	-5.68772500	2.04104400
C	-5.68311600	-4.50113500	2.14802600
C	-6.44461300	-0.87239000	2.46464600
C	-5.17201600	-0.32957000	2.58851100
C	-4.04263300	-1.16480800	2.56221700
C	-5.48827200	-3.08920400	2.28887200
C	-6.60838000	-2.24481300	2.31796400
H	-7.31376900	-0.22327800	2.48006600
C	2.31030800	-1.06270500	0.21696500
C	3.27825000	-1.77019300	0.39070900
C	6.83016600	-2.82697400	0.79708500
C	6.70091100	-4.20842400	0.86780500
C	5.42938300	-4.80116900	0.79867800

C	4.43111500	-2.60141600	0.56725100
C	5.70543200	-2.02093600	0.64944500
H	7.81498200	-2.37421900	0.85385000
C	5.29462800	-6.22364700	0.89326100
C	5.19301300	-7.42774000	0.98684500
C	6.09505700	-11.03508300	1.29152900
C	4.83898000	-11.62765500	1.34272900
C	3.68415700	-10.83126900	1.27949500
C	5.07323800	-8.85012600	1.10391700
C	6.21992200	-9.65481900	1.17391000
H	6.98526200	-11.65388200	1.33757200
C	1.28081000	-11.92616900	1.41309000
C	2.38389200	-11.42707000	1.34732400
C	-1.14023200	-11.60575800	1.44109700
C	-5.18187500	-8.02747200	1.83162900
C	-4.20267800	-2.54530200	2.40197400
C	4.29767800	-3.99338300	0.64269200
C	3.80677000	-9.44407700	1.15536400
H	-3.64269200	-13.84261000	1.98675100
H	0.60524900	-14.49870900	1.82535900
H	-8.33729800	-6.76623000	1.92583900
H	-7.05579100	-10.85647500	1.57978400
H	-5.03642300	0.74016800	2.70814800
H	-7.59856800	-2.67618200	2.21684300
H	7.57516900	-4.84013500	0.98347100
H	5.80043500	-0.94189500	0.58062700
H	4.73841100	-12.70383600	1.43504600
H	7.19925400	-9.19081600	1.12394600
H	-0.98336100	-10.55131100	1.23599100
H	-4.14651600	-7.70418200	1.85462900
H	-3.33490900	-3.19445700	2.34570000
H	3.31359400	-4.44603000	0.57487400
H	2.91685900	-8.82526800	1.09949000
C	0.72029300	2.81285400	3.05082300
C	-1.66887900	-0.03164000	2.82808200
C	-2.74158900	-0.58044300	2.69632800
C	1.92332300	2.15259400	3.27834600
C	1.95136600	0.75241200	3.37138800
C	-0.44075000	0.68907200	2.98031600
C	-0.45786000	2.09104700	2.90891000
H	0.70056700	3.89626400	2.98577800
C	0.76736300	0.02294000	3.21304900
H	2.84568000	2.71136000	3.39940600
H	-1.40137100	2.59837600	2.73504700
H	0.78715800	-1.06026000	3.27058000
C	3.18278800	0.07777500	3.66949900
C	4.22344800	-0.48016500	3.96959700
Si	5.76959100	-1.31706800	4.55143400
C	7.24725900	-0.54795800	3.68362200

C	5.60800300	-3.15421300	4.21268800
C	5.91737200	-1.01668300	6.40110900
H	7.37034700	0.49428900	3.99293700
H	7.14375600	-0.57326800	2.59654700
H	8.15958900	-1.09047600	3.95183300
H	5.33499500	-3.34754000	3.17176300
H	4.83980600	-3.59188000	4.85797200
H	6.55511900	-3.66362600	4.41819000
H	5.05869400	-1.42966700	6.93833300
H	5.98102600	0.05216900	6.62377300
H	6.82260800	-1.49721000	6.78657800
C	-0.04255000	-14.38926600	-1.60471400
C	1.14518600	-13.67907100	-1.73496500
C	1.11532900	-12.28265700	-1.87390500
C	-1.30747200	-12.33409500	-1.74830800
C	-1.26694200	-13.72854300	-1.61065000
H	-0.01440800	-15.46763700	-1.48908300
C	2.32778200	-11.52888700	-1.98242900
C	3.33689600	-10.86214900	-2.05862000
C	6.92734200	-9.84811900	-2.14824300
C	6.81594400	-8.46745200	-2.25823000
C	5.54814200	-7.86635800	-2.31604700
C	4.51786500	-10.05591600	-2.13531100
C	5.78899100	-10.64534500	-2.08726900
H	7.90943500	-10.30724300	-2.10140300
C	5.42865700	-6.44369300	-2.43171200
C	5.33741900	-5.23850900	-2.52327300
C	6.37755400	-1.66464500	-2.68926600
C	5.15273900	-1.02789200	-2.83970800
C	3.96738900	-1.78023800	-2.89556300
C	5.26411400	-3.81223900	-2.63368200
C	6.44060700	-3.04995600	-2.58684000
H	7.28937200	-1.07814600	-2.64709200
C	-2.32839000	-0.70845600	-0.58156500
C	-3.38789100	-1.27546500	-0.73763300
C	-7.04856400	-1.93051900	-1.05108000
C	-7.06849300	-3.31653100	-1.15407100
C	-5.86470800	-4.04006200	-1.13999400
C	-4.63463700	-1.96203100	-0.90005200
C	-5.84122400	-1.24834300	-0.92805400
H	-7.98154800	-1.37577100	-1.06163700
C	-5.87431000	-5.46670400	-1.26481300
C	-5.88638400	-6.67345000	-1.37845000
C	-7.21768600	-10.13812000	-1.73374900
C	-6.04439700	-10.88245500	-1.76454200
C	-4.80131600	-10.23706100	-1.67348400
C	-5.93298800	-8.09946400	-1.51068700
C	-7.16986400	-8.75373800	-1.60976500
H	-8.17712000	-10.63994900	-1.80442100

C	-2.55250300	-11.62697900	-1.73122100
C	-3.58581200	-10.99423900	-1.70706500
C	-0.11294300	-11.61575800	-1.87715300
C	4.40271100	-8.66521000	-2.25090000
C	4.02715600	-3.17276800	-2.78733600
C	-4.65095900	-3.35851100	-1.00434000
C	-4.74817500	-8.84510900	-1.54112600
H	2.10045900	-14.19287700	-1.72362600
H	-2.19398700	-14.27994600	-1.49648500
H	7.70239700	-7.84374700	-2.30154600
H	5.87296500	-11.72254000	-1.99042400
H	5.09754600	0.05257900	-2.91968500
H	7.39390900	-3.55196900	-2.46134600
H	-8.00865300	-3.84876100	-1.25244200
H	-5.82192100	-0.16705100	-0.83441300
H	-6.07764100	-11.96239700	-1.86192100
H	-8.08374300	-8.16994700	-1.57937400
H	-0.14154200	-10.53514600	-1.96915700
H	3.42024500	-8.20600200	-2.28422400
H	3.11575700	-3.76043900	-2.82001900
H	-3.72085800	-3.91506800	-0.95673200
H	-3.79134400	-8.34074000	-1.45021100
C	-0.25609400	2.70350300	-3.52472600
C	1.71455600	-0.43391600	-3.20579600
C	2.72090100	-1.09369900	-3.05923900
C	-1.53975300	2.21235100	-3.73767100
C	-1.76545800	0.82773800	-3.78316100
C	0.59341300	0.44043700	-3.37910700
C	0.80799400	1.82775800	-3.35232500
H	-0.08304700	3.77479700	-3.49711700
C	-0.69674300	-0.05641200	-3.59423000
H	-2.37307300	2.89176400	-3.88409800
H	1.81342500	2.20374700	-3.19148500
H	-0.86972600	-1.12740300	-3.61638000
C	-3.08078900	0.33075900	-4.07119600
C	-4.19380400	-0.06814000	-4.36461400
Si	-5.84917600	-0.66911700	-4.93553500
C	-7.18877200	0.32560800	-4.07526800
C	-5.96870500	-2.49930700	-4.55236700
C	-5.95152600	-0.37951200	-6.78965100
H	-7.10981400	1.38501300	-4.33574400
H	-7.12541600	0.23212900	-2.98875900
H	-8.17532800	-0.02847900	-4.39129100
H	-5.73093800	-2.69539000	-3.50347800
H	-5.27201900	-3.06812500	-5.17532100
H	-6.98051600	-2.86818700	-4.74858700
H	-5.15627200	-0.91322800	-7.31749500
H	-5.86769600	0.68458200	-7.02769200
H	-6.91283500	-0.73779500	-7.17183700

TS-d	N	-0.00917600	-0.86429700	-0.22411200
	C	-0.08164100	-2.89338800	-0.41842900
	H	0.23826600	-2.97975400	0.61017300
	H	0.65976800	-2.80910600	-1.19843400
	H	-1.12986900	-2.79255900	-0.64039700
	O	-0.12264200	-4.74088400	-0.68646700
	S	-1.19438100	-5.52975700	0.06963600
	O	-1.94074600	-6.41066300	-0.84050700
	O	-2.02209600	-4.63486300	0.89760200
	C	-0.23809600	-6.56401000	1.17223500
	H	0.38119800	-5.88199300	1.76274300
	H	0.41657800	-7.16202700	0.53092700
	C	-1.11481500	-7.43985600	2.05631500
	H	-1.77295800	-6.80153700	2.65818700
	C	-0.27779700	-8.33885800	2.96511700
	H	-1.75791300	-8.06197500	1.41926100
	H	0.36205100	-8.98230900	2.34317500
	C	-1.14174800	-9.21400100	3.87174400
	H	0.40269000	-7.72677400	3.57114800
	H	-1.64106100	-8.58748600	4.62270100
	C	-0.35297500	-10.32650700	4.55924200
	H	-1.94553300	-9.66511300	3.27382900
	H	0.25984100	-10.84595600	3.80893600
	C	-1.25068000	-11.34836100	5.25221300
	H	0.35088800	-9.89536000	5.28424400
	H	-1.97952500	-11.72561200	4.52199200
	H	-1.82959900	-10.85159300	6.04105700
	C	-0.46478800	-12.51863100	5.83636700
	H	0.07600200	-13.04863300	5.04481800
	H	-1.12117500	-13.23757400	6.33405000
	H	0.27144600	-12.17142500	6.56857600
	C	1.17023000	-0.24512900	-0.03252700
	C	1.32005800	1.13334800	-0.04231400
	H	2.30611100	1.54775200	0.11845800
	C	0.18686600	1.95511100	-0.23467300
	N	0.28222200	3.30438400	-0.25405800
	C	-1.05121600	1.29658500	-0.40521700
	H	-1.97339000	1.84035200	-0.55836800
	C	-1.09473700	-0.08952300	-0.40729600
	C	1.58800500	3.93840900	-0.18647100
C	-0.92328700	4.11174400	-0.33819200	
H	1.46333600	5.01604000	-0.27464700	
H	2.23079900	3.59688900	-1.00571900	
H	2.09021200	3.72288500	0.76409300	
H	-1.46368800	3.92504100	-1.27342300	
H	-0.64880100	5.16421800	-0.30274300	
H	-1.59613600	3.89982800	0.50061300	
C	-1.47558000	-14.34596500	1.80006500	
C	-2.57637900	-13.49571100	1.80652500	



C	-2.39567100	-12.11371800	1.64344200
C	0.00176900	-12.45971500	1.47260500
C	-0.18975500	-13.83845700	1.64251900
H	-1.62075900	-15.41369100	1.92556100
C	-3.50147200	-11.20552400	1.69974400
C	-4.39745600	-10.39272300	1.78090800
C	-7.80659200	-8.90036800	2.04120600
C	-7.50496400	-7.54604800	2.10890800
C	-6.16773900	-7.11878300	2.06939300
C	-5.45137800	-9.42895400	1.88817300
C	-6.78986000	-9.84341100	1.93289000
H	-8.84146800	-9.22479400	2.06970700
C	-5.86990200	-5.72006800	2.14275900
C	-5.66112900	-4.52795600	2.20449500
C	-6.45100600	-0.89444300	2.37357100
C	-5.18388700	-0.33980400	2.50142900
C	-4.05099200	-1.16987800	2.52047900
C	-5.47969900	-3.11017000	2.29255100
C	-6.60482900	-2.27238300	2.27376800
H	-7.32402200	-0.25074900	2.35285200
C	2.31359400	-1.08269000	0.19865400
C	3.28567300	-1.78244100	0.37762700
C	6.83698400	-2.81365800	0.83632500
C	6.71760400	-4.19752400	0.86460000
C	5.45364300	-4.79989700	0.75189600
C	4.44347900	-2.60418900	0.56203000
C	5.70863900	-2.01247300	0.68939200
H	7.81664000	-2.35547000	0.92588200
C	5.33030900	-6.22478000	0.80935900
C	5.23896900	-7.43135500	0.87300200
C	6.12950600	-11.05149600	1.02049500
C	4.87299600	-11.63659800	1.12095000
C	3.72335900	-10.83097900	1.14248300
C	5.11872000	-8.85576300	0.95540000
C	6.26048800	-9.66907100	0.93877900
H	7.01516900	-11.67773300	1.00083100
C	1.31721700	-11.90892700	1.34260100
C	2.42230700	-11.41868300	1.25094200
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C	-4.19846000	-2.55574300	2.40229000
C	4.31814300	-3.99831600	0.59309300
C	3.85152300	-9.44187800	1.05485200
H	-3.57703300	-13.89040900	1.94598200
H	0.67054700	-14.49909100	1.64552800
H	-8.29487400	-6.80759700	2.19548600
H	-7.02096000	-10.90161200	1.87335600
H	-5.05629800	0.73398100	2.58880900
H	-7.59122300	-2.71270300	2.17381200

H	7.59507400	-4.82457800	0.98119100
H	5.79435800	-0.93106800	0.65582200
H	4.76833900	-12.71441300	1.18447500
H	7.23965300	-9.21080500	0.85086500
H	-0.96251300	-10.53995000	1.30894100
H	-4.11011200	-7.73676900	1.90758100
H	-3.32516800	-3.19985500	2.37110900
H	3.33932000	-4.45524900	0.48582400
H	2.96556100	-8.81557900	1.06170000
C	0.77017800	2.75412200	3.03140600
C	-1.67699500	-0.04103200	2.79705600
C	-2.75318900	-0.58184100	2.66242700
C	1.95704300	2.06711200	3.26563700
C	1.95256200	0.66674700	3.36091800
C	-0.43759000	0.65752900	2.95375400
C	-0.42354400	2.05949500	2.88308100
H	0.77474600	3.83786800	2.96962700
C	0.75368400	-0.03567100	3.19454900
H	2.89050700	2.60524600	3.39349400
H	-1.35489700	2.58823500	2.70710300
H	0.74723100	-1.11889000	3.25741500
C	3.16251100	-0.03599000	3.67897900
C	4.18376000	-0.61628800	4.00145800
Si	5.69140200	-1.48677000	4.63248700
C	7.21236500	-0.70261000	3.86086500
C	5.53016900	-3.30999600	4.22895800
C	5.74558900	-1.24219200	6.49470100
H	7.32732700	0.32699600	4.21209400
H	7.15667700	-0.68812100	2.77055600
H	8.10847100	-1.26109100	4.14937500
H	5.31481000	-3.46809000	3.16941400
H	4.72101500	-3.75668300	4.81441100
H	6.45746100	-3.83840300	4.47210300
H	4.85741900	-1.66305300	6.97387600
H	5.80425500	-0.18083100	6.75142800
H	6.62582300	-1.74137400	6.91234500
C	-0.00182400	-14.35678900	-1.75033900
C	1.17507900	-13.63054800	-1.88989400
C	1.12998300	-12.22972700	-1.96866000
C	-1.28615800	-12.30887000	-1.76519300
C	-1.23069000	-13.70741100	-1.68772500
H	0.03856400	-15.43891500	-1.68331700
C	2.33282700	-11.46344800	-2.09413300
C	3.33914700	-10.79487100	-2.18826600
C	6.93126600	-9.81794200	-2.43444500
C	6.83347200	-8.43263400	-2.48510900
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C	4.52307600	-9.99615700	-2.29294800
C	5.78663900	-10.60233300	-2.34047700

H	7.90739200	-10.29057200	-2.46444900
C	5.46856400	-6.38777200	-2.51327400
C	5.38927000	-5.17987200	-2.57193000
C	6.43892900	-1.60405100	-2.62373000
C	5.21823500	-0.96148300	-2.78383100
C	4.03426000	-1.71147900	-2.87945400
C	5.32259000	-3.75106200	-2.64258900
C	6.49848800	-2.99169300	-2.55393000
H	7.35069800	-1.02072800	-2.54934500
C	-2.34912200	-0.75852600	-0.61134500
C	-3.40641200	-1.33182000	-0.75548300
C	-7.05882700	-1.96899800	-1.13313800
C	-7.08875600	-3.35754200	-1.17711300
C	-5.89477600	-4.09235200	-1.09109500
C	-4.65206400	-2.02086500	-0.91000300
C	-5.84789400	-1.29527300	-1.00550500
H	-7.98495000	-1.40693100	-1.19772600
C	-5.92119300	-5.52175000	-1.16271800
C	-5.95001600	-6.73052700	-1.23970700
C	-7.22293600	-10.23012600	-1.44558000
C	-6.03504100	-10.94596200	-1.52826000
C	-4.80473300	-10.27012000	-1.51762400
C	-5.97962300	-8.15861500	-1.33375100
C	-7.20339700	-8.84238700	-1.35247200
H	-8.17144100	-10.75693200	-1.45102000
C	-2.53644300	-11.61649700	-1.68481900
C	-3.57746200	-11.00135300	-1.60796100
C	-0.10266800	-11.57437200	-1.90277900
C	4.42148800	-8.60095100	-2.34769500
C	4.08957300	-3.10605800	-2.80248200
C	-4.67601600	-3.42107000	-0.94367000
C	-4.77956200	-8.87593600	-1.41069300
H	2.13404900	-14.13552500	-1.93583100
H	-2.14945900	-14.27138300	-1.56785000
H	7.72470000	-7.81842000	-2.55702100
H	5.85986200	-11.68353500	-2.29205800
H	5.16614600	0.12054800	-2.84053900
H	7.44887500	-3.49775100	-2.42244400
H	-8.03060100	-3.88493200	-1.28493200
H	-5.81671900	-0.21115800	-0.96437000
H	-6.04597400	-12.02809900	-1.60288600
H	-8.12854400	-8.28004000	-1.28404700
H	-0.14285700	-10.49135800	-1.95085600
H	3.44596600	-8.12818000	-2.30479400
H	3.17718400	-3.69016400	-2.86379200
H	-3.75369500	-3.98419100	-0.83309900
H	-3.83295200	-8.34486700	-1.37617700
C	-0.27979200	2.70274700	-3.52872700
C	1.77409700	-0.38174900	-3.20863000

	C	2.78863900	-1.02699300	-3.05451000
	C	-1.54748800	2.17585100	-3.75284200
	C	-1.73222700	0.78565300	-3.80996400
	C	0.63366400	0.46496300	-3.38974800
	C	0.80855300	1.85751500	-3.35421100
	H	-0.13789200	3.77843400	-3.49558000
	C	-0.63952000	-0.06800800	-3.61925400
	H	-2.39912100	2.83167900	-3.90096000
	H	1.80224000	2.26125900	-3.18774400
	H	-0.78007500	-1.14349100	-3.65442700
	C	-3.02873100	0.25028600	-4.11245000
	C	-4.12591100	-0.18134100	-4.41811800
	Si	-5.75267100	-0.83261900	-5.01560900
	C	-7.13177700	0.16927600	-4.23113600
	C	-5.85441300	-2.65075300	-4.57516200
	C	-5.80108900	-0.60837200	-6.88058800
	H	-7.05862200	1.22048500	-4.52419600
	H	-7.10261400	0.11313800	-3.14080100
	H	-8.10272900	-0.20931400	-4.56603500
	H	-5.64388500	-2.81106800	-3.51466900
	H	-5.13133400	-3.22669300	-5.16005100
	H	-6.85429000	-3.04175100	-4.78844800
	H	-4.98482500	-1.15078200	-7.36545900
	H	-5.72122300	0.44752100	-7.15362500
	H	-6.74649500	-0.99106200	-7.27823500
4d	N	0.01566600	-0.84746800	-0.19264200
	C	-0.02239100	-2.32014000	-0.24461300
	H	0.44117100	-2.72048800	0.65942200
	H	0.53075000	-2.66159100	-1.12177400
	H	-1.05044700	-2.66863900	-0.29721600
	O	-0.34189200	-5.07064300	-1.15655500
	S	-1.33080300	-5.69632600	-0.24545300
	O	-2.24152800	-6.64572500	-0.92949100
	O	-2.05728400	-4.70549000	0.59205600
	C	-0.35510700	-6.68151800	0.89525900
	H	0.31166400	-5.98382600	1.41229900
	H	0.25726200	-7.34534100	0.27628700
	C	-1.20693100	-7.47489000	1.87341600
	H	-1.84765300	-6.78572900	2.43776300
	C	-0.35903600	-8.31254700	2.82873600
	H	-1.87201000	-8.13550800	1.30049000
	H	0.28839700	-8.98046300	2.24042500
	C	-1.20545100	-9.15293200	3.78357400
	H	0.31673500	-7.66145400	3.39879800
	H	-1.70955100	-8.49836900	4.50719300
	C	-0.39561700	-10.22096800	4.51630800
	H	-2.00644900	-9.64355300	3.21281200
	H	0.23154600	-10.75368000	3.78737300
	C	-1.27023000	-11.23842000	5.24383300

H	0.29596900	-9.74722100	5.22655400
H	-1.98472200	-11.66149900	4.52421600
H	-1.86640000	-10.72785300	6.01093300
C	-0.45618800	-12.36468400	5.87485200
H	0.10079900	-12.91055600	5.10538800
H	-1.09454700	-13.08085700	6.39911900
H	0.26879100	-11.97017100	6.59430000
C	1.21775100	-0.22005600	-0.00953600
C	1.33061500	1.15097900	-0.01853000
H	2.31347700	1.57405200	0.13300300
C	0.18010400	1.96263300	-0.18779000
N	0.25873200	3.30129500	-0.19394100
C	-1.05503000	1.28721600	-0.34994400
H	-1.98290600	1.82188600	-0.49436800
C	-1.10853000	-0.09014200	-0.37031400
C	1.55953400	3.95569300	-0.12504200
C	-0.95769300	4.10120200	-0.26680400
H	1.41595200	5.03178600	-0.19011600
H	2.19623500	3.63881500	-0.95733000
H	2.06680900	3.72678500	0.81835100
H	-1.49526700	3.91389700	-1.20219000
H	-0.69035700	5.15453700	-0.22523000
H	-1.62025800	3.87475700	0.57472000
C	-1.47663400	-14.36700400	1.85939300
C	-2.59173200	-13.53626000	1.81616600
C	-2.42946700	-12.15538900	1.62789500
C	-0.02250700	-12.46221600	1.53232200
C	-0.19577500	-13.84038600	1.72699800
H	-1.60709100	-15.43430000	2.00360300
C	-3.54863100	-11.26231400	1.63389300
C	-4.45348900	-10.45667600	1.67599800
C	-7.85495100	-8.92457000	1.80801600
C	-7.53753600	-7.57580000	1.90732000
C	-6.19369000	-7.16832800	1.92572900
C	-5.50365700	-9.48568900	1.74292900
C	-6.84820000	-9.88162100	1.72909900
H	-8.89470700	-9.23411100	1.79091100
C	-5.87116400	-5.77827100	2.03866200
C	-5.62797700	-4.59500500	2.13363200
C	-6.31071100	-0.94827600	2.42366200
C	-5.02692000	-0.43539100	2.55590200
C	-3.91813700	-1.29813900	2.53334300
C	-5.40416900	-3.18695600	2.26097300
C	-6.50465600	-2.31757600	2.28147300
H	-7.16487300	-0.27957200	2.43282100
C	2.35970700	-1.04512200	0.20347200
C	3.33169900	-1.74543000	0.38030900
C	6.88269800	-2.80193700	0.76250300
C	6.74557400	-4.18324400	0.82694500

C	5.47134900	-4.77272000	0.77269900
C	4.48779500	-2.56812800	0.56023000
C	5.76159600	-1.98733400	0.63388800
H	7.87113100	-2.35650700	0.80866700
C	5.32735500	-6.19323800	0.87298300
C	5.21705400	-7.39606000	0.97016700
C	6.09619900	-11.00719200	1.27574700
C	4.83672600	-11.59066200	1.33954400
C	3.68584800	-10.78748700	1.28412600
C	5.08646500	-8.81701700	1.09228800
C	6.22880800	-9.62802500	1.15379600
H	6.98252600	-11.63191400	1.31482900
C	1.28696600	-11.89123100	1.42839700
C	2.38506400	-11.38158500	1.35980500
C	-1.14352800	-11.62826500	1.47098600
C	-5.18037100	-8.12599100	1.83469900
C	-4.10523000	-2.67411400	2.36954700
C	4.34286300	-3.95926300	0.63013900
C	3.81567300	-9.40136200	1.15535100
H	-3.58913400	-13.94541200	1.93601300
H	0.67497600	-14.48614200	1.76739600
H	-8.31999600	-6.82736600	1.97439600
H	-7.09177600	-10.93565300	1.64876700
H	-4.86645500	0.63061200	2.67766400
H	-7.50401900	-2.72712000	2.17939000
H	7.61875600	-4.81878600	0.92867500
H	5.86015800	-0.90837100	0.57104900
H	4.72974300	-12.66605900	1.43438100
H	7.21032000	-9.17004700	1.09352700
H	-1.01561600	-10.56405200	1.29951700
H	-4.14084100	-7.81326900	1.82651600
H	-3.25242800	-3.34244300	2.29679900
H	3.35511300	-4.40449600	0.56603500
H	2.92947800	-8.77670900	1.10412800
C	0.82377000	2.66348800	3.09716100
C	-1.53081500	-0.20215400	2.82202300
C	-2.60678600	-0.74106800	2.67654700
C	2.03770800	2.01404100	3.30022200
C	2.08367800	0.61271500	3.36869100
C	-0.31031000	0.52627500	2.99154000
C	-0.34650600	1.92973000	2.94848900
H	0.78870100	3.74797300	3.06109900
C	0.90732200	-0.12910700	3.20694600
H	2.95350200	2.58218700	3.42623400
H	-1.29875100	2.42805900	2.79601600
H	0.94036600	-1.21289000	3.25448800
C	3.32264400	-0.05180700	3.65588800
C	4.36876000	-0.60055300	3.95271600
Si	5.91476400	-1.42467400	4.55588700

C	7.39594700	-0.63738600	3.71240100
C	5.76271100	-3.26011400	4.20822000
C	6.02814300	-1.12711500	6.40749500
H	7.51046900	0.39998600	4.04031500
H	7.30182400	-0.64379900	2.62460600
H	8.30876700	-1.17947100	3.97922500
H	5.47985400	-3.44684000	3.16919100
H	5.00036100	-3.70395600	4.85596600
H	6.71257700	-3.76868000	4.40201000
H	5.16365400	-1.54835200	6.92816500
H	6.07942300	-0.05846500	6.63368100
H	6.93009900	-1.60182500	6.80725000
C	-0.00120700	-14.36636300	-1.64854900
C	1.19384400	-13.66634900	-1.76867700
C	1.17762800	-12.26731700	-1.87841600
C	-1.24478700	-12.29484300	-1.74419700
C	-1.21829900	-13.69262500	-1.63643700
H	0.01568900	-15.44720900	-1.55537900
C	2.39436000	-11.52074500	-1.98487500
C	3.40495000	-10.85587800	-2.05644200
C	6.98589200	-9.80801400	-2.16994200
C	6.85940300	-8.42814700	-2.27526600
C	5.58496100	-7.84033200	-2.32124500
C	4.57895800	-10.04045800	-2.13680600
C	5.85630900	-10.61703400	-2.10181200
H	7.97301300	-10.25712700	-2.13394500
C	5.44688100	-6.41931000	-2.43603200
C	5.33438100	-5.21606800	-2.52867700
C	6.32673800	-1.62940800	-2.71414000
C	5.09288200	-1.00798400	-2.85256600
C	3.91717200	-1.77652800	-2.89342400
C	5.23924600	-3.79145700	-2.64099100
C	6.40646900	-3.01380800	-2.61011900
H	7.23209000	-1.03236600	-2.68306700
C	-2.35170500	-0.75337500	-0.58680400
C	-3.40798200	-1.32440100	-0.74827300
C	-7.05991900	-1.94253900	-1.11131600
C	-7.09382000	-3.32998400	-1.18602900
C	-5.90192900	-4.07157700	-1.13959700
C	-4.65205500	-2.01028100	-0.92360600
C	-5.84508200	-1.27563000	-0.99006200
H	-7.98550700	-1.37721900	-1.14712300
C	-5.93445400	-5.49856900	-1.25020100
C	-5.96425700	-6.70577400	-1.34914500
C	-7.17246900	-10.21969900	-1.67374400
C	-5.97082200	-10.91523900	-1.71270700
C	-4.75224700	-10.22163600	-1.63368400
C	-5.96646700	-8.13279100	-1.47097600
C	-7.17764800	-8.83363500	-1.55590500

H	-8.11157400	-10.75995700	-1.73270000
C	-2.48404000	-11.57837800	-1.71128600
C	-3.51748400	-10.94641600	-1.67572500
C	-0.04344000	-11.58705900	-1.86219000
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C	3.99205100	-3.16791300	-2.77989100
C	-4.67680000	-3.40976300	-0.99089900
C	-4.75016900	-8.82837700	-1.50576800
H	2.14353500	-14.19059400	-1.77375200
H	-2.15074100	-14.23666100	-1.53081400
H	7.73898700	-7.79528600	-2.32539100
H	5.95218000	-11.69370400	-2.00991500
H	5.02284700	0.07139400	-2.93526900
H	7.36718900	-3.50420500	-2.49531100
H	-8.03931700	-3.85169500	-1.29001400
H	-5.80884700	-0.19261300	-0.92760100
H	-5.96090800	-11.99611700	-1.80525600
H	-8.11310200	-8.28538700	-1.51921500
H	-0.06017200	-10.50464100	-1.93243000
H	3.46095900	-8.20162000	-2.26992900
H	3.08600900	-3.76493800	-2.79606800
H	-3.75474400	-3.97700800	-0.89069900
H	-3.81584900	-8.27927300	-1.41935900
C	-0.36361100	2.66299500	-3.46287100
C	1.65015300	-0.45133700	-3.18825300
C	2.66231200	-1.10373700	-3.04817900
C	-1.64306900	2.15610200	-3.66720300
C	-1.84917600	0.76912200	-3.73227300
C	0.51864800	0.41069600	-3.35334400
C	0.71509000	1.80068200	-3.31139900
H	-0.20472600	3.73635600	-3.42838500
C	-0.76595200	-0.10225600	-3.56707600
H	-2.48733200	2.82536800	-3.79587100
H	1.71752900	2.18872400	-3.16035100
H	-0.92277500	-1.17525400	-3.61076000
C	-3.15723600	0.25738200	-4.02433500
C	-4.26377000	-0.14914600	-4.33011400
Si	-5.89874900	-0.75915200	-4.95127100
C	-7.26685900	0.23246200	-4.13449300
C	-6.01100700	-2.59195900	-4.58016700
C	-5.94279100	-0.46367800	-6.80627700
H	-7.18702500	1.28906900	-4.40585600
H	-7.23296300	0.15390300	-3.04590100
H	-8.24224900	-0.13123300	-4.47288600
H	-5.76495800	-2.79656200	-3.53522000
H	-5.31403200	-3.15086800	-5.21165600
H	-7.02154400	-2.96515500	-4.77403400
H	-5.13191300	-0.99601400	-7.31084300
H	-5.85229400	0.60099500	-7.03895400



	H	-6.89190800	-0.82160700	-7.21796400
3e	N	0.05658500	-0.84413000	-0.18621500
	C	-0.13207700	-3.72765500	-0.46099900
	H	0.19207800	-3.51752800	0.55754300
	H	0.63760700	-3.42547400	-1.16881500
	H	-1.06472000	-3.20618200	-0.67147500
	O	-0.28671700	-5.16071800	-0.66064200
	S	-1.43210500	-5.90485100	0.18460700
	O	-2.28375200	-6.60777300	-0.76715700
	O	-2.05377300	-4.95096400	1.09606000
	C	-0.45888300	-7.10064100	1.11529900
	H	0.30764400	-6.49031600	1.60594100
	C	-1.37682900	-7.74907500	2.14885500
	H	-0.77784800	-8.39761300	2.79407500
	H	-2.13529700	-8.36316200	1.64854100
	H	-1.86994500	-7.00192800	2.77559800
	C	0.15968100	-8.11223500	0.15549300
	H	0.83763700	-7.63703000	-0.55754000
	H	-0.63192100	-8.63140300	-0.39369000
	H	0.72396600	-8.85387200	0.72965700
	C	1.21894400	-0.19441800	-0.02180200
	C	1.36415100	1.18903800	-0.04627600
	H	2.34850800	1.61550200	0.09561000
	C	0.22268800	1.99676100	-0.22899400
	N	0.30261900	3.35354100	-0.25039300
	C	-1.00537900	1.32232300	-0.39042100
	H	-1.93384300	1.85508800	-0.54839900
	C	-1.02265100	-0.06907600	-0.37301600
	C	1.59995100	4.00028200	-0.19000100
	C	-0.91219100	4.14431800	-0.31438700
	H	1.46423900	5.07747300	-0.27252800
	H	2.24260200	3.67020700	-1.01493600
	H	2.11458700	3.78708400	0.75524500
	H	-1.46433700	3.95800400	-1.24357700
	H	-0.65191000	5.20081200	-0.27540300
	H	-1.57343900	3.91892500	0.53110000
	C	-1.41609800	-14.17554500	1.93539000
	C	-2.52022300	-13.32955100	1.93451700
	C	-2.34198400	-11.94449600	1.79624300
	C	0.06023800	-12.28155800	1.65333400
	C	-0.12970500	-13.66299400	1.80139200
H	-1.55974600	-15.24549400	2.04310700	
C	-3.45814000	-11.04592000	1.82389600	
C	-4.38410000	-10.26449700	1.87261300	
C	-7.83567700	-8.84448700	1.98985600	
C	-7.56732100	-7.48302700	2.06453000	
C	-6.23881500	-7.02950400	2.07703300	
C	-5.46615400	-9.32660700	1.93295300	
C	-6.79679900	-9.76789000	1.92622300	

H	-8.86382200	-9.19071100	1.97766900
C	-5.95064000	-5.62950500	2.16220000
C	-5.71355100	-4.44316700	2.23444300
C	-6.43648300	-0.79887400	2.44462300
C	-5.15896400	-0.26744700	2.56778400
C	-4.03910500	-1.11579100	2.57543000
C	-5.50412900	-3.03007800	2.33846100
C	-6.61459800	-2.17277000	2.33285300
H	-7.29824600	-0.13989000	2.43465800
C	2.38042900	-1.01713600	0.19843100
C	3.36774900	-1.69658400	0.37463900
C	6.93833500	-2.68078600	0.81123700
C	6.83572100	-4.06488300	0.87731600
C	5.57693500	-4.68162900	0.79312800
C	4.53795800	-2.50123300	0.55767800
C	5.79969500	-1.89607500	0.65439600
H	7.91347600	-2.20909600	0.87985500
C	5.46182000	-6.10573300	0.88545700
C	5.36336400	-7.31010200	0.97810300
C	6.19900700	-10.94078900	1.20911500
C	4.93263900	-11.50386500	1.31366500
C	3.79514400	-10.68000800	1.31281800
C	5.22461600	-8.73098200	1.09090700
C	6.35311500	-9.56253800	1.09885400
H	7.07468500	-11.58145600	1.20700900
C	1.37610400	-11.72928700	1.52477400
C	2.48467100	-11.24775300	1.42606900
C	-1.05011300	-11.43139500	1.64638600
C	-5.19467700	-7.95480200	2.00534900
C	-4.21321200	-2.49832400	2.45139200
C	4.43154200	-3.89555700	0.62691100
C	3.94794100	-9.29546000	1.19736300
H	-3.52179100	-13.73032400	2.04764900
H	0.73169500	-14.32218300	1.80173200
H	-8.37633000	-6.76220700	2.11666200
H	-7.00503300	-10.83046400	1.86142400
H	-5.01221300	0.80344700	2.66100500
H	-7.60863600	-2.59566500	2.23336600
H	7.72117700	-4.67908900	1.00198500
H	5.87454900	-0.81525100	0.58970200
H	4.81076000	-12.57851000	1.39799300
H	7.34004300	-9.12206500	1.00636900
H	-0.90655500	-10.36517300	1.51930200
H	-4.17053900	-7.60010400	2.00233200
H	-3.35212900	-3.15882400	2.42546100
H	3.45760900	-4.36758300	0.54600600
H	3.07526700	-8.65090000	1.18964200
C	0.73158500	2.84784400	3.03324400
C	-1.65813400	0.00269600	2.83654000

C	-2.73350100	-0.54204500	2.70996500
C	1.93444100	2.18972300	3.26817900
C	1.96248800	0.79035500	3.37368700
C	-0.42886700	0.72317900	2.97983300
C	-0.44623700	2.12468800	2.89665500
H	0.71174100	3.93074500	2.95925500
C	0.77900600	0.05918700	3.21908200
H	2.85648800	2.74966900	3.38601700
H	-1.38995800	2.63052100	2.71915700
H	0.79839300	-1.02337700	3.28770300
C	3.19326400	0.12014900	3.68405900
C	4.23691300	-0.42570500	3.99542600
Si	5.78430200	-1.24685200	4.59505400
C	7.26561300	-0.43959900	3.77064500
C	5.66408800	-3.08067100	4.22394800
C	5.88960200	-0.97321600	6.45120400
H	7.36047900	0.60144200	4.09295500
H	7.18812800	-0.45602100	2.68169300
H	8.18179900	-0.96707500	4.05497800
H	5.40721200	-3.26184200	3.17714500
H	4.89831400	-3.54513300	4.85247000
H	6.61937800	-3.57357200	4.43142700
H	5.03057000	-1.41317200	6.96510500
H	5.92515500	0.09293700	6.69171100
H	6.79756400	-1.44009500	6.84644400
C	0.05628100	-14.27605600	-1.52371400
C	1.23517500	-13.55245600	-1.66092400
C	1.18969100	-12.15417800	-1.77548300
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C	-1.17380500	-13.62650500	-1.49172500
H	0.09602800	-15.35644200	-1.43143800
C	2.39144500	-11.38678700	-1.90305100
C	3.39467600	-10.71506600	-2.00713600
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C	4.57600500	-9.91506500	-2.12784600
C	5.84225400	-10.51717300	-2.14910300
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C	5.42616100	-5.10415100	-2.53565600
C	6.48239100	-1.53367600	-2.68422700
C	5.26093100	-0.89167400	-2.84140400
C	4.07351200	-1.63958200	-2.90574400
C	5.36110600	-3.67711200	-2.64047200
C	6.54009400	-2.91945300	-2.58445700
H	7.39609000	-0.95068200	-2.63493400
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C	-3.33244100	-1.32904500	-0.71120500

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C	-5.87472800	-4.05037400	-1.06361600
C	-4.58716000	-2.00429200	-0.86095700
C	-5.77352800	-1.25867100	-0.92621600
H	-7.91419700	-1.32588000	-1.09317200
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C	-7.18874400	-8.81461900	-1.37075200
H	-8.13144300	-10.74069600	-1.48737800
C	-2.48283300	-11.53855400	-1.55363600
C	-3.53073100	-10.93134700	-1.50777600
C	-0.04458300	-11.49982300	-1.74581100
C	4.46877100	-8.52225900	-2.22345100
C	4.12779500	-3.03248400	-2.79965800
C	-4.64198100	-3.40225500	-0.92390000
C	-4.76412700	-8.82095100	-1.35719900
H	2.19504100	-14.05761100	-1.67844300
H	-2.09360700	-14.18872700	-1.37139400
H	7.77036500	-7.73194200	-2.42911300
H	5.91975300	-11.59625900	-2.06853200
H	5.21053500	0.18913400	-2.91973900
H	7.49089500	-3.42499100	-2.45421800
H	-8.00889200	-3.80196600	-1.22313100
H	-5.72271000	-0.17632700	-0.86269000
H	-5.98870400	-11.98921400	-1.56448300
H	-8.12203000	-8.26277500	-1.33326400
H	-0.08257000	-10.41983500	-1.83742400
H	3.49038400	-8.05311200	-2.20346100
H	3.21404400	-3.61615500	-2.83766100
H	-3.73023800	-3.98716900	-0.85521800
H	-3.82513000	-8.27861400	-1.30419800
C	-0.23357700	2.78687700	-3.50837200
C	1.81437900	-0.30453200	-3.22039500
C	2.82749500	-0.95358600	-3.07354200
C	-1.50459500	2.26532900	-3.72497400
C	-1.69473300	0.87610100	-3.78674300
C	0.67385000	0.54515800	-3.38917500
C	0.85301600	1.93694000	-3.34791500
H	-0.08849500	3.86187100	-3.46736900
C	-0.60334200	0.01777900	-3.60953000
H	-2.35558100	2.92470900	-3.86106900
H	1.84885500	2.33650600	-3.18452700
H	-0.74862700	-1.05686000	-3.64368200
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	C	-4.10370400	-0.07208600	-4.36600100
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	C	-7.10332500	0.28196200	-4.09548500
	C	-5.84251500	-2.53737000	-4.50606900
	C	-5.84814600	-0.46959900	-6.78761800
	H	-7.05465500	1.33017000	-4.40421400
	H	-7.02659800	0.23996700	-3.00692700
	H	-8.08364300	-0.11107800	-4.38330500
	H	-5.60713700	-2.71153800	-3.45304300
	H	-5.13652300	-3.10869800	-5.11593400
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	H	-5.04364700	-1.00325800	-7.30092500
	H	-5.78002900	0.58969300	-7.05058700
	H	-6.80269000	-0.85155800	-7.16351400
	N	0.04154900	-0.84239200	-0.19967400
	C	-0.02605400	-2.88830000	-0.34257900
	H	0.55872600	-2.94270200	0.56236300
	H	0.47828500	-2.79514900	-1.29350200
	H	-1.09912500	-2.81045000	-0.27801800
	O	-0.04463100	-4.74702300	-0.53968000
	S	-1.23455900	-5.50572700	0.05459800
	O	-2.05002400	-6.13486500	-0.99751700
	O	-1.98153600	-4.65237800	0.99625000
	C	-0.46437600	-6.82928900	1.00806800
	H	0.21797800	-6.30252000	1.68312800
	C	-1.54187300	-7.55711500	1.80236800
	H	-1.07220900	-8.26317200	2.49225900
	H	-2.19723800	-8.11636800	1.12446900
	H	-2.14151400	-6.85485300	2.38583900
	C	0.30063300	-7.76484500	0.07848500
	H	1.10623400	-7.24434500	-0.44457000
	H	-0.38570100	-8.18963900	-0.66042600
	H	0.73160700	-8.58813600	0.65814800
	C	1.21511400	-0.20900600	-0.02001200
	C	1.34983200	1.17115800	-0.02876500
	H	2.33278400	1.59521500	0.12526000
	C	0.20602200	1.98090400	-0.20660900
	N	0.28626300	3.33118200	-0.21732300
	C	-1.02500700	1.30834100	-0.37311800
	H	-1.95384600	1.84191200	-0.52209800
	C	-1.05238800	-0.07869000	-0.37922500
	C	1.58516000	3.97928500	-0.14553600
	C	-0.92843800	4.12623700	-0.28775200
	H	1.44845300	5.05611600	-0.22481100
	H	2.23106300	3.65175800	-0.96799300
	H	2.09047600	3.76162800	0.80295500
	H	-1.47242100	3.94049400	-1.22109000
	H	-0.66482600	5.18133500	-0.24668500
	H	-1.59339400	3.90128100	0.55393300

C	-1.42333400	-14.15918100	1.95471800
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C	-0.14386300	-13.62791900	1.83221000
H	-1.55310500	-15.23107500	2.06068000
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C	-5.50248300	-3.09139200	2.31827700
C	-6.58553600	-2.20045100	2.33422500
H	-7.20380700	-0.14781700	2.46143200
C	2.37358000	-1.02872800	0.19962700
C	3.36360000	-1.70415200	0.37342400
C	6.94084100	-2.68293200	0.74599000
C	6.83747800	-4.06596100	0.82858900
C	5.57659400	-4.68252000	0.78545100
C	4.53721800	-2.50493000	0.54930300
C	5.79963000	-1.89768400	0.61125200
H	7.91811300	-2.21249300	0.78350000
C	5.46259800	-6.10380600	0.90591700
C	5.36493800	-7.30563000	1.02475600
C	6.17755800	-10.93141800	1.37549100
C	4.90560700	-11.48582400	1.45556300
C	3.77315300	-10.65731100	1.39830500
C	5.21870600	-8.72226000	1.16918800
C	6.34233500	-9.55726900	1.23378200
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C	-5.27225100	-8.00375300	1.99090100
C	-4.19303500	-2.60212900	2.41436600
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C	3.93656200	-9.27753400	1.25099900
H	-3.53524400	-13.74088500	2.05074500
H	0.72711100	-14.27426600	1.84029200
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H	-7.08421800	-10.87567300	1.80403300

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H	-7.59354600	-2.59134100	2.24474100
H	7.72512000	-4.68009700	0.93659600
H	5.87376100	-0.81755700	0.53561200
H	4.77525000	-12.55723300	1.56440400
H	7.33374000	-9.12341500	1.15978100
H	-0.96483500	-10.33816800	1.53389300
H	-4.24622300	-7.65678800	2.00608300
H	-3.35309600	-3.28754800	2.35752200
H	3.45136800	-4.36823200	0.58276500
H	3.06765700	-8.63034200	1.19997700
C	0.78088700	2.70797900	3.07132500
C	-1.57341300	-0.15913800	2.81997600
C	-2.65461100	-0.69090800	2.68657200
C	1.99342000	2.06174900	3.28860400
C	2.04117500	0.66097200	3.36434400
C	-0.34983500	0.56833500	2.97509600
C	-0.38681700	1.97110600	2.92173400
H	0.74507900	3.79184200	3.02321700
C	0.86769700	-0.08391100	3.19764100
H	2.90783100	2.63158100	3.41738800
H	-1.33832700	2.46685800	2.75803000
H	0.90252300	-1.16741500	3.24506500
C	3.28177800	0.00430400	3.66307200
C	4.33357600	-0.52859300	3.96879700
Si	5.89223000	-1.33023900	4.56612200
C	7.36035400	-0.51178300	3.72950000
C	5.78177200	-3.16508300	4.20008700
C	6.00296600	-1.04802100	6.42042400
H	7.44917900	0.53004000	4.05103900
H	7.27332700	-0.52864200	2.64125600
H	8.28328800	-1.03150100	4.00582200
H	5.50231300	-3.34522300	3.15921200
H	5.03225600	-3.63527700	4.84355200
H	6.74433800	-3.65209000	4.38558300
H	5.15065100	-1.49487300	6.93948900
H	6.02913200	0.01917700	6.65731500
H	6.91717700	-1.50476800	6.81302700
C	0.06300500	-14.29161700	-1.50799500
C	1.26329700	-13.60041600	-1.62702300
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C	-1.16323900	-12.20843400	-1.57267000
C	-1.14798200	-13.60765600	-1.48081200
H	0.07097400	-15.37364700	-1.42883000
C	2.47751400	-11.46031600	-1.83970900
C	3.48698000	-10.79660500	-1.93278700
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C	5.40466600	-5.16688700	-2.51820500
C	6.38237900	-1.57952600	-2.74830400
C	5.14539900	-0.96467800	-2.88899200
C	3.97207900	-1.73726900	-2.91560000
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C	-2.30192900	-0.75660800	-0.58632800
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C	-7.03332300	-1.89011200	-1.04390700
C	-7.09001100	-3.27691900	-1.11087000
C	-5.90738000	-4.03268400	-1.06974100
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C	-5.80760000	-1.24037500	-0.93378200
H	-7.95019400	-1.31032900	-1.07434300
C	-5.95082500	-5.45992700	-1.16124700
C	-5.95929800	-6.66842800	-1.24474800
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H	-8.03523500	-10.76720200	-1.55572000
C	-2.39878800	-11.48671100	-1.53324400
C	-3.43934700	-10.86682100	-1.49601700
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C	4.52848600	-8.59619400	-2.17294900
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C	-4.67265500	-3.38624900	-0.94164800
C	-4.71351600	-8.77115200	-1.36185300
H	2.20813400	-14.13293700	-1.64560800
H	-2.08465200	-14.14471700	-1.37751800
H	7.81745200	-7.74053400	-2.28710900
H	6.03510900	-11.63354800	-1.88992400
H	5.07106200	0.11339500	-2.98395200
H	7.43167600	-3.44747700	-2.51166700
H	-8.04350900	-3.78604200	-1.20268400
H	-5.75635200	-0.15789600	-0.87269200
H	-5.86217300	-11.96444000	-1.60111400
H	-8.08393600	-8.28921600	-1.38941200
H	0.03731500	-10.42810000	-1.75977700
H	3.54059800	-8.14846300	-2.19877100
H	3.15119600	-3.72788900	-2.79307900
H	-3.75890500	-3.97050900	-0.87886700
H	-3.78799500	-8.20556800	-1.29608600



	C	-0.30626600	2.69726200	-3.49318900
	C	1.69996800	-0.42111800	-3.21270100
	C	2.71361300	-1.07096200	-3.07114100
	C	-1.58555300	2.19381700	-3.70432300
	C	-1.79554700	0.80735700	-3.76584400
	C	0.56938800	0.44267200	-3.37697100
	C	0.76883500	1.83196200	-3.33587900
	H	-0.14516900	3.77008500	-3.45565400
	C	-0.71575800	-0.06655700	-3.59351800
	H	-2.42734400	2.86521800	-3.83817100
	H	1.77093000	2.21755100	-3.17725600
	H	-0.87616600	-1.13907900	-3.63093300
	C	-3.10605300	0.29858100	-4.05374100
	C	-4.21631000	-0.10699500	-4.34758600
	Si	-5.86434000	-0.72484200	-4.92285100
	C	-7.21346100	0.27279600	-4.08177900
	C	-5.97133900	-2.55264800	-4.52556000
	C	-5.95661800	-0.45304000	-6.77980300
	H	-7.15308900	1.32437600	-4.37662600
	H	-7.14071900	0.21610000	-2.99364300
	H	-8.19669700	-0.10628200	-4.37807100
	H	-5.72325300	-2.74204800	-3.47812600
	H	-5.27647000	-3.12046500	-5.15118200
	H	-6.98238000	-2.92866700	-4.71132800
	H	-5.15533400	-0.98688000	-7.29791300
	H	-5.87778600	0.60916800	-7.02743900
	H	-6.91344900	-0.82074200	-7.16404100
4e	N	0.07391900	-0.80158500	-0.19197800
	C	0.05983800	-2.27463900	-0.25799300
	H	0.59389400	-2.67303000	0.60440600
	H	0.55847100	-2.59806000	-1.17345200
	H	-0.96230900	-2.64186900	-0.24082100
	O	-0.04322100	-5.09061400	-1.00365400
	S	-1.23158000	-5.68244600	-0.33983300
	O	-2.14385700	-6.37690200	-1.28214200
	O	-1.93982600	-4.71786000	0.54333400
	C	-0.57889700	-6.96912300	0.75463300
	H	0.12977600	-6.43754000	1.39946500
	C	-1.70602300	-7.56298100	1.58718500
	H	-1.30201600	-8.23737000	2.34816000
	H	-2.38427100	-8.13527800	0.94231500
	H	-2.27126600	-6.77309600	2.08774700
	C	0.13905900	-8.02911100	-0.07240800
	H	0.95057800	-7.59350900	-0.66105700
	H	-0.57940100	-8.49620500	-0.75464000
	H	0.55554700	-8.80746800	0.57716300
	C	1.26443600	-0.15324000	-0.00578400
	C	1.35284600	1.21973600	-0.00916900
	H	2.32786400	1.65864100	0.14777300

C	0.18927800	2.01244100	-0.17748700
N	0.24467700	3.35197100	-0.17738300
C	-1.03300000	1.31580400	-0.34543200
H	-1.97001900	1.83422800	-0.49050900
C	-1.06199100	-0.06239900	-0.36990700
C	1.53430600	4.02803000	-0.10576100
C	-0.98521100	4.13111400	-0.25074500
H	1.37299400	5.10158000	-0.17056800
H	2.17730600	3.72178500	-0.93719800
H	2.04372500	3.80715400	0.83838700
H	-1.51370800	3.94314900	-1.19132000
H	-0.73671300	5.18860600	-0.19732300
H	-1.64842700	3.88505100	0.58472000
C	-1.42815100	-14.17069100	1.99459500
C	-2.55549200	-13.35615900	1.97628700
C	-2.41510100	-11.96765400	1.83148300
C	-0.00411000	-12.23479900	1.72047200
C	-0.15651200	-13.62077200	1.87394000
H	-1.54195800	-15.24383400	2.10633200
C	-3.55763900	-11.10329200	1.84085000
C	-4.50906200	-10.35250400	1.87125200
C	-7.95210400	-8.89286100	1.91723500
C	-7.66394000	-7.53525300	1.99893600
C	-6.32908500	-7.10435400	2.04891100
C	-5.59109600	-9.41431900	1.91794600
C	-6.92780600	-9.83426100	1.87637200
H	-8.98535700	-9.22170200	1.87922800
C	-6.00774100	-5.71167900	2.13796500
C	-5.71584900	-4.53733300	2.20611200
C	-6.26550300	-0.86367900	2.43908900
C	-4.96420400	-0.39502900	2.55819600
C	-3.88597500	-1.29608900	2.54376700
C	-5.44017200	-3.13579500	2.30714400
C	-6.50858900	-2.22724900	2.31970400
H	-7.09530800	-0.16491700	2.44174700
C	2.42405800	-0.95322700	0.20776900
C	3.40703800	-1.63625700	0.39122000
C	6.97087900	-2.65917900	0.75062500
C	6.84512000	-4.04036000	0.83756900
C	5.57487900	-4.63917800	0.80662000
C	4.57210100	-2.44621700	0.56971500
C	5.84216300	-1.85515000	0.62218800
H	7.95610000	-2.20533800	0.77960300
C	5.43782500	-6.05775200	0.93445300
C	5.32060600	-7.25704000	1.06053000
C	6.12976100	-10.87814000	1.43823000
C	4.85837200	-11.43386600	1.51279600
C	3.72433200	-10.60834600	1.44190400
C	5.16708400	-8.67240000	1.21137400

C	6.29204000	-9.50462000	1.28938700
H	7.00248300	-11.52056700	1.48940400
C	1.30205300	-11.65700400	1.60799200
C	2.41106900	-11.17362800	1.52727900
C	-1.13736100	-11.41527500	1.69297800
C	-5.30043500	-8.04826000	2.00710300
C	-4.12290300	-2.66671500	2.40144900
C	4.43860200	-3.83679300	0.66233000
C	3.88446400	-9.22875300	1.28627800
H	-3.54683900	-13.78386000	2.08095700
H	0.72402600	-14.25399100	1.88865800
H	-8.46301500	-6.80202400	2.02851700
H	-7.15290600	-10.89281600	1.80146700
H	-4.76566500	0.66619000	2.66387600
H	-7.52242300	-2.60260700	2.22975800
H	7.72410500	-4.66769600	0.94041200
H	5.93226100	-0.77656200	0.54309000
H	4.72884600	-12.50480300	1.62731300
H	7.28282300	-9.06857700	1.22000100
H	-1.02805300	-10.34497700	1.55486700
H	-4.26958000	-7.71817400	2.03621700
H	-3.29279100	-3.36377100	2.34122300
H	3.45395500	-4.29080700	0.61436200
H	3.01345700	-8.58468000	1.22408300
C	0.81877200	2.67265400	3.10445300
C	-1.48425000	-0.23218400	2.82570700
C	-2.56035100	-0.77162200	2.68199200
C	2.04461100	2.04631900	3.30769200
C	2.11759400	0.64605800	3.37208800
C	-0.27359000	0.51369400	2.99279200
C	-0.33659200	1.91643200	2.95260300
H	0.76267900	3.75625000	3.07083100
C	0.95620100	-0.11850700	3.20713900
H	2.94916400	2.63151900	3.43683300
H	-1.29807100	2.39671300	2.80040600
H	1.01018800	-1.20149600	3.25228600
C	3.36982300	0.00756000	3.66022200
C	4.43139900	-0.51048000	3.95708000
Si	6.00096000	-1.28961100	4.55820300
C	7.45776400	-0.47248100	3.70093900
C	5.89661600	-3.13043800	4.22154400
C	6.11608100	-0.97645600	6.40699700
H	7.54069800	0.57417100	4.00818600
H	7.36543700	-0.50391300	2.61340500
H	8.38595400	-0.98165800	3.97918100
H	5.60060800	-3.32819700	3.18845400
H	5.15965800	-3.59421700	4.88404800
H	6.86442500	-3.61001600	4.39868700
H	5.26856400	-1.42124600	6.93564000

H	6.13532100	0.09457500	6.62668600
H	7.03473000	-1.42044600	6.80378800
C	0.06095400	-14.28189700	-1.46321800
C	1.27026700	-13.60604500	-1.58313100
C	1.28072100	-12.20742600	-1.69360600
C	-1.14135200	-12.18534600	-1.55109800
C	-1.14225800	-13.58397900	-1.44602700
H	0.05591100	-15.36321900	-1.37407400
C	2.50490700	-11.47467400	-1.80568600
C	3.51159800	-10.80613600	-1.89448700
C	7.08264400	-9.72666100	-2.02597800
C	6.94234100	-8.35087700	-2.16264100
C	5.66212800	-7.77738000	-2.22595200
C	4.67850800	-9.98310600	-1.99353600
C	5.96132300	-10.54568300	-1.94281200
H	8.07412100	-10.16453300	-1.97712700
C	5.50890700	-6.36073300	-2.37094700
C	5.38070900	-5.16140700	-2.48965900
C	6.34899100	-1.57341100	-2.74432000
C	5.11053400	-0.96121500	-2.88160900
C	3.93875100	-1.73656600	-2.89805700
C	5.27415000	-3.73963100	-2.62497800
C	6.43714300	-2.95528000	-2.61788600
H	7.25118900	-0.97121100	-2.73111100
C	-2.29611500	-0.74049500	-0.59343400
C	-3.35762200	-1.30584400	-0.74003100
C	-7.02350000	-1.85963700	-1.05601100
C	-7.08588700	-3.24676300	-1.11318100
C	-5.90814800	-4.00970900	-1.06735600
C	-4.61492000	-1.97302600	-0.88969500
C	-5.79447200	-1.21628300	-0.95212400
H	-7.93764400	-1.27606600	-1.09023100
C	-5.96069900	-5.43682000	-1.15376100
C	-5.96409000	-6.64533000	-1.23571800
C	-7.07585200	-10.19636300	-1.49710100
C	-5.85454700	-10.85674500	-1.51799700
C	-4.65644800	-10.12646300	-1.44909100
C	-5.93195600	-8.07305700	-1.32946300
C	-7.12220400	-8.80900000	-1.40491200
H	-7.99836100	-10.76523800	-1.54733600
C	-2.36836900	-11.44863300	-1.51586700
C	-3.40496700	-10.82171600	-1.47798400
C	0.07319000	-11.50393000	-1.67638000
C	4.53402600	-8.59779700	-2.13669300
C	4.02204500	-3.12537200	-2.76178200
C	-4.66795800	-3.37170900	-0.94126200
C	-4.69527800	-8.73234300	-1.34927000
H	2.20882300	-14.14984000	-1.59153200
H	-2.08515500	-14.10946300	-1.33967900

	H	7.81553100	-7.71017900	-2.22402200
	H	6.06804500	-11.61892400	-1.82656900
	H	5.03351300	0.11617500	-2.98171200
	H	7.40143900	-3.43878600	-2.50403700
	H	-8.04221500	-3.75122800	-1.20195900
	H	-5.73622000	-0.13364600	-0.90157600
	H	-5.81198600	-11.93848800	-1.58816800
	H	-8.07304300	-8.28727500	-1.38010000
	H	0.08196400	-10.42272400	-1.75603200
	H	3.54202600	-8.16005800	-2.17381100
	H	3.11919100	-3.72733300	-2.75867800
	H	-3.75605400	-3.95854900	-0.86256700
	H	-3.77692300	-8.15206900	-1.28773400
	C	-0.34594200	2.69749700	-3.45343400
	C	1.66776800	-0.41816800	-3.19206400
	C	2.68007000	-1.07042100	-3.05166900
	C	-1.62529700	2.19162300	-3.66054700
	C	-1.83151000	0.80497100	-3.73159800
	C	0.53633200	0.44465500	-3.35438000
	C	0.73270100	1.83448500	-3.30544700
	H	-0.18717000	3.77067700	-3.41375300
	C	-0.74818200	-0.06715300	-3.57128200
	H	-2.46947600	2.86150700	-3.78629100
	H	1.73486400	2.22211600	-3.15188200
	H	-0.90510500	-1.13987600	-3.62048300
	C	-3.14071100	0.29414900	-4.02019900
	C	-4.24980200	-0.11077900	-4.31866200
	Si	-5.89123800	-0.72709000	-4.91653600
	C	-7.24918100	0.26985300	-4.08927100
	C	-5.99745200	-2.55722300	-4.53107400
	C	-5.95937100	-0.44531400	-6.77285500
	H	-7.18717300	1.32023900	-4.38801700
	H	-7.18655700	0.21846800	-3.00041700
	H	-8.22923300	-0.11137000	-4.39311000
	H	-5.74260100	-2.75487100	-3.48701400
	H	-5.30529600	-3.11939100	-5.16473600
	H	-7.00904500	-2.93287900	-4.71409500
	H	-5.15299100	-0.97820200	-7.28387300
	H	-5.87584400	0.61796800	-7.01418600
	H	-6.91224900	-0.80952400	-7.17009500
3f	N	-0.03814500	-0.90102400	-0.22789800
	C	-0.23998300	-3.86275100	-0.46101000
	H	0.27388700	-3.61731400	0.47085300
	H	0.32782000	-3.46207000	-1.29896100
	H	-1.25132700	-3.45375300	-0.46041600
	O	-0.27167200	-5.29915600	-0.66593000
	S	-1.23255800	-6.17757900	0.27421100
	O	-1.23167700	-7.50333300	-0.32527900
	O	-2.50287100	-5.47900800	0.44297000

C	-0.35405900	-6.23028400	1.84521400
H	-0.24144400	-5.17615000	2.13207200
C	-1.23325100	-6.96441900	2.87387300
H	-0.55697300	-7.38128300	3.62750400
H	-1.70586500	-7.82996800	2.38887600
C	-2.27337300	-6.08043500	3.55799600
H	-1.78275300	-5.26922500	4.10462600
H	-2.85855700	-6.66509400	4.27310600
H	-2.96304900	-5.63658800	2.83555100
C	1.02423500	-6.87544400	1.64072300
H	1.45534600	-6.54217300	0.68995500
H	0.88897800	-7.96138200	1.57061400
C	1.98204900	-6.51782500	2.77715100
H	2.15705800	-5.43738100	2.80866500
H	2.94968500	-7.00652800	2.63022700
H	1.59277400	-6.82804100	3.75131000
C	1.12893500	-0.25754400	-0.06593700
C	1.28770100	1.12401000	-0.11287000
H	2.27544400	1.54261400	0.02849600
C	0.15686700	1.94063700	-0.31881700
N	0.24923200	3.29645100	-0.35913800
C	-1.07487300	1.27504000	-0.48117700
H	-1.99667100	1.81255600	-0.66000400
C	-1.10615800	-0.11569300	-0.43876400
C	1.55304000	3.93145500	-0.31959400
C	-0.95698700	4.09621600	-0.46273200
H	1.42620200	5.00937700	-0.40669600
H	2.18414900	3.59038700	-1.14905800
H	2.07616000	3.71942200	0.62069400
H	-1.48929400	3.90448100	-1.40247500
H	-0.68887300	5.15088500	-0.42821100
H	-1.64052000	3.88578800	0.36845800
C	-1.46436100	-14.18106200	1.52649500
C	-2.50198900	-13.26363400	1.63846200
C	-2.22544800	-11.88686600	1.64018000
C	0.13893600	-12.37579600	1.40754200
C	-0.14674400	-13.74800200	1.41486200
H	-1.68352900	-15.24362100	1.52365000
C	-3.28481600	-10.93310300	1.76656900
C	-4.18523800	-10.12982400	1.87850100
C	-7.63610100	-8.80520200	2.34394900
C	-7.40584300	-7.43492200	2.35223000
C	-6.10145300	-6.94004900	2.19503900
C	-5.27244200	-9.21088400	2.02625300
C	-6.57867800	-9.69464900	2.18862900
H	-8.64580100	-9.18408800	2.46095000
C	-5.86487600	-5.52863500	2.22116300
C	-5.69290600	-4.32964000	2.25485400
C	-6.49098200	-0.69213700	2.30633600

C	-5.22487300	-0.13376500	2.43224800
C	-4.09306000	-0.96241000	2.49728300
C	-5.52324600	-2.90943900	2.30812600
C	-6.64698600	-2.07221900	2.24760400
H	-7.36231300	-0.04791000	2.25352000
C	2.28562900	-1.08174500	0.17041900
C	3.26259100	-1.76744600	0.37738600
C	6.81705300	-2.75845600	0.90692600
C	6.71883900	-4.14403000	0.91163000
C	5.46657500	-4.76124900	0.75928100
C	4.42591700	-2.57778800	0.57671500
C	5.68009300	-1.97222200	0.74613700
H	7.78731000	-2.28716900	1.02653400
C	5.36780700	-6.18829200	0.79897500
C	5.31629900	-7.39797300	0.85320100
C	6.30809600	-10.99193800	1.04978200
C	5.06558500	-11.61121700	1.12552800
C	3.89556400	-10.83719700	1.11142700
C	5.24050600	-8.82500000	0.93809300
C	6.40435900	-9.60721100	0.96022400
H	7.21045000	-11.59404200	1.05822700
C	1.48255200	-11.89632100	1.29626800
C	2.60105100	-11.43922900	1.20662400
C	-0.90513100	-11.44928900	1.51602700
C	-5.03899100	-7.83096100	2.01815800
C	-4.24528400	-2.35063300	2.42523500
C	4.32360900	-3.97431500	0.58314600
C	3.98972800	-9.44606700	1.00783300
H	-3.52955500	-13.59975100	1.72700700
H	0.66433300	-14.46239700	1.32318500
H	-8.22536600	-6.73638700	2.48235400
H	-6.75240000	-10.76533000	2.18374200
H	-5.09780800	0.94229500	2.48407700
H	-7.63241800	-2.51395900	2.14602400
H	7.60197300	-4.76043000	1.04133600
H	5.75074500	-0.88922100	0.73433600
H	4.98975900	-12.69069600	1.20047400
H	7.37295100	-9.12322500	0.89565100
H	-0.68846400	-10.38623700	1.49492300
H	-4.03569600	-7.44788800	1.85851500
H	-3.37230800	-2.99554900	2.44893600
H	3.35566400	-4.44562000	0.44451100
H	3.08598400	-8.84647500	0.97260500
C	0.85242700	2.83995700	2.94825500
C	-1.70516900	0.13874100	2.76614000
C	-2.79282100	-0.37955700	2.63566300
C	2.00712500	2.11133900	3.21467900
C	1.94310500	0.71573900	3.34880800
C	-0.44170600	0.79508800	2.91534300

C	-0.36815400	2.19211800	2.80528000
H	0.90312000	3.92041300	2.85733700
C	0.71739200	0.06021700	3.18807200
H	2.96071900	2.61383600	3.33861000
H	-1.27344700	2.75499400	2.60153500
H	0.66473000	-1.01950800	3.27984200
C	3.11860200	-0.02851100	3.70125500
C	4.10859500	-0.64543500	4.05269900
Si	5.56705500	-1.57749000	4.71074200
C	7.13391800	-0.82069800	4.00601700
C	5.36495800	-3.38423200	4.25384600
C	5.57024600	-1.38517200	6.57998500
H	7.27519500	0.19085600	4.39766600
H	7.10445600	-0.76475800	2.91590000
H	8.00352700	-1.41994700	4.29394900
H	5.19590500	-3.50819100	3.18144900
H	4.51391100	-3.81723200	4.78817900
H	6.26135900	-3.95000900	4.52691900
H	4.65289100	-1.78640600	7.01943900
H	5.65865900	-0.33428100	6.86914300
H	6.41826000	-1.92774600	7.01016900
C	0.00267500	-14.18913100	-1.98815700
C	1.17952300	-13.45531000	-2.07187200
C	1.13831000	-12.05271500	-2.02219000
C	-1.27471000	-12.14422100	-1.79491700
C	-1.22244700	-13.54408400	-1.85374900
H	0.03949300	-15.27280000	-2.02568000
C	2.34653100	-11.29032600	-2.11646200
C	3.36835900	-10.64451900	-2.20096000
C	6.97847000	-9.72444500	-2.41315900
C	6.90188000	-8.33814300	-2.47489400
C	5.65046000	-7.70255300	-2.45496300
C	4.56709900	-9.86758700	-2.29836400
C	5.82184200	-10.49235100	-2.32582600
H	7.94795600	-10.21144800	-2.42699000
C	5.55983400	-6.27500600	-2.51925900
C	5.47700000	-5.06701500	-2.56908500
C	6.47815500	-1.47679900	-2.54816000
C	5.25300600	-0.85021000	-2.73654000
C	4.08327100	-1.61539700	-2.87650800
C	5.39549300	-3.63846900	-2.62523800
C	6.55727100	-2.86421300	-2.49418400
H	7.37833200	-0.88081700	-2.43995000
C	-2.36410700	-0.78900000	-0.62878400
C	-3.43187800	-1.34198100	-0.77686500
C	-7.10120400	-1.88757000	-1.16481100
C	-7.17123800	-3.27583800	-1.17467100
C	-5.99762100	-4.03833900	-1.06486500
C	-4.69608300	-1.99736200	-0.92623400



C	-5.87312600	-1.24385700	-1.04473800
H	-8.01111600	-1.30161400	-1.24756400
C	-6.04604100	-5.46864700	-1.09345300
C	-6.06235500	-6.67951400	-1.13335000
C	-7.23597200	-10.22202400	-1.15512400
C	-6.03340000	-10.90385800	-1.29629800
C	-4.82715000	-10.19072000	-1.38328800
C	-6.05745200	-8.11025300	-1.18470500
C	-7.25661000	-8.83197900	-1.10239100
H	-8.16545200	-10.77734200	-1.08411100
C	-2.52864400	-11.46844000	-1.65122800
C	-3.58329600	-10.88428000	-1.52976900
C	-0.09027900	-11.40178200	-1.87666300
C	4.48666200	-8.47156100	-2.36212700
C	4.15815500	-3.00958600	-2.81337400
C	-4.76186100	-3.39555800	-0.93165900
C	-4.84272700	-8.79411000	-1.31796900
H	2.13638800	-13.95488400	-2.17915900
H	-2.14275800	-14.11402600	-1.78410800
H	7.80280900	-7.73754800	-2.54025100
H	5.87944800	-11.57400000	-2.26751500
H	5.18657900	0.23161800	-2.78186700
H	7.51078500	-3.35823400	-2.34152600
H	-8.12694500	-3.77944200	-1.27336200
H	-5.81406900	-0.16019800	-1.02684700
H	-6.01454500	-11.98757500	-1.34107500
H	-8.19364100	-8.29728900	-0.98887800
H	-0.12768900	-10.31873600	-1.81896300
H	3.51781400	-7.98418000	-2.33166100
H	3.25682100	-3.60622000	-2.90773300
H	-3.85813300	-3.98630700	-0.81576200
H	-3.90994200	-8.24007800	-1.35832200
C	-0.27498100	2.73175000	-3.63686000
C	1.80891400	-0.32406800	-3.25787800
C	2.83246500	-0.94876000	-3.08143000
C	-1.53607000	2.18964800	-3.86149000
C	-1.70777100	0.79716600	-3.89876100
C	0.65858900	0.50460200	-3.46040100
C	0.81954400	1.89912800	-3.44416900
H	-0.14368000	3.80908000	-3.61635500
C	-0.60835700	-0.04360800	-3.68855300
H	-2.39324600	2.83503100	-4.02361700
H	1.80829900	2.31406000	-3.27608300
H	-0.73968500	-1.12042600	-3.70425300
C	-3.00128100	0.24956200	-4.19503300
C	-4.09686000	-0.19152300	-4.49402400
Si	-5.72398600	-0.86253100	-5.06931400
C	-7.10424700	0.16575200	-4.32074000
C	-5.83361400	-2.66496300	-4.56706700

	C	-5.77437900	-0.70452900	-6.94168700
	H	-7.04213800	1.20298800	-4.66253500
	H	-7.06703100	0.15995200	-3.22903200
	H	-8.07466700	-0.23546900	-4.63025600
	H	-5.62954900	-2.79090100	-3.50015000
	H	-5.11131100	-3.26436100	-5.12978000
	H	-6.83484100	-3.05727900	-4.77209500
	H	-4.95876500	-1.26384700	-7.40850400
	H	-5.69546300	0.34128300	-7.25249500
	H	-6.72025000	-1.10135000	-7.32435500
	N	0.00324400	-0.85838000	-0.22879200
	C	0.02952700	-2.89104000	-0.36617200
	H	0.48190400	-2.91397600	0.61383700
	H	0.66623500	-2.77639000	-1.23146300
	H	-1.04525700	-2.88821600	-0.46627100
	O	0.14791300	-4.74822400	-0.57351600
	S	-0.87445100	-5.61513000	0.16532700
	O	-1.01723000	-6.91464100	-0.50588800
	O	-2.12622200	-4.86362900	0.38127200
	C	-0.12556900	-5.91941100	1.77768500
	H	0.04808700	-4.91421900	2.18638100
	C	-1.08721700	-6.70180100	2.68368700
	H	-0.48037600	-7.16463500	3.46977000
	H	-1.50771300	-7.53132700	2.09963800
	C	-2.19599700	-5.87424500	3.32937000
	H	-1.77003000	-5.04934400	3.91043900
	H	-2.78859400	-6.49286000	4.00982800
	H	-2.86546700	-5.45178700	2.57765200
	C	1.21382000	-6.64754700	1.59399100
	H	1.70899100	-6.29643700	0.68208300
	H	1.00300000	-7.71451900	1.45037400
	C	2.14388900	-6.43474100	2.78726600
	H	2.42360600	-5.37923500	2.87273900
	H	3.06497700	-7.01255000	2.67136600
	H	1.67330300	-6.73552700	3.72794400
	C	1.16927600	-0.21058600	-0.04288600
	C	1.29212300	1.16947600	-0.07485500
	H	2.26956400	1.60481300	0.08257100
	C	0.14204900	1.96546000	-0.27820900
	N	0.20955800	3.31642400	-0.30875100
	C	-1.07993700	1.27872300	-0.44903200
	H	-2.01098100	1.80097500	-0.62228400
	C	-1.09518200	-0.10915400	-0.43482500
	C	1.50358500	3.97676500	-0.26650100
	C	-1.01093600	4.09884300	-0.41339600
	H	1.35580300	5.05152900	-0.35325300
	H	2.13919000	3.64669200	-1.09612900
	H	2.02614500	3.77329400	0.67524700
	H	-1.53087100	3.90667000	-1.35922400

H	-0.75920500	5.15663000	-0.36610200
H	-1.69430800	3.86819800	0.41144600
C	-1.46821800	-14.25152100	1.61918000
C	-2.52637200	-13.35469000	1.70448700
C	-2.27936300	-11.97275000	1.68300400
C	0.09732600	-12.41469000	1.47781900
C	-0.15949500	-13.79231700	1.50873100
H	-1.66449600	-15.31838700	1.63547400
C	-3.35661900	-11.03553200	1.78205800
C	-4.25864000	-10.23093000	1.86741800
C	-7.69512600	-8.82271700	2.19503000
C	-7.43061200	-7.45902900	2.21447200
C	-6.10824500	-6.99741800	2.11486300
C	-5.33138300	-9.28953700	1.97724500
C	-6.65531300	-9.73928200	2.08143100
H	-8.71855100	-9.17531800	2.26767600
C	-5.84328400	-5.59116700	2.14654700
C	-5.65623600	-4.39463600	2.18724900
C	-6.45082100	-0.75832000	2.29334700
C	-5.18424900	-0.20183200	2.42216100
C	-4.05252000	-1.03190900	2.46627600
C	-5.48192600	-2.97541700	2.25358800
C	-6.60616600	-2.13744900	2.21428200
H	-7.32284300	-0.11405700	2.25634700
C	2.32626100	-1.02427900	0.20414400
C	3.29398900	-1.72732700	0.39281600
C	6.83048900	-2.78703500	0.89320500
C	6.70213900	-4.17006200	0.89475600
C	5.43666200	-4.76360800	0.75229700
C	4.44327400	-2.55868500	0.58458400
C	5.70891900	-1.97670500	0.74515700
H	7.81137000	-2.33687400	1.00599600
C	5.31657600	-6.18899700	0.79703000
C	5.26227000	-7.39794200	0.86463600
C	6.24908300	-10.98952900	1.10534600
C	5.00641800	-11.60661900	1.19179900
C	3.83640900	-10.83236600	1.16987500
C	5.18210000	-8.82380000	0.96716300
C	6.34563500	-9.60621800	0.99650700
H	7.15119300	-11.59194900	1.11942900
C	1.43239600	-11.91146500	1.36459500
C	2.54428600	-11.43893200	1.27191600
C	-0.96672700	-11.50904300	1.56315600
C	-5.06199700	-7.91522200	1.98717000
C	-4.20280900	-2.41875100	2.36846300
C	4.30856200	-3.95289800	0.58705900
C	3.93040300	-9.44261900	1.04833700
H	-3.54702100	-13.71157000	1.79153100
H	0.66736300	-14.49065600	1.43649200

H	-8.23732300	-6.73996700	2.30847200
H	-6.85706300	-10.80493600	2.06316600
H	-5.05694100	0.87306200	2.49386300
H	-7.59220400	-2.57827200	2.11420400
H	7.57336000	-4.80499600	1.01526700
H	5.80063900	-0.89533400	0.73644200
H	4.92987100	-12.68501800	1.28033300
H	7.31430900	-9.12368200	0.92282400
H	-0.77085200	-10.44228300	1.53110600
H	-4.04138000	-7.55984600	1.88322700
H	-3.32895600	-3.06307100	2.36644800
H	3.32792600	-4.39973600	0.45083000
H	3.02733200	-8.84207000	1.00992900
C	0.87363200	2.77919800	3.00177200
C	-1.66671000	0.06687600	2.76062800
C	-2.75254000	-0.45179500	2.61701300
C	2.03285400	2.05234900	3.25370100
C	1.97738100	0.65396400	3.36045000
C	-0.40756400	0.72709300	2.92626600
C	-0.34296100	2.12678300	2.84516700
H	0.91727400	3.86168700	2.93514500
C	0.75589200	-0.00615600	3.18559900
H	2.98312300	2.55808500	3.38875800
H	-1.25219700	2.68782500	2.65415400
H	0.70954700	-1.08791300	3.25818300
C	3.15613800	-0.08870100	3.70460500
C	4.14834800	-0.70428700	4.05174800
Si	5.60557200	-1.63523100	4.71515700
C	7.17563600	-0.87648300	4.02005000
C	5.40250200	-3.44075300	4.25412400
C	5.59772100	-1.44458600	6.58438200
H	7.31426600	0.13405200	4.41525400
H	7.15311700	-0.81749700	2.92997100
H	8.04361900	-1.47620600	4.31183100
H	5.22031200	-3.56069800	3.18339000
H	4.55774500	-3.87633100	4.79646000
H	6.30224300	-4.00720900	4.51417000
H	4.67721600	-1.84552800	7.01750400
H	5.68521100	-0.39400600	6.87499200
H	6.44252200	-1.98837200	7.01932900
C	-0.01208500	-14.30356900	-1.87367800
C	1.16623900	-13.57321200	-1.96902500
C	1.12579000	-12.17000500	-1.95558700
C	-1.28927600	-12.25405100	-1.74228300
C	-1.23775700	-13.65488200	-1.76328700
H	0.02410300	-15.38784200	-1.88231500
C	2.33239400	-11.40631900	-2.05933600
C	3.34728900	-10.75044000	-2.14949300
C	6.94563600	-9.78465700	-2.36650400

C	6.85045100	-8.40038400	-2.44288700
C	5.59046100	-7.78154600	-2.43177700
C	4.53587500	-9.95883700	-2.25344700
C	5.79909600	-10.56671300	-2.27242700
H	7.92158500	-10.25867400	-2.37371800
C	5.48196000	-6.35599600	-2.50877700
C	5.38641500	-5.14940500	-2.56635700
C	6.36245000	-1.55264900	-2.58386100
C	5.13072000	-0.93570900	-2.75861300
C	3.96444400	-1.71040500	-2.87448600
C	5.29302600	-3.72232200	-2.63156900
C	6.45103600	-2.93920000	-2.52182800
H	7.26015700	-0.95017700	-2.49291200
C	-2.33528900	-0.80017400	-0.65015500
C	-3.39746600	-1.36034700	-0.81048300
C	-7.06177700	-1.93261900	-1.18327000
C	-7.11849600	-3.32127900	-1.20640800
C	-5.93767800	-4.07595400	-1.11852500
C	-4.65596300	-2.02561900	-0.96988700
C	-5.83836200	-1.27866600	-1.07181700
H	-7.97834500	-1.35513500	-1.24856400
C	-5.98199300	-5.50656400	-1.16233100
C	-6.00446300	-6.71721200	-1.20895300
C	-7.23897000	-10.23736700	-1.27256800
C	-6.04576200	-10.94218800	-1.37299300
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C	-6.01991200	-8.14807000	-1.26392300
C	-7.23437400	-8.84732200	-1.22087700
H	-8.18057500	-10.77475800	-1.23115000
C	-2.54179600	-11.56986100	-1.62854900
C	-3.59001500	-10.96953500	-1.53344600
C	-0.10354400	-11.51533800	-1.83583000
C	4.43673600	-8.56481400	-2.33327700
C	4.04803100	-3.10342000	-2.80321000
C	-4.70555500	-3.42485900	-0.98835500
C	-4.81530300	-8.85538000	-1.36095400
H	2.12310300	-14.07654000	-2.05726700
H	-2.15863100	-14.22260800	-1.68354200
H	7.74328100	-7.78825200	-2.51242100
H	5.87112500	-11.64679500	-2.20213000
H	5.05546900	0.14522600	-2.80991600
H	7.40993900	-3.42598700	-2.38018000
H	-8.07114600	-3.83192200	-1.29904100
H	-5.78816600	-0.19475700	-1.04439400
H	-6.04606100	-12.02611100	-1.41526400
H	-8.16401000	-8.29452000	-1.13788600
H	-0.13983600	-10.43118900	-1.81048300
H	3.46139800	-8.09020700	-2.30906300
H	3.14920200	-3.70683900	-2.87746500

	H	-3.79173600	-4.00076700	-0.87287700
	H	-3.87229100	-8.31835100	-1.37731800
	C	-0.35954000	2.66741000	-3.58210900
	C	1.68848900	-0.41528000	-3.22851100
	C	2.70837900	-1.04907500	-3.06244400
	C	-1.62886200	2.14124300	-3.79851500
	C	-1.81757100	0.75101600	-3.84086000
	C	0.54798700	0.42870400	-3.42118700
	C	0.72656000	1.82116500	-3.39967500
	H	-0.21486800	3.74304100	-3.56112200
	C	-0.72664200	-0.10369000	-3.64399800
	H	-2.47914400	2.79756800	-3.95230300
	H	1.72142300	2.22363300	-3.23704000
	H	-0.87019500	-1.17905100	-3.66609900
	C	-3.11707700	0.21878100	-4.13638200
	C	-4.21760600	-0.20617000	-4.43956800
	Si	-5.84621500	-0.84964900	-5.04112200
	C	-7.22451600	0.15042700	-4.25224100
	C	-5.94599600	-2.67229900	-4.61841400
	C	-5.89785200	-0.60935100	-6.90419500
	H	-7.16637700	1.19660500	-4.56628400
	H	-7.17932500	0.11587700	-3.16180600
	H	-8.19635800	-0.24386300	-4.56614000
	H	-5.70708300	-2.84634200	-3.56627000
	H	-5.24112100	-3.24336400	-5.22971100
	H	-6.95254800	-3.05753400	-4.80953300
	H	-5.08342300	-1.14806400	-7.39610300
	H	-5.81844300	0.44889100	-7.16816200
	H	-6.84468800	-0.98791900	-7.30257400
4f	N	0.00812100	-0.82940800	-0.21582800
	C	-0.01560800	-2.30526200	-0.22882900
	H	0.49005600	-2.67662200	0.66289800
	H	0.51062800	-2.66651500	-1.11434600
	H	-1.04182100	-2.66493400	-0.23433500
	O	0.07258800	-5.15368600	-0.64439900
	S	-0.97654500	-5.80384200	0.18054300
	O	-1.34032200	-7.16292500	-0.30092900
	O	-2.16003300	-4.92077300	0.38575800
	C	-0.22018100	-6.03679200	1.81186100
	H	-0.00675600	-5.01255300	2.15018500
	C	-1.18038600	-6.72669900	2.78906900
	H	-0.58109600	-7.12546800	3.61656600
	H	-1.61019900	-7.59815100	2.27662500
	C	-2.28461500	-5.83723600	3.35682700
	H	-1.85406000	-4.97857500	3.88490500
	H	-2.90190400	-6.39368400	4.06983900
	H	-2.92846800	-5.45689900	2.56130400
	C	1.09854900	-6.81016300	1.66935900
	H	1.59231700	-6.52066500	0.73499100

H	0.86440900	-7.88061000	1.58997200
C	2.04753300	-6.55432100	2.84011700
H	2.34257000	-5.49942800	2.87199200
H	2.96108700	-7.14841900	2.74392700
H	1.58634500	-6.80202400	3.80127500
C	1.20369400	-0.18616700	-0.03803300
C	1.30373700	1.18497800	-0.08198000
H	2.28162200	1.61994100	0.06827500
C	0.14791400	1.98316300	-0.27850000
N	0.21403100	3.32222600	-0.30807000
C	-1.07829300	1.29295900	-0.44206800
H	-2.00860500	1.81502000	-0.61467900
C	-1.11866700	-0.08496900	-0.42908600
C	1.50916500	3.98974000	-0.26082600
C	-1.00890700	4.10943400	-0.40794600
H	1.35492100	5.06321600	-0.34166700
H	2.14224800	3.66523300	-1.09287200
H	2.02593500	3.78101100	0.68166300
H	-1.52605000	3.91642500	-1.35377200
H	-0.75338800	5.16547600	-0.36002400
H	-1.68600200	3.87643700	0.41980300
C	-1.46227600	-14.23480400	1.61465400
C	-2.51951600	-13.33632200	1.69385600
C	-2.27093300	-11.95487300	1.66416300
C	0.10511300	-12.40022000	1.46569500
C	-0.15289400	-13.77738200	1.50475900
H	-1.65966300	-15.30136900	1.63648400
C	-3.34612000	-11.01541900	1.76058600
C	-4.24633000	-10.20903900	1.84666900
C	-7.68643800	-8.81998000	2.20236900
C	-7.42983800	-7.45484000	2.22143300
C	-6.11143800	-6.98556500	2.10765600
C	-5.32130100	-9.27110900	1.96128300
C	-6.64144400	-9.72913000	2.07882900
H	-8.70674500	-9.17940000	2.28496500
C	-5.85352400	-5.57856500	2.14140500
C	-5.66282300	-4.38285200	2.18073500
C	-6.40808800	-0.73456900	2.26954300
C	-5.13369700	-0.19652500	2.39894700
C	-4.01482400	-1.04390200	2.44841400
C	-5.47197100	-2.96604200	2.24099500
C	-6.58356600	-2.11187100	2.19669500
H	-7.27038800	-0.07759500	2.22806000
C	2.35062200	-0.99408100	0.20675600
C	3.31594500	-1.70145300	0.39132200
C	6.84659800	-2.77440800	0.86927200
C	6.70928600	-4.15657800	0.87313600
C	5.43990700	-4.74556100	0.74285300
C	4.46048600	-2.53719500	0.58022300

C	5.72854200	-1.95795900	0.73025000
H	7.83107900	-2.33030000	0.97290700
C	5.31506400	-6.16997800	0.79199100
C	5.26017100	-7.37838600	0.86526000
C	6.25714000	-10.96538200	1.12019300
C	5.01604200	-11.58653600	1.19996400
C	3.84355500	-10.81652300	1.16749900
C	5.18283200	-8.80416700	0.96945500
C	6.34921800	-9.58195800	1.00937100
H	7.16131700	-11.56446400	1.14198100
C	1.44085200	-11.89863800	1.35601500
C	2.55276400	-11.42580000	1.26610200
C	-0.95817900	-11.49289700	1.54127700
C	-5.05946900	-7.89523200	1.96527200
C	-4.18416100	-2.42855800	2.35352100
C	4.31442700	-3.93041000	0.58532700
C	3.93263500	-9.42696500	1.04106300
H	-3.54062400	-13.69153200	1.78243900
H	0.67365500	-14.47675400	1.43916800
H	-8.23950800	-6.74053600	2.32588000
H	-6.83597100	-10.79620500	2.06388900
H	-4.99029800	0.87656900	2.46731200
H	-7.57589900	-2.53868300	2.09756700
H	7.57822800	-4.79594500	0.98650700
H	5.82460500	-0.87709500	0.71958800
H	4.94266300	-12.66488600	1.29171200
H	7.31655500	-9.09573900	0.94222200
H	-0.76331200	-10.42638300	1.49630600
H	-4.04293200	-7.53205200	1.84047000
H	-3.32064200	-3.08709000	2.35074500
H	3.33055500	-4.37225500	0.45760000
H	3.02704200	-8.83081800	0.99095200
C	0.91675700	2.74557500	2.99987900
C	-1.61934200	0.03119300	2.75006700
C	-2.70786900	-0.48040600	2.60096400
C	2.07928100	2.01941400	3.23974700
C	2.02656300	0.62061500	3.34302400
C	-0.36107900	0.69114900	2.92165400
C	-0.29980700	2.09172100	2.84673900
H	0.95736300	3.82875800	2.94257100
C	0.80469700	-0.04117400	3.17495500
H	3.02940700	2.52627300	3.37092300
H	-1.21198700	2.65195400	2.66717000
H	0.75998400	-1.12289000	3.25072800
C	3.20787400	-0.12066600	3.68006500
C	4.20194900	-0.73408400	4.02509700
Si	5.65946700	-1.66148100	4.69502100
C	7.22941900	-0.90484800	3.99780600
C	5.45222200	-3.46807500	4.24182500



C	5.64794600	-1.45981900	6.56265600
H	7.36767400	0.10653500	4.39092400
H	7.20786900	-0.84786500	2.90772000
H	8.09732400	-1.50373000	4.29138600
H	5.26393800	-3.59118200	3.17272500
H	4.60896600	-3.90006200	4.78927100
H	6.35203700	-4.03550300	4.49918900
H	4.72661100	-1.85816800	6.99623500
H	5.73529200	-0.40763400	6.84729100
H	6.49185100	-2.00134800	7.00201100
C	0.01211500	-14.27652600	-1.88627600
C	1.18748200	-13.54125500	-1.97969500
C	1.14155800	-12.13820900	-1.96360300
C	-1.27301900	-12.23221300	-1.75271000
C	-1.21616700	-13.63271400	-1.77619000
H	0.05268800	-15.36064200	-1.89621900
C	2.34587600	-11.37058000	-2.06430200
C	3.35937400	-10.71225200	-2.15184500
C	6.95702500	-9.74028500	-2.35076900
C	6.85975300	-8.35646500	-2.43254300
C	5.59846000	-7.74023800	-2.43163600
C	4.54675400	-9.91859300	-2.25285400
C	5.81126900	-10.52406500	-2.26138800
H	7.93387900	-10.21250900	-2.34993600
C	5.48750800	-6.31509500	-2.51223500
C	5.38876700	-5.10890700	-2.57193100
C	6.35564100	-1.50904800	-2.59852100
C	5.12148700	-0.89530200	-2.76744700
C	3.95741500	-1.67408600	-2.87822200
C	5.29147200	-3.68229900	-2.63972400
C	6.44774000	-2.89546600	-2.53639400
H	7.25235600	-0.90446600	-2.51243200
C	-2.35021500	-0.76622000	-0.64718300
C	-3.40873900	-1.32969100	-0.81767300
C	-7.06372600	-1.92067100	-1.21041600
C	-7.10855300	-3.31002600	-1.22316000
C	-5.92429800	-4.05804900	-1.12018600
C	-4.66217200	-1.99898700	-0.98087900
C	-5.84594300	-1.25694800	-1.09870200
H	-7.98452200	-1.35156800	-1.28659000
C	-5.96339500	-5.48850400	-1.16245400
C	-5.98356500	-6.69910100	-1.20637300
C	-7.22475100	-10.21548300	-1.29063500
C	-6.03247300	-10.92195100	-1.39119700
C	-4.80936200	-10.23441900	-1.43117500
C	-6.00062800	-8.12960000	-1.26532900
C	-7.21711100	-8.82580500	-1.23171100
H	-8.16764800	-10.75111100	-1.25626500
C	-2.52759400	-11.55240500	-1.63750200

	C	-3.57611100	-10.95292100	-1.54130300
	C	-0.09019000	-11.48827200	-1.84296800
	C	4.44540300	-8.52506300	-2.33805200
	C	4.04406100	-3.06688900	-2.80616200
	C	-4.69734100	-3.39934100	-0.98187000
	C	-4.79636000	-8.83778600	-1.35812600
	H	2.14644800	-14.04060200	-2.06790200
	H	-2.13493300	-14.20407200	-1.69800200
	H	7.75181700	-7.74279100	-2.49821200
	H	5.88484900	-11.60374200	-2.18653700
	H	5.04283800	0.18533100	-2.81944500
	H	7.40871900	-3.37955400	-2.39941300
	H	-8.05696600	-3.82779700	-1.31996900
	H	-5.80141300	-0.17264000	-1.08296200
	H	-6.03486800	-12.00559700	-1.44094700
	H	-8.14582400	-8.27108700	-1.15100000
	H	-0.13119400	-10.40435600	-1.81188200
	H	3.46916300	-8.05198300	-2.32091100
	H	3.14620000	-3.67215200	-2.87575300
	H	-3.78013200	-3.96760000	-0.84321200
	H	-3.85126800	-8.30343600	-1.35707800
	C	-0.40386700	2.67240800	-3.57693600
	C	1.67444100	-0.39058300	-3.22856700
	C	2.69871800	-1.01754100	-3.06412000
	C	-1.66942700	2.13387000	-3.78683900
	C	-1.84452600	0.74178000	-3.83095500
	C	0.52590600	0.44249800	-3.41966600
	C	0.69163000	1.83682400	-3.39925200
	H	-0.26880700	3.74945700	-3.56110200
	C	-0.74442400	-0.10262400	-3.63913300
	H	-2.52646100	2.78196400	-3.93775800
	H	1.68424400	2.24859200	-3.24600700
	H	-0.87660900	-1.17942800	-3.66728000
	C	-3.13823600	0.19785700	-4.12943000
	C	-4.23360800	-0.23433100	-4.44050800
	Si	-5.85084500	-0.88857400	-5.06379700
	C	-7.24478600	0.10837600	-4.29887300
	C	-5.94329200	-2.71073700	-4.63842000
	C	-5.87515500	-0.65198100	-6.92768300
	H	-7.18733200	1.15276800	-4.61878800
	H	-7.21545800	0.08147600	-3.20779100
	H	-8.21006500	-0.29260300	-4.62426500
	H	-5.70984000	-2.88266300	-3.58481400
	H	-5.23048500	-3.27796200	-5.24405100
	H	-6.94605600	-3.10253500	-4.83591000
	H	-5.05113600	-1.18803000	-7.40639500
	H	-5.79691800	0.40609900	-7.19250700
	H	-6.81440000	-1.03578500	-7.33891200
3g	N	0.03231200	-0.96693200	-0.28875700

C	-0.22658700	-3.95149300	-0.23141300
H	0.32999100	-3.65210100	0.66076300
H	0.32209000	-3.64214300	-1.11838400
H	-1.22379700	-3.50639300	-0.23295600
O	-0.30937500	-5.39848600	-0.31321600
S	-1.34295200	-6.15006000	0.65564700
O	-1.32076500	-7.53886700	0.22047300
O	-2.61311300	-5.43013500	0.64278800
C	-0.58218600	-6.02006600	2.28270200
H	-0.52873500	-4.93978800	2.47329000
C	-1.51069000	-6.68982800	3.30953500
H	-0.88957300	-6.95566600	4.17273700
H	-1.87050500	-7.64439200	2.89758100
C	-2.68183700	-5.82941300	3.78431100
H	-2.28602700	-4.89660900	4.20702200
C	-3.52645500	-6.55354700	4.82841200
H	-3.30954800	-5.54586700	2.93353500
H	-3.90692400	-7.50059700	4.43022400
H	-4.38719200	-5.94728900	5.12440200
H	-2.94080400	-6.77781800	5.72595500
C	0.82534600	-6.62858600	2.24568600
H	1.32203500	-6.37907800	1.30085200
H	0.73517600	-7.72139700	2.28295500
C	1.69358100	-6.12740600	3.40191900
H	1.80521200	-5.03880800	3.31699400
C	3.06885100	-6.78887400	3.39918800
H	1.19493200	-6.31761500	4.35919200
H	2.97802100	-7.87803500	3.47132400
H	3.67589400	-6.44632700	4.24132200
H	3.61393400	-6.55833100	2.47737900
C	1.19779700	-0.32495300	-0.11081900
C	1.35283600	1.05806900	-0.12277100
H	2.33946800	1.47569100	0.02920800
C	0.21982000	1.87722600	-0.30438300
N	0.30953100	3.23392200	-0.30691700
C	-1.01059000	1.21293500	-0.48117200
H	-1.93477400	1.75266100	-0.64076800
C	-1.03783400	-0.17861000	-0.47792100
C	1.61212400	3.86997300	-0.24613700
C	-0.89920200	4.03391000	-0.37215300
H	1.48408200	4.94919800	-0.31322600
H	2.24791700	3.54571100	-1.07858200
H	2.13059200	3.64042600	0.69290100
H	-1.44045100	3.87005600	-1.31185300
H	-0.63279900	5.08763600	-0.30733400
H	-1.57338000	3.79567700	0.45933500
C	-1.29541700	-14.03086500	1.71417500
C	-2.34583100	-13.12374100	1.77359400
C	-2.09286300	-11.74641500	1.66802400

C	0.27418900	-12.21253900	1.43553600
C	0.01178300	-13.58471100	1.54922400
H	-1.49593100	-15.09408000	1.79427300
C	-3.17380200	-10.81184900	1.74428500
C	-4.10569400	-10.04092900	1.81991700
C	-7.61866300	-8.87800100	2.24866100
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C	-6.17635400	-6.94298900	2.07626200
C	-5.23673300	-9.17197200	1.93823100
C	-6.51896400	-9.71673100	2.10657600
H	-8.60891100	-9.30393400	2.37158600
C	-5.99210500	-5.52452000	2.09884800
C	-5.82069800	-4.32579500	2.13767300
C	-6.50619400	-0.66367800	2.21816900
C	-5.22181800	-0.15000500	2.35015600
C	-4.11804600	-1.01651500	2.40857900
C	-5.61343900	-2.91140700	2.19755100
C	-6.70875100	-2.03729900	2.14792200
H	-7.35493300	0.01040400	2.17164000
C	2.35934000	-1.14695200	0.11135000
C	3.35832500	-1.81292500	0.27337700
C	6.95341800	-2.68466100	0.73029000
C	6.90875000	-4.07301400	0.70068400
C	5.67956800	-4.73267900	0.54579800
C	4.55209500	-2.58756800	0.43299300
C	5.78524000	-1.93953600	0.60339400
H	7.90600600	-2.17895400	0.85092700
C	5.62420800	-6.16212200	0.56156100
C	5.57087300	-7.37152000	0.61410500
C	6.44362400	-10.99984000	0.76306900
C	5.18490100	-11.57054500	0.91335000
C	4.04593900	-10.75222900	0.96582700
C	5.45468000	-8.79470500	0.70638100
C	6.58699900	-9.61969800	0.66261500
H	7.32151800	-11.63585700	0.72240900
C	1.61330200	-11.73699000	1.26838700
C	2.73815000	-11.30871300	1.13032900
C	-0.78246900	-11.29523700	1.49121100
C	-5.07152600	-7.78320100	1.90438100
C	-4.31656000	-2.39782300	2.31926100
C	4.50373000	-3.98647700	0.40422300
C	4.18613000	-9.36622600	0.85396100
H	-3.36629400	-13.46769000	1.90439600
H	0.83469600	-14.28954200	1.49734300
H	-8.30759000	-6.83855600	2.36682000
H	-6.63989700	-10.79462600	2.11963900
H	-5.05883300	0.92058900	2.41396200
H	-7.70850000	-2.44553900	2.04573100
H	7.81644400	-4.65766600	0.80500500

H	5.81506100	-0.85479600	0.62213600
H	5.07203200	-12.64632800	0.99479000
H	7.56779300	-9.17278300	0.54117600
H	-0.58674300	-10.23256700	1.38716600
H	-4.08823500	-7.35190900	1.73665800
H	-3.46835900	-3.07590700	2.33336300
H	3.55302000	-4.49289200	0.26815200
H	3.30689700	-8.73048500	0.87768300
C	0.87116200	2.69357700	2.97336600
C	-1.70414300	0.01760000	2.71184700
C	-2.80134500	-0.47557400	2.56369100
C	2.02139100	1.95126600	3.22027800
C	1.94956000	0.55284500	3.31358800
C	-0.43421400	0.65707300	2.88029400
C	-0.35240000	2.05640800	2.81111400
H	0.92752700	3.77587600	2.91270800
C	0.72058500	-0.09176900	3.13213800
H	2.97763500	2.44458000	3.35954600
H	-1.25468600	2.62951100	2.62288900
H	0.66238400	-1.17357200	3.19271600
C	3.12083000	-0.20544000	3.64976900
C	4.10847700	-0.83275900	3.98913400
Si	5.55001300	-1.79017900	4.64766600
C	7.13757900	-0.99810900	4.03768900
C	5.37139200	-3.56945600	4.08581700
C	5.48265100	-1.70122600	6.52321800
H	7.24476100	0.01056600	4.44670400
H	7.16179000	-0.93194000	2.94780800
H	7.99982100	-1.58912700	4.36243700
H	5.28069800	-3.63678600	2.99859400
H	4.47708300	-4.01483500	4.53267800
H	6.23848300	-4.16140500	4.39556000
H	4.55137600	-2.12872500	6.90487000
H	5.55487100	-0.66822400	6.87444100
H	6.31637500	-2.26502600	6.95396600
C	0.09293200	-14.26565200	-1.80712000
C	1.25446900	-13.52015900	-1.96738800
C	1.18817000	-12.11873300	-2.02088900
C	-1.21971800	-12.23516200	-1.74489200
C	-1.14190300	-13.63402600	-1.69806000
H	0.14951400	-15.34817400	-1.76216900
C	2.37981100	-11.34211400	-2.18663300
C	3.38405500	-10.67844800	-2.32612400
C	6.96349400	-9.71194800	-2.74641400
C	6.86633400	-8.32683100	-2.79932800
C	5.61054300	-7.70606500	-2.70272000
C	4.56461200	-9.88461900	-2.48982700
C	5.82332200	-10.49389800	-2.59296600
H	7.93627800	-10.18667400	-2.82019800

C	5.50606800	-6.27865700	-2.75197500
C	5.42765400	-5.06984900	-2.78678900
C	6.47348400	-1.49436700	-2.69850100
C	5.25525400	-0.84745000	-2.86144000
C	4.07456300	-1.59425600	-3.00619000
C	5.36184800	-3.63948900	-2.81603700
C	6.53474800	-2.88343800	-2.67633700
H	7.38239400	-0.91319000	-2.58289400
C	-2.29423500	-0.84885200	-0.68887200
C	-3.36426600	-1.39294700	-0.85297400
C	-7.02902600	-1.95766900	-1.26096000
C	-7.08913000	-3.34606900	-1.28887200
C	-5.91009400	-4.10175900	-1.18732200
C	-4.62406400	-2.05248200	-1.02126100
C	-5.80585700	-1.30597500	-1.13157500
H	-7.94355200	-1.37784100	-1.33570000
C	-5.95215000	-5.53241400	-1.22301400
C	-5.97485000	-6.74349300	-1.25701400
C	-7.19140100	-10.27098200	-1.24745100
C	-5.99524900	-10.97086600	-1.35207000
C	-4.77870200	-10.27496100	-1.42774400
C	-5.98563100	-8.17492700	-1.29067100
C	-7.19527200	-8.88032600	-1.21932700
H	-8.12913600	-10.81310500	-1.18558800
C	-2.48222100	-11.56858500	-1.63277900
C	-3.53900500	-10.98285900	-1.53907400
C	-0.05044200	-11.48107800	-1.90347000
C	4.46366000	-8.48928100	-2.54483700
C	4.13155500	-2.99055800	-2.97734400
C	-4.67996400	-3.45107100	-1.04487900
C	-4.77852900	-8.87702300	-1.38905500
H	2.21863200	-14.00994500	-2.05268500
H	-2.04962500	-14.21313600	-1.56608700
H	7.75435000	-7.71481100	-2.91609500
H	5.89708700	-11.57486200	-2.54076500
H	5.20260200	0.23585600	-2.88029800
H	7.48277700	-3.39290000	-2.54136700
H	-8.04140500	-3.85498100	-1.39332200
H	-5.75496700	-0.22229300	-1.09772500
H	-5.99024400	-12.05526300	-1.37746000
H	-8.12730200	-8.33195400	-1.13442100
H	-0.10718300	-10.39789000	-1.92867800
H	3.49220400	-8.01486500	-2.45555700
H	3.22135600	-3.57257600	-3.07671000
H	-3.77231800	-4.03498900	-0.92853500
H	-3.83863300	-8.33574200	-1.42027500
C	-0.29789400	2.77821600	-3.60929600
C	1.80725400	-0.27454200	-3.32547500
C	2.82903700	-0.90931500	-3.17831200

	C	-1.55787400	2.23337400	-3.83379400
	C	-1.72079100	0.84110000	-3.90310900
	C	0.65209100	0.55436100	-3.49573800
	C	0.80422800	1.94889900	-3.44743800
	H	-0.17353300	3.85562600	-3.56538900
	C	-0.61355800	0.00349500	-3.72466100
	H	-2.42072800	2.87683700	-3.97128000
	H	1.79171400	2.36714500	-3.28039800
	H	-0.73766400	-1.07350800	-3.76556600
	C	-3.01213100	0.29042700	-4.20296000
	C	-4.10636100	-0.15136100	-4.50577700
	Si	-5.72999600	-0.81633000	-5.09729500
	C	-7.11674800	0.17325300	-4.30941500
	C	-5.81670700	-2.63823900	-4.66660100
	C	-5.79225400	-0.58805200	-6.96176100
	H	-7.07135000	1.21844100	-4.62869000
	H	-7.06852800	0.14438100	-3.21895200
	H	-8.08489500	-0.23370200	-4.61865500
	H	-5.58883600	-2.80755700	-3.61111300
	H	-5.10213900	-3.20669500	-5.26911800
	H	-6.81879700	-3.03055300	-4.86713100
	H	-4.97563300	-1.12290500	-7.45421400
	H	-5.72319800	0.46913900	-7.23288900
	H	-6.73766700	-0.97725500	-7.35330100
TS-g	N	0.01953700	-0.96478800	-0.26338700
	C	-0.03202900	-3.00433700	-0.20458300
	H	0.46528700	-2.94620200	0.75220200
	H	0.56583900	-3.00885900	-1.10340400
	H	-1.11023000	-2.96816300	-0.26075000
	O	0.01177100	-4.87952000	-0.21502100
	S	-1.05238600	-5.63323800	0.58564300
	O	-1.16950200	-7.01610200	0.09992700
	O	-2.30825500	-4.85854300	0.62188900
	C	-0.39856200	-5.70681000	2.26719100
	H	-0.31989000	-4.65243600	2.56792100
	C	-1.36899000	-6.45097900	3.19383900
	H	-0.80579300	-6.72343600	4.09514100
	H	-1.64641800	-7.39978300	2.71293700
	C	-2.62299500	-5.68564900	3.61471400
	H	-2.32673900	-4.71056000	4.02460000
	C	-3.43050600	-6.45589600	4.65615400
	H	-3.24522200	-5.47609700	2.73989100
	H	-3.69660500	-7.45181900	4.28540300
	H	-4.35972200	-5.93298700	4.89932000
	H	-2.86011000	-6.58702400	5.58150300
	C	0.99268200	-6.35303900	2.25131000
	H	1.53315100	-6.05108800	1.34747700
	H	0.87051100	-7.44300600	2.20263100
	C	1.82903000	-5.97275900	3.47425300

H	1.99613800	-4.88753400	3.46642800
C	3.17006500	-6.70085100	3.49206100
H	1.27669800	-6.19636300	4.39429300
H	3.02390300	-7.78644400	3.49104100
H	3.75474100	-6.44192100	4.37883800
H	3.76647500	-6.44409700	2.61001900
C	1.19534100	-0.33247700	-0.08607200
C	1.33401900	1.04700100	-0.10771000
H	2.31894100	1.46861500	0.04015500
C	0.19269800	1.85944400	-0.29003000
N	0.27477700	3.20994400	-0.29487400
C	-1.03698000	1.18864900	-0.46731600
H	-1.96215900	1.72319500	-0.63490200
C	-1.06932400	-0.19885200	-0.46344400
C	1.57538100	3.85575900	-0.23545700
C	-0.93871200	4.00663900	-0.36649900
H	1.43884900	4.93355500	-0.30048900
H	2.20940200	3.53653600	-1.07036100
H	2.09409400	3.62726200	0.70286800
H	-1.47232600	3.83891600	-1.30914200
H	-0.67547500	5.06065600	-0.30123500
H	-1.61348500	3.76553500	0.46265100
C	-1.31479400	-14.08090000	1.70790700
C	-2.37985000	-13.19067700	1.76632600
C	-2.14837700	-11.80935200	1.66645100
C	0.22701900	-12.23724100	1.43915500
C	-0.01439700	-13.61380400	1.54832400
H	-1.49879200	-15.14732600	1.78472400
C	-3.24163100	-10.88893200	1.74154900
C	-4.17385800	-10.11835600	1.81466800
C	-7.68065500	-8.91785000	2.19147600
C	-7.50210100	-7.53950500	2.18808600
C	-6.21473000	-6.99838100	2.04764500
C	-5.29715500	-9.23792800	1.92146800
C	-6.58800500	-9.76825400	2.06639600
H	-8.67741100	-9.33313000	2.29608300
C	-6.01678300	-5.58178500	2.07160500
C	-5.83429400	-4.38461400	2.11091400
C	-6.47822700	-0.71564400	2.23804000
C	-5.18745600	-0.21862900	2.36929800
C	-4.09353900	-1.09904000	2.40310400
C	-5.61075700	-2.97276900	2.17905600
C	-6.69644500	-2.08611900	2.15069700
H	-7.31986300	-0.03185400	2.20767700
C	2.35494200	-1.14982900	0.13758500
C	3.35217300	-1.81679900	0.30357900
C	6.94290500	-2.70249100	0.75820900
C	6.89043500	-4.09033000	0.71872400
C	5.65833600	-4.74470800	0.56251800



C	4.54393400	-2.59330700	0.46733500
C	5.77846200	-1.94988400	0.64046400
H	7.89874000	-2.20317800	0.87876500
C	5.59719300	-6.17378800	0.57250500
C	5.53757600	-7.38276700	0.62575500
C	6.38891800	-11.01500400	0.77983100
C	5.12699100	-11.57798000	0.93072500
C	3.99203100	-10.75351000	0.98139200
C	5.41198000	-8.80500700	0.71962500
C	6.53974400	-9.63589400	0.67626100
H	7.26322400	-11.65604600	0.74035600
C	1.56016800	-11.74321000	1.27698400
C	2.68278400	-11.30813500	1.14195100
C	-0.84405900	-11.33733100	1.49549800
C	-5.11582200	-7.85056400	1.89728000
C	-4.30581700	-2.47648700	2.29066200
C	4.48620900	-3.99161200	0.42772100
C	4.13964000	-9.36828400	0.86912400
H	-3.39497200	-13.55145100	1.89297100
H	0.81969700	-14.30538700	1.49753900
H	-8.34961200	-6.87128300	2.29716700
H	-6.72138900	-10.84471000	2.07335800
H	-5.01200600	0.84880000	2.45083600
H	-7.70178500	-2.48170700	2.05292800
H	7.79582700	-4.67967800	0.81633600
H	5.81332000	-0.86549800	0.66615200
H	5.00781100	-12.65303400	1.01314000
H	7.52280700	-9.19435300	0.55354600
H	-0.66322000	-10.27138900	1.39870000
H	-4.12264200	-7.43269900	1.75373100
H	-3.46455200	-3.16325200	2.26889300
H	3.53223900	-4.48959900	0.28375100
H	3.26524000	-8.72585000	0.89438200
C	0.89144700	2.59762500	2.99010700
C	-1.67073200	-0.08837500	2.71453300
C	-2.77045200	-0.57425600	2.56042600
C	2.04598300	1.85993000	3.23103800
C	1.98097700	0.46081900	3.32078400
C	-0.40354800	0.55437500	2.88927900
C	-0.32891000	1.95467200	2.82562400
H	0.94154400	3.68060000	2.93674600
C	0.75477200	-0.18957100	3.14065200
H	2.99999700	2.35726200	3.37091700
H	-1.23478500	2.52357300	2.64184500
H	0.70122500	-1.27162600	3.20667500
C	3.15592700	-0.29170100	3.65587900
C	4.14642200	-0.91271300	3.99810100
Si	5.58972300	-1.85979100	4.66850800
C	7.17657200	-1.06388900	4.06199300

C	5.41188600	-3.64139800	4.11551600
C	5.51354500	-1.75896300	6.54294300
H	7.27866600	-0.05452700	4.47070000
H	7.20494400	-0.99808000	2.97232500
H	8.03963500	-1.65153900	4.39059900
H	5.30740200	-3.71284900	3.02981900
H	4.52254400	-4.08533300	4.57353300
H	6.28218200	-4.23251400	4.41753600
H	4.58126200	-2.18563300	6.92300900
H	5.58236500	-0.72351200	6.88765200
H	6.34628300	-2.31839600	6.98120600
C	0.06671400	-14.29969000	-1.80433900
C	1.23524500	-13.56409100	-1.96028700
C	1.18045800	-12.16242800	-2.01812700
C	-1.22972100	-12.25849000	-1.75545700
C	-1.16352200	-13.65791100	-1.70376900
H	0.11431400	-15.38251600	-1.75611800
C	2.37811000	-11.39430500	-2.17964400
C	3.38597100	-10.73547700	-2.31593200
C	6.96589600	-9.76469400	-2.72898500
C	6.86681800	-8.37961000	-2.78139100
C	5.60997500	-7.76104100	-2.68601700
C	4.56679000	-9.94114200	-2.47507100
C	5.82663600	-10.54829400	-2.57723300
H	7.93934700	-10.23805500	-2.80253200
C	5.50070000	-6.33413200	-2.73594000
C	5.41152900	-5.12610900	-2.76805300
C	6.40705500	-1.53556300	-2.68080500
C	5.17910200	-0.90660000	-2.83997300
C	4.00942200	-1.67143000	-2.98139400
C	5.32680500	-3.69705400	-2.79695100
C	6.48855500	-2.92370900	-2.65982200
H	7.30764300	-0.94123300	-2.56699500
C	-2.31866100	-0.86934200	-0.68758300
C	-3.39031700	-1.40770800	-0.85852200
C	-7.05444600	-1.96992500	-1.26307000
C	-7.11153300	-3.35851900	-1.29310300
C	-5.93191100	-4.11415600	-1.19672300
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C	-5.83200400	-1.31591100	-1.13829800
H	-7.97050200	-1.39220600	-1.33352400
C	-5.97433800	-5.54496400	-1.23948600
C	-5.99229100	-6.75590000	-1.28101500
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H	-8.13205400	-10.83370900	-1.23574700

C	-2.48749000	-11.58180900	-1.65123100
C	-3.54124100	-10.98975500	-1.56398400
C	-0.05365800	-11.51451100	-1.90996500
C	4.46396400	-8.54599200	-2.52970400
C	4.08615700	-3.06651300	-2.95353500
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C	-4.78713200	-8.88509900	-1.41800500
H	2.19576800	-14.06202300	-2.03928400
H	-2.07652800	-14.22924500	-1.57453400
H	7.75406700	-7.76629800	-2.89730600
H	5.90200900	-11.62923000	-2.52642900
H	5.10980300	0.17577300	-2.85758500
H	7.44441100	-3.41915600	-2.52792500
H	-8.06371200	-3.86804900	-1.39577200
H	-5.78210500	-0.23216400	-1.10553000
H	-5.98774900	-12.06746700	-1.41903800
H	-8.13916300	-8.35260000	-1.17623200
H	-0.10112400	-10.43108300	-1.94044500
H	3.49184700	-8.07279500	-2.44115000
H	3.18450500	-3.66211400	-3.05080000
H	-3.78922600	-4.03710400	-0.92530600
H	-3.84947200	-8.33956500	-1.44368000
C	-0.35597400	2.69082500	-3.58114000
C	1.72883200	-0.37410800	-3.29560100
C	2.75474300	-1.00268300	-3.14987200
C	-1.62023800	2.15434500	-3.80226200
C	-1.79294600	0.76306700	-3.87024600
C	0.57793000	0.46023200	-3.46554900
C	0.74052100	1.85390600	-3.41964600
H	-0.22344100	3.76744100	-3.54114800
C	-0.69154700	-0.08245000	-3.69279900
H	-2.47861700	2.80360100	-3.94017100
H	1.73167900	2.26497700	-3.25619800
H	-0.82303800	-1.15870400	-3.73475400
C	-3.08701700	0.22191200	-4.17359900
C	-4.18320800	-0.20915400	-4.48390800
Si	-5.80549000	-0.85652700	-5.09847200
C	-7.19253800	0.13608400	-4.31543200
C	-5.90260500	-2.68150600	-4.68498100
C	-5.84550900	-0.60826900	-6.96082400
H	-7.13584700	1.18333900	-4.62596000
H	-7.15508000	0.09855700	-3.22486700
H	-8.16071800	-0.26058000	-4.63739000
H	-5.67053700	-2.86053700	-3.63213800
H	-5.19215400	-3.24748100	-5.29460400
H	-6.90683600	-3.06830400	-4.88497300
H	-5.02726100	-1.14363200	-7.45003800
H	-5.76598100	0.45125400	-7.21954100
H	-6.78931200	-0.98639200	-7.36674000

4g	N	0.03913900	-0.88358100	-0.26700600
	C	-0.00838200	-2.35860600	-0.27588100
	H	0.57196600	-2.73750300	0.56390900
	H	0.42638300	-2.73076400	-1.20532500
	H	-1.03661600	-2.69848100	-0.18031500
	O	-0.01651600	-5.26096600	-0.33104700
	S	-1.12650200	-5.74194100	0.53035900
	O	-1.55270300	-7.12864600	0.21676900
	O	-2.26016600	-4.77566100	0.56750900
	C	-0.45007500	-5.78873300	2.21727500
	H	-0.30887000	-4.72696400	2.46514500
	C	-1.43417200	-6.43362600	3.19876500
	H	-0.88821000	-6.63892800	4.12891300
	H	-1.72794800	-7.41172100	2.79186000
	C	-2.67813500	-5.61368300	3.53651100
	H	-2.36830000	-4.61314900	3.86986600
	C	-3.52341100	-6.27570100	4.62140300
	H	-3.27692100	-5.46201000	2.63405800
	H	-3.80827100	-7.29201800	4.32692700
	H	-4.44370600	-5.71255000	4.80331300
	H	-2.97295900	-6.34589300	5.56583700
	C	0.91078500	-6.49592000	2.22461800
	H	1.45791300	-6.23550800	1.31235600
	H	0.74790000	-7.58249700	2.20280200
	C	1.76672400	-6.12520400	3.43761500
	H	1.95327600	-5.04298600	3.42229700
	C	3.09660800	-6.87426200	3.45165900
	H	1.22082600	-6.33262100	4.36524500
	H	2.93405800	-7.95769800	3.45205100
	H	3.68921600	-6.62438700	4.33621700
	H	3.69459000	-6.62664200	2.56752100
	C	1.24037000	-0.25347200	-0.08887100
	C	1.34885200	1.11838800	-0.10203300
	H	2.33146400	1.54343000	0.04394000
	C	0.19633600	1.92836900	-0.26502400
	N	0.26965000	3.26728800	-0.24963600
	C	-1.03417000	1.25029400	-0.44602400
	H	-1.96125100	1.78199000	-0.60542100
	C	-1.08249600	-0.12704500	-0.46521900
	C	1.56827700	3.92599800	-0.17482900
	C	-0.94949000	4.06371300	-0.31929000
	H	1.41895400	5.00266800	-0.20836300
	H	2.19910100	3.63534700	-1.02098500
	H	2.08526600	3.67359800	0.75691800
	H	-1.47000900	3.90400700	-1.26928600
	H	-0.68816200	5.11632600	-0.23792900
	H	-1.62529800	3.80736500	0.50269600
	C	-1.26553200	-14.03920900	1.85114400
	C	-2.34743300	-13.16789000	1.88768100

C	-2.14318500	-11.78622700	1.74474900
C	0.23916100	-12.17453600	1.52066800
C	0.02481600	-13.55179200	1.67334200
H	-1.42864100	-15.10621100	1.96112700
C	-3.25213500	-10.88295000	1.79990900
C	-4.19165300	-10.12001400	1.85844300
C	-7.70489500	-8.91797200	2.18476300
C	-7.52564900	-7.53953500	2.16554600
C	-6.23658900	-7.00083500	2.03041500
C	-5.31881600	-9.24182600	1.94413300
C	-6.61128800	-9.77031900	2.08235500
H	-8.70293400	-9.33145900	2.28461100
C	-6.03641700	-5.58440200	2.03627600
C	-5.84536700	-4.38831900	2.06861600
C	-6.43844200	-0.70874500	2.21726600
C	-5.14007500	-0.23248500	2.34908000
C	-4.06035400	-1.13079500	2.37124000
C	-5.60603400	-2.97904600	2.13897600
C	-6.67828200	-2.07559600	2.12259000
H	-7.26965100	-0.01198500	2.19420100
C	2.39371500	-1.06465700	0.11886800
C	3.38969100	-1.73539300	0.27653100
C	6.97739200	-2.64015000	0.68688000
C	6.91402200	-4.02756300	0.64225100
C	5.67623600	-4.67542800	0.50428600
C	4.57763200	-2.51778000	0.42987500
C	5.81671400	-1.87915000	0.59035300
H	7.93830100	-2.14806800	0.79499300
C	5.60701900	-6.10353800	0.52804300
C	5.54100900	-7.31126900	0.59861200
C	6.38833600	-10.94043600	0.81526900
C	5.12623200	-11.49911300	0.97959100
C	3.99152000	-10.67326500	1.01352000
C	5.41229900	-8.73180100	0.71208200
C	6.53974200	-9.56365300	0.68483000
H	7.26228800	-11.58255900	0.78851200
C	1.56458300	-11.66490700	1.34232100
C	2.68357800	-11.22522800	1.19229400
C	-0.84879300	-11.29396300	1.55211300
C	-5.13601300	-7.85509900	1.90274300
C	-4.29267600	-2.50341900	2.24337600
C	4.50700200	-3.91524800	0.38694100
C	4.13906700	-9.29114700	0.86956200
H	-3.35475700	-13.54431200	2.03075200
H	0.87237100	-14.22798500	1.64161000
H	-8.37425800	-6.86994600	2.25695000
H	-6.74532600	-10.84661400	2.10302000
H	-4.94803900	0.83133700	2.44053000
H	-7.69037600	-2.45470200	2.02832500

H	7.81705600	-4.62282400	0.72448000
H	5.85830400	-0.79532300	0.62183600
H	5.00643800	-12.57200500	1.08628400
H	7.52306000	-9.12459200	0.55541400
H	-0.69160700	-10.22831400	1.41661000
H	-4.14056900	-7.44376800	1.75374700
H	-3.46260200	-3.20299100	2.19998400
H	3.54756900	-4.40661200	0.25825200
H	3.26424300	-8.64889400	0.88040100
C	0.96545700	2.49348000	3.04696800
C	-1.62497400	-0.15801800	2.70375800
C	-2.72963500	-0.62868700	2.53777300
C	2.11372000	1.73701600	3.25988800
C	2.03418400	0.33676100	3.31288200
C	-0.35136100	0.46725200	2.89378600
C	-0.26299300	1.86832200	2.87016000
H	1.02580700	3.57710600	3.03006800
C	0.80008800	-0.29578700	3.12086100
H	3.07315200	2.22054100	3.41008100
H	-1.16458200	2.45173500	2.71224800
H	0.73440400	-1.37860800	3.16277200
C	3.19983900	-0.43575100	3.63421700
C	4.18075800	-1.07133600	3.97715200
Si	5.59995400	-2.04338900	4.66627900
C	7.20654300	-1.24156700	4.12391100
C	5.43293100	-3.80957800	4.06402100
C	5.46435200	-1.98628600	6.53887600
H	7.30045600	-0.24097600	4.55554200
H	7.26698600	-1.15425700	3.03665000
H	8.05734600	-1.83938900	4.46574500
H	5.37221900	-3.85191400	2.97393400
H	4.52375800	-4.26042600	4.47380500
H	6.28811700	-4.41277300	4.38472900
H	4.51977900	-2.41975800	6.87884400
H	5.52416600	-0.95953300	6.91010700
H	6.28179800	-2.55817700	6.98967400
C	0.14076600	-14.30368900	-1.66179000
C	1.30308300	-13.56386000	-1.84357300
C	1.23659000	-12.16526700	-1.94603400
C	-1.17191200	-12.27281400	-1.67482900
C	-1.09483900	-13.66915900	-1.57937100
H	0.19754400	-15.38410400	-1.57883100
C	2.42586000	-11.38960200	-2.13178300
C	3.42397400	-10.72011300	-2.28627200
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C	6.87401100	-8.32917000	-2.80052700
C	5.60997500	-7.72427400	-2.71158800
C	4.59340000	-9.91337400	-2.46638800
C	5.86027200	-10.50676200	-2.56306100

H	7.96870800	-10.17474800	-2.79788600
C	5.48537000	-6.29901000	-2.77595400
C	5.38479500	-5.09203000	-2.81460900
C	6.36277400	-1.49595900	-2.74781400
C	5.12988000	-0.87292200	-2.89061300
C	3.96275000	-1.64444300	-3.01633700
C	5.29107900	-3.66362600	-2.84886400
C	6.45055000	-2.88377400	-2.72743100
H	7.26205500	-0.89754700	-2.64616200
C	-2.31838900	-0.79440700	-0.70277800
C	-3.38307700	-1.34084100	-0.88932600
C	-7.03261000	-1.97743700	-1.28872200
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C	-5.89503800	-6.74048700	-1.28385600
C	-7.13554000	-10.25767400	-1.33450100
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C	-4.71813000	-10.28013400	-1.43504500
C	-5.91073400	-8.17199600	-1.32363900
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H	-8.07917500	-10.79246900	-1.30682500
C	-2.43191800	-11.59841000	-1.58662100
C	-3.48285400	-10.99973200	-1.51408100
C	-0.00243300	-11.52446900	-1.85549600
C	4.47346600	-8.52044200	-2.54208900
C	4.04525000	-3.03925600	-2.98898500
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H	7.75357800	-7.70674700	-2.92619800
H	5.94873300	-11.58585500	-2.49605700
H	5.05449200	0.20903300	-2.90742300
H	7.41044400	-3.37445100	-2.60737100
H	-7.99738800	-3.89846200	-1.40876700
H	-5.79811200	-0.21023100	-1.14566800
H	-5.94491300	-12.05052900	-1.44077900
H	-8.05785300	-8.31093500	-1.24242000
H	-0.05912800	-10.44294400	-1.91864800
H	3.49605900	-8.05751500	-2.45697800
H	3.14467900	-3.63853300	-3.07240600
H	-3.71993800	-3.97204300	-0.92980100
H	-3.76060800	-8.34889200	-1.36050200
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	C	2.70357800	-0.98073700	-3.16932800
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	C	0.52067500	0.47779000	-3.46081600
	C	0.67747600	1.87217200	-3.40817100
	H	-0.29654700	3.78140600	-3.51881300
	C	-0.74734100	-0.07002300	-3.68465800
	H	-2.54989600	2.80848600	-3.90725800
	H	1.66830000	2.28709600	-3.25254900
	H	-0.87269600	-1.14665600	-3.73694400
	C	-3.14321300	0.22279700	-4.16134000
	C	-4.23500900	-0.21243700	-4.48065700
	Si	-5.84773800	-0.86451200	-5.11759200
	C	-7.24940400	0.10981800	-4.33764100
	C	-5.92867200	-2.69516200	-4.72617800
	C	-5.87234200	-0.59393100	-6.97692800
	H	-7.19925900	1.15946000	-4.64127100
	H	-7.22112100	0.06617500	-3.24715100
	H	-8.21125400	-0.29318300	-4.67048800
	H	-5.69075300	-2.88614400	-3.67674400
	H	-5.21460300	-3.24631900	-5.34508500
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	H	-5.04608900	-1.11734700	-7.46550000
	H	-5.79897900	0.46921900	-7.22220300
	H	-6.80991200	-0.97429600	-7.39508000
3h	N	0.03836800	-0.98037200	-0.26053000
	C	-0.60632400	-3.91842000	-0.10901400
	H	0.15365000	-3.77119500	0.66271200
	H	-0.23938500	-3.53471000	-1.05709900
	H	-1.53572200	-3.41082400	0.15825500
	O	-0.83471100	-5.33582900	-0.31778200
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	O	-1.89112400	-7.45785000	0.18531700
	O	-3.03274700	-5.32401900	0.85648000
	C	-0.90044500	-6.09565300	2.26004300
	H	-0.86042400	-5.03465300	2.54295600
	C	-1.70659400	-6.89579400	3.29547100
	H	-1.00255200	-7.18101900	4.08625700
	H	-2.03354700	-7.83816200	2.83156300
	C	-2.89224700	-6.16511600	3.92288600
	H	-2.52807400	-5.26413600	4.43562600
	C	-3.64023000	-7.05228300	4.91606900
	H	-3.58708000	-5.82084800	3.14787300
	H	-3.95517900	-7.97156300	4.40422000
	C	-4.85975100	-6.35369400	5.50902900
	H	-2.95660400	-7.36206900	5.71689700
	C	0.51215600	-6.65114900	2.04895500
	H	0.89683400	-6.36236200	1.06449300
	H	0.46498000	-7.74750500	2.06460900



C	1.48566200	-6.14710200	3.11577700
H	1.60614000	-5.06012100	3.00415200
C	2.84502100	-6.82785200	2.98687500
H	1.08018900	-6.31608200	4.12157700
H	2.72996200	-7.90066500	3.19119700
C	3.91009600	-6.22777400	3.89684500
H	3.18533800	-6.74415200	1.94763700
C	1.21048900	-0.35724800	-0.06128100
C	1.38442300	1.02396500	-0.05470100
H	2.37433900	1.42711500	0.11490200
C	0.26453000	1.85995600	-0.23774300
N	0.37213100	3.21521400	-0.22617300
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H	-1.88877000	1.76991700	-0.59368100
C	-1.02010400	-0.17563500	-0.45176600
C	1.67968700	3.83397900	-0.11693500
C	-0.82694800	4.03085600	-0.27052800
H	1.56943800	4.91431300	-0.19889200
H	2.34149000	3.49445800	-0.92246600
H	2.15882800	3.60465200	0.84334500
H	-1.37647000	3.88358800	-1.20825600
H	-0.54646100	5.08048100	-0.19812900
H	-1.49712800	3.79270800	0.56455600
C	-1.37861700	-14.05505200	1.69176000
C	-2.44563600	-13.16747300	1.75042400
C	-2.21668300	-11.78454000	1.66602500
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C	-0.07796500	-13.58379000	1.54897000
H	-1.56110800	-15.12256200	1.75604400
C	-3.31834500	-10.87268100	1.74149200
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C	-5.05827500	-0.30378900	2.34775000
C	-4.01292100	-1.24145500	2.41094300
C	-5.62573800	-3.02960000	2.15457400
C	-6.66120900	-2.08637900	2.10223400
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C	2.35920700	-1.19675700	0.16735800
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C	6.95649400	-2.72634900	0.72958100
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C	5.68014600	-4.78147300	0.68726500
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C	5.78451500	-1.98701700	0.60188700
H	7.91241400	-2.21567500	0.79029700
C	5.62146700	-6.21150700	0.71949100
C	5.55508400	-7.42109500	0.76327700
C	6.36259400	-11.06114400	1.00588600
C	5.08960400	-11.61267700	1.10142300
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C	5.41145200	-8.84292700	0.85898800
C	6.53175700	-9.68486900	0.89194800
H	7.23230500	-11.70933200	1.02264400
C	1.50213900	-11.71806900	1.31684700
C	2.63742000	-11.31057300	1.19880700
C	-0.91147100	-11.30857200	1.51000200
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C	-4.29777700	-2.60523700	2.30111500
C	4.49880000	-4.04006500	0.56169700
C	4.12879700	-9.39795700	0.93641600
H	-3.46099100	-13.53134300	1.86538300
H	0.75801500	-14.27321800	1.49985600
H	-8.49197500	-6.92849000	2.26332300
H	-6.81668900	-10.88518800	2.07666600
H	-4.82576400	0.75319900	2.42428600
H	-7.68401100	-2.42747700	1.98199000
H	7.82579600	-4.69380500	0.85901000
H	5.81330400	-0.90320000	0.55105000
H	4.95819000	-12.68479300	1.20189400
H	7.52460500	-9.25397000	0.81926000
H	-0.73454000	-10.24133900	1.42285100
H	-4.26360900	-7.44428200	1.71016300
H	-3.50011800	-3.34233200	2.31772200
H	3.54428800	-4.55184700	0.48236300
H	3.25679700	-8.75491800	0.89029100
C	0.71923500	2.63508000	3.05065300
C	-1.58264700	-0.26359200	2.75949100
C	-2.67434200	-0.76122900	2.58365600
C	1.94342200	2.01133300	3.26596700
C	2.02112800	0.61097200	3.32811500
C	-0.36548300	0.47155200	2.93337400
C	-0.43087100	1.87421000	2.89062700
H	0.66156200	3.71843300	3.00756100
C	0.86394100	-0.15826100	3.15527200
H	2.84652900	2.59813700	3.39968400
H	-1.39202700	2.35020300	2.72467300
H	0.92256900	-1.24148000	3.18815400
C	3.28610000	-0.00952600	3.60382200
C	4.36619600	-0.49545900	3.89012000
Si	5.97940600	-1.21390000	4.44675900

C	7.38035600	-0.35562400	3.53484300
C	5.93740800	-3.06524300	4.15239000
C	6.14815600	-0.87442800	6.28758100
H	7.45472900	0.68819700	3.85434800
H	7.24261600	-0.37175200	2.45161700
H	8.33043200	-0.84840200	3.76551100
H	5.61609500	-3.30746100	3.13515300
H	5.24233900	-3.53397100	4.85626700
H	6.92822800	-3.50315200	4.31190500
H	5.33510700	-1.34266600	6.84957400
H	6.13708500	0.19894700	6.49612500
H	7.09455400	-1.28186200	6.65772600
C	0.06556000	-14.26513300	-1.81092100
C	1.23534900	-13.52683400	-1.94395200
C	1.18001000	-12.12457700	-1.98756300
C	-1.23328500	-12.22556700	-1.75533800
C	-1.16646600	-13.62546100	-1.71805500
H	0.11363500	-15.34844800	-1.77450800
C	2.37976600	-11.35404900	-2.12036500
C	3.39086900	-10.69501500	-2.22961700
C	6.98666400	-9.73585500	-2.49400500
C	6.89391200	-8.35148600	-2.56864600
C	5.63568500	-7.72861800	-2.54147200
C	4.57822800	-9.90412900	-2.35393100
C	5.83940500	-10.51533000	-2.38647200
H	7.96135700	-10.21221600	-2.51266900
C	5.53799300	-6.30135800	-2.60971300
C	5.46992900	-5.09243600	-2.66124100
C	6.57077700	-1.53275900	-2.69872100
C	5.35871000	-0.87070400	-2.84687200
C	4.16295000	-1.60154500	-2.93882500
C	5.42229900	-3.66222000	-2.72232200
C	6.61030100	-2.92127200	-2.63826600
H	7.49158000	-0.96359900	-2.62676700
C	-2.28199500	-0.82784500	-0.68778700
C	-3.35213600	-1.37058500	-0.85690200
C	-7.01381200	-1.92738000	-1.30637400
C	-7.07523400	-3.31543800	-1.34457100
C	-5.89876100	-4.07453800	-1.23798900
C	-4.61119100	-2.02792400	-1.04288800
C	-5.79120800	-1.27908700	-1.15751600
H	-7.92639400	-1.34535600	-1.38699200
C	-5.94725500	-5.50503800	-1.28630900
C	-5.97832400	-6.71592800	-1.32623000
C	-7.20079100	-10.24283700	-1.33302200
C	-6.00446200	-10.94397400	-1.42525600
C	-4.78671100	-10.24845400	-1.48579800
C	-5.99281300	-8.14765800	-1.36354900
C	-7.20376800	-8.85191400	-1.30516700

H	-8.13967400	-10.78412400	-1.27987000
C	-2.49225700	-11.55031200	-1.65851900
C	-3.54648900	-10.95778100	-1.58066500
C	-0.05611600	-11.47914300	-1.88838400
C	4.48147900	-8.50926200	-2.43131800
C	4.19873500	-2.99756600	-2.87003900
C	-4.66871500	-3.42626200	-1.08237500
C	-4.78466600	-8.85064100	-1.44654300
H	2.19727400	-14.02325500	-2.01613400
H	-2.08050000	-14.19893800	-1.60630200
H	7.78742900	-7.74137600	-2.64658600
H	5.90955100	-11.59554200	-2.31629200
H	5.32288400	0.21225100	-2.89762600
H	7.55388200	-3.44234900	-2.51683300
H	-8.02736400	-3.82191000	-1.46159400
H	-5.73940800	-0.19585400	-1.11249400
H	-5.99982600	-12.02845100	-1.44967400
H	-8.13633800	-8.30301500	-1.22915500
H	-0.10451800	-10.39549400	-1.90866300
H	3.50737700	-8.03297500	-2.39643500
H	3.27693800	-3.56652800	-2.92813000
H	-3.76416200	-4.01300600	-0.96633000
H	-3.84372800	-8.30995500	-1.46059600
C	-0.19726100	2.79606000	-3.51875100
C	1.90786300	-0.26050300	-3.25908500
C	2.92468000	-0.90257800	-3.10889400
C	-1.45304800	2.25346200	-3.77014700
C	-1.61259100	0.86219300	-3.86539200
C	0.75498700	0.57192600	-3.42925100
C	0.90427000	1.96575400	-3.35685400
H	-0.07516000	3.87275400	-3.45407300
C	-0.50673500	0.02345700	-3.68437900
H	-2.31485000	2.89798700	-3.90928100
H	1.88854700	2.38322200	-3.16984000
H	-0.62838100	-1.05298700	-3.74507900
C	-2.89753200	0.31420000	-4.19589700
C	-3.98851600	-0.11854200	-4.52245800
Si	-5.61235200	-0.75768200	-5.14049900
C	-6.99468200	0.24928600	-4.36723000
C	-5.73554700	-2.57826200	-4.71406500
C	-5.64228800	-0.52466400	-7.00533300
H	-6.91679400	1.29998000	-4.66111500
H	-6.97454700	0.19415600	-3.27655500
H	-7.96398000	-0.12724300	-4.70943900
H	-5.55229000	-2.74864100	-3.65006000
H	-5.00336500	-3.15492700	-5.28700200
H	-6.73294900	-2.95985600	-4.95453600
H	-4.82565100	-1.07046900	-7.48616600
H	-5.55345900	0.53192600	-7.27325400

	H	-6.58697300	-0.89943100	-7.41228700
	H	-5.38561100	-6.99757200	6.21896300
	H	-5.56203100	-6.07251100	4.71726700
	H	-4.56731400	-5.43921700	6.03528300
	H	4.09934300	-5.18400400	3.62448200
	H	4.85605600	-6.77058500	3.80732600
	H	3.59869500	-6.25323400	4.94652800
TS-h	N	-0.09496300	-1.04234600	-0.19368300
	C	-0.39607000	-3.06480200	-0.17655800
	H	0.45965000	-3.16304200	0.47632500
	H	-0.24641000	-3.05449100	-1.24567000
	H	-1.38349900	-2.89250800	0.23045700
	O	-0.63121500	-4.92583000	-0.27170900
	S	-1.61226700	-5.60252900	0.68669100
	O	-1.94018400	-6.95258600	0.19995000
	O	-2.76366700	-4.72020300	0.94937700
	C	-0.70474200	-5.78589800	2.23750700
	H	-0.53515100	-4.75065000	2.56596700
	C	-1.55300000	-6.54517000	3.26495100
	H	-0.87382600	-6.86953500	4.06346800
	H	-1.92006100	-7.46657000	2.78970000
	C	-2.71270300	-5.77535600	3.89424100
	H	-2.32762800	-4.85233400	4.35137200
	C	-3.43462100	-6.60420900	4.95486200
	H	-3.42712200	-5.46369700	3.12433800
	H	-3.78820000	-7.53823900	4.49740200
	C	-4.61457500	-5.85648100	5.56904500
	H	-2.72400000	-6.89393000	5.73987200
	C	0.63363900	-6.48179100	1.97519200
	H	1.03542500	-6.15987900	1.00862200
	H	0.45416500	-7.56232800	1.90228800
	C	1.67913400	-6.20112700	3.05554600
	H	1.98163600	-5.14546700	3.00108800
	C	2.89850600	-7.09895200	2.87124900
	H	1.25768800	-6.35408600	4.05730800
	H	2.58910300	-8.14495900	3.00034600
	C	4.05816600	-6.77733300	3.80536600
	H	3.24700500	-7.00361700	1.83590700
	C	1.12217500	-0.49490300	-0.01964300
	C	1.35967600	0.87296500	-0.06112500
	H	2.37215600	1.22369400	0.08701700
	C	0.28435200	1.76372900	-0.27038400
	N	0.46375200	3.10432000	-0.30774200
	C	-0.98988100	1.17994300	-0.44916700
	H	-1.87199800	1.77661200	-0.63839600
	C	-1.12272800	-0.20001400	-0.42315600
	C	1.80305400	3.65977300	-0.21167600
	C	-0.69119400	3.98355100	-0.37852100
	H	1.74740100	4.74004500	-0.33322800

H	2.44884100	3.25766200	-0.99989100
H	2.26149000	3.44054100	0.76006700
H	-1.25392500	3.82655000	-1.30551900
H	-0.35224600	5.01738500	-0.35196000
H	-1.36480200	3.81623200	0.47007300
C	-1.32068100	-14.02215800	1.57998600
C	-2.33040300	-13.07350700	1.67788000
C	-2.01921000	-11.70434400	1.62848100
C	0.32672200	-12.26480100	1.36840000
C	0.00467800	-13.62747000	1.42906800
H	-1.56752100	-15.07800100	1.61708000
C	-3.06971600	-10.73721400	1.74067100
C	-3.99657300	-9.96204300	1.84024600
C	-7.53837300	-8.91354000	2.29967800
C	-7.42511900	-7.52858400	2.28868100
C	-6.16924000	-6.92759900	2.11313000
C	-5.14776500	-9.11997300	1.97565100
C	-6.40935900	-9.71037400	2.14997100
H	-8.51160600	-9.37538300	2.42837700
C	-6.04378700	-5.50249500	2.11512300
C	-5.90455200	-4.29937000	2.13556900
C	-6.60545600	-0.63556200	2.16634600
C	-5.32538700	-0.11999600	2.32850600
C	-4.22452900	-0.98739600	2.42189700
C	-5.71188600	-2.88265900	2.18544500
C	-6.80586100	-2.01040300	2.10018500
H	-7.45284400	0.03795700	2.09266300
C	2.23312900	-1.37566100	0.21764800
C	3.22456000	-2.05015900	0.39247800
C	6.84104300	-2.77525300	0.87853500
C	6.85560100	-4.16446800	0.86563000
C	5.65857900	-4.88131900	0.70852500
C	4.44048000	-2.78682300	0.57265100
C	5.64364500	-2.08251700	0.73195200
H	7.77098500	-2.22811800	0.99449300
C	5.67049100	-6.31304100	0.69468700
C	5.66214600	-7.52511000	0.69955700
C	6.55405300	-11.15376000	0.86983200
C	5.29307200	-11.73370800	0.96299200
C	4.14887500	-10.92209500	0.95273000
C	5.55873300	-8.95282100	0.76074600
C	6.69595900	-9.77259100	0.77747600
H	7.43679000	-11.78426300	0.87428100
C	1.68583200	-11.84291800	1.21105300
C	2.82993100	-11.46466200	1.08181800
C	-0.69019700	-11.30544900	1.46639400
C	-5.03173100	-7.72549700	1.94115700
C	-4.41807800	-2.36905800	2.33862400
C	4.45018800	-4.18747900	0.56314200

C	4.28918900	-9.53680700	0.83173100
H	-3.36503800	-13.37768800	1.79539800
H	0.79544300	-14.36520200	1.34531000
H	-8.30099800	-6.90100500	2.41523300
H	-6.49058000	-10.79207300	2.16150100
H	-5.16451400	0.95122100	2.38778500
H	-7.80293300	-2.41898100	1.97467000
H	7.78836800	-4.70688300	0.97619700
H	5.62614200	-0.99733800	0.72506300
H	5.18523000	-12.80957600	1.05003100
H	7.68036200	-9.32178400	0.71099000
H	-0.44648400	-10.24961400	1.41034400
H	-4.06475400	-7.26164100	1.76159200
H	-3.57463400	-3.05172100	2.36953300
H	3.52333000	-4.73575800	0.42440200
H	3.40336700	-8.91335700	0.79521000
C	0.71376700	2.75841000	2.98351700
C	-1.81048600	0.03599600	2.76186700
C	-2.90936300	-0.44971200	2.60066600
C	1.87922400	2.04177800	3.23490500
C	1.83608800	0.64379200	3.35288600
C	-0.55034500	0.69377900	2.93148800
C	-0.49727800	2.09404700	2.84037100
H	0.74967600	3.84030800	2.90110200
C	0.61926900	-0.02921500	3.19213000
H	2.82726500	2.55499700	3.35846100
H	-1.41365300	2.64414400	2.65227800
H	0.58263900	-1.11112400	3.26955300
C	3.03529600	-0.07457500	3.67746500
C	4.06166000	-0.64432700	4.00269900
Si	5.58576900	-1.48294000	4.63757500
C	7.09384900	-0.67007400	3.87033900
C	5.45336400	-3.30870600	4.23815400
C	5.63203400	-1.24020700	6.50008100
H	7.20866500	0.34904900	4.25080900
H	7.02605600	-0.62252400	2.78172500
H	7.99548400	-1.23288600	4.13212900
H	5.28235900	-3.47844700	3.17132800
H	4.61896700	-3.74842700	4.79351200
H	6.36785900	-3.83687900	4.52695700
H	4.75514400	-1.68479800	6.97853400
H	5.66352200	-0.17819500	6.75875000
H	6.52497000	-1.71726100	6.91666900
C	0.06196700	-14.23951300	-1.94460500
C	1.25348300	-13.53781000	-2.08262900
C	1.24403300	-12.13414400	-2.09117600
C	-1.16628000	-12.15927900	-1.81242400
C	-1.14529300	-13.56144600	-1.81150100
H	0.07354400	-15.32431100	-1.93574700

C	2.46343800	-11.39673200	-2.23055800
C	3.48650700	-10.75688500	-2.34132600
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C	6.98818100	-8.40784000	-2.66258800
C	5.72930200	-7.78874100	-2.60699800
C	4.67680900	-9.96982400	-2.45975000
C	5.93848200	-10.57797900	-2.51732500
H	8.05830400	-10.26769400	-2.65897900
C	5.61812700	-6.36154300	-2.63640800
C	5.51663000	-5.15413800	-2.64873000
C	6.47006800	-1.55305900	-2.52463700
C	5.23681000	-0.93723200	-2.69496600
C	4.07764500	-1.71414100	-2.85618700
C	5.41552000	-3.72594900	-2.66287300
C	6.56701200	-2.94020200	-2.51020500
H	7.36250300	-0.94911100	-2.39799100
C	-2.41033800	-0.78865400	-0.65899200
C	-3.50004100	-1.28464700	-0.84377000
C	-7.15654300	-1.88630900	-1.31609800
C	-7.19528900	-3.27633900	-1.32071100
C	-6.00765400	-4.01301400	-1.18692100
C	-4.75868500	-1.94100600	-1.03134300
C	-5.94664900	-1.21172600	-1.17512400
H	-8.07849100	-1.32277600	-1.41802400
C	-6.01580000	-5.44489700	-1.20322600
C	-5.98278600	-6.65623000	-1.22029700
C	-7.10386200	-10.21339300	-1.21428600
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C	-5.94991200	-8.08786100	-1.25231000
C	-7.14112100	-8.82359300	-1.17626900
H	-8.02716600	-10.77938200	-1.14837800
C	-2.40314400	-11.45133400	-1.67196100
C	-3.44633000	-10.84651300	-1.55102500
C	0.03254700	-11.45015000	-1.95177900
C	4.57786500	-8.57405600	-2.50403300
C	4.16996900	-3.10841800	-2.83231300
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H	2.19665900	-14.06371600	-2.18509800
H	-2.07577900	-14.10669800	-1.69486800
H	7.88011700	-7.79492900	-2.73614000
H	6.01160900	-11.65922500	-2.47154200
H	5.15583900	0.14442200	-2.71003000
H	7.52708900	-3.42566100	-2.37181700
H	-8.13886800	-3.79974600	-1.43287700
H	-5.91433200	-0.12698100	-1.15779600
H	-5.85902700	-11.96448800	-1.37505500
H	-8.08551900	-8.29869300	-1.07999200



	H	0.02129800	-10.36549700	-1.94648300
	H	3.60351700	-8.10048000	-2.44754700
	H	3.27626100	-3.71326900	-2.94392200
	H	-3.87605700	-3.90061400	-0.88173300
	H	-3.79850300	-8.18971500	-1.37835000
	C	-0.29122800	2.61605400	-3.58223300
	C	1.79060400	-0.44213200	-3.22390200
	C	2.81956400	-1.05865900	-3.05071200
	C	-1.55239300	2.07736700	-3.81395600
	C	-1.72504400	0.68537400	-3.86596700
	C	0.63968800	0.38661900	-3.42225000
	C	0.80189500	1.78086300	-3.39275300
	H	-0.15772900	3.69291200	-3.55793100
	C	-0.62687800	-0.15855700	-3.66136200
	H	-2.40810100	2.72482200	-3.97449000
	H	1.79046100	2.19445100	-3.22003900
	H	-0.75839100	-1.23504900	-3.69600300
	C	-3.01560800	0.14585800	-4.18706500
	C	-4.11055100	-0.27371200	-4.51706500
	Si	-5.72947000	-0.89334600	-5.16820000
	C	-7.11587000	0.15271800	-4.45777500
	C	-5.89436300	-2.70186500	-4.70878900
	C	-5.69818800	-0.69495500	-7.03660500
	H	-7.00048400	1.19935700	-4.75348600
	H	-7.14367900	0.10345100	-3.36714500
	H	-8.07850000	-0.20299000	-4.83902200
	H	-5.70582500	-2.85465700	-3.64315600
	H	-5.17892200	-3.30572200	-5.27466400
	H	-6.90153300	-3.06641000	-4.93413100
	H	-4.88087500	-1.26902900	-7.48171900
	H	-5.57550600	0.35381700	-7.32090800
	H	-6.63896900	-1.05500500	-7.46534400
	H	-5.12432900	-6.45818000	6.32646700
	H	-5.34265200	-5.58991500	4.79608100
	H	-4.28053500	-4.92850000	6.04517100
	H	4.46753200	-5.78627600	3.58387500
	H	4.86719200	-7.50414400	3.68735100
	H	3.73981600	-6.78693900	4.85368600
4h	N	-0.07776800	-0.97084500	-0.17136900
	C	-0.27967000	-2.43210600	-0.12519300
	H	0.53489600	-2.88456400	0.43327600
	H	-0.29373600	-2.83849000	-1.13689900
	H	-1.22712500	-2.65272900	0.36554100
	O	-0.65344100	-5.24275800	-0.35819400
	S	-1.62931400	-5.75533800	0.63948900
	O	-2.09530300	-7.13228800	0.33574800
	O	-2.74267000	-4.79915000	0.87991300
	C	-0.73022700	-5.85985900	2.21258500
	H	-0.56054700	-4.80872800	2.48572200

C	-1.57046600	-6.56450600	3.28274500
H	-0.89591200	-6.84100200	4.10388000
H	-1.93400800	-7.50990900	2.85539500
C	-2.74000000	-5.77416400	3.86597400
H	-2.36517200	-4.82948100	4.28729700
C	-3.46683500	-6.56102000	4.95486000
H	-3.44403000	-5.50081300	3.07280000
H	-3.82926200	-7.50604900	4.52796200
C	-4.63851100	-5.78798200	5.55412900
H	-2.75544900	-6.83271600	5.74618300
C	0.61411000	-6.55886800	2.00199600
H	1.02155100	-6.27022900	1.02763200
H	0.44337600	-7.64356800	1.96807400
C	1.64887600	-6.23604200	3.08037400
H	1.92756600	-5.17469800	3.00866800
C	2.89045700	-7.10605100	2.91502100
H	1.22877500	-6.38060900	4.08413000
H	2.60594100	-8.15815400	3.05129800
C	4.03862500	-6.74967800	3.85069700
H	3.24227800	-7.01055300	1.88129900
C	1.16319100	-0.42318600	-0.00775100
C	1.36367300	0.93949500	-0.06399600
H	2.37226300	1.30151900	0.07574700
C	0.27427400	1.82099000	-0.27392000
N	0.44044300	3.15191300	-0.30833400
C	-0.99857600	1.22416500	-0.45637600
H	-1.88353800	1.81092300	-0.65714100
C	-1.14008400	-0.14554600	-0.42520200
C	1.77704600	3.72406800	-0.20939400
C	-0.72223000	4.02625700	-0.39334500
H	1.70716900	4.80298400	-0.32871900
H	2.42517300	3.32975700	-0.99806700
H	2.22962300	3.50632900	0.76427500
H	-1.26983100	3.86185200	-1.32684000
H	-0.38827300	5.06084000	-0.36447000
H	-1.39886100	3.85290600	0.45003800
C	-1.31372800	-14.06417400	1.58872000
C	-2.34228800	-13.13579700	1.68864100
C	-2.05920500	-11.76105800	1.63804300
C	0.29776600	-12.27393200	1.37329200
C	0.00297100	-13.64302700	1.43502600
H	-1.53925300	-15.12473600	1.62698100
C	-3.12509800	-10.81128200	1.75273200
C	-4.05498500	-10.04006600	1.85344600
C	-7.58040600	-8.93778800	2.31614200
C	-7.44600300	-7.55493200	2.29256800
C	-6.18199700	-6.97422700	2.10720500
C	-5.19391000	-9.18064200	1.98572200
C	-6.46306800	-9.75147300	2.16953300

H	-8.55967400	-9.38446700	2.45225500
C	-6.03857800	-5.55045500	2.09841600
C	-5.88112300	-4.34974500	2.11172900
C	-6.52380900	-0.67558200	2.15054200
C	-5.23582300	-0.18062200	2.30951100
C	-4.14775300	-1.06588500	2.39192100
C	-5.66339900	-2.93661600	2.15784800
C	-6.74406800	-2.04745800	2.08167700
H	-7.36165700	0.01044300	2.08329400
C	2.27289800	-1.29056200	0.22599200
C	3.26254100	-1.96794300	0.39989900
C	6.86359200	-2.75513100	0.88158600
C	6.85072200	-4.14430000	0.86644200
C	5.64103100	-4.84140300	0.71497600
C	4.46459400	-2.72448300	0.58409300
C	5.67907400	-2.03960800	0.74040900
H	7.80428500	-2.22642500	0.99491100
C	5.63327800	-6.27334900	0.70307100
C	5.61506900	-7.48539300	0.70555600
C	6.51054000	-11.11264200	0.86325900
C	5.25115800	-11.69533800	0.95848600
C	4.10472700	-10.88656600	0.95128200
C	5.50960400	-8.91369100	0.76064800
C	6.64874900	-9.73091100	0.77373500
H	7.39479200	-11.74105600	0.86472800
C	1.64933900	-11.82780000	1.21505200
C	2.78880900	-11.43618600	1.08385400
C	-0.73811400	-11.33552900	1.47257700
C	-5.05416700	-7.78780200	1.93803900
C	-4.35916200	-2.44450700	2.30025700
C	4.44468800	-4.12584400	0.57468700
C	4.24104800	-9.50079000	0.83068100
H	-3.37018000	-13.46109000	1.80917400
H	0.80821700	-14.36492600	1.35104800
H	-8.31190200	-6.91299600	2.41667400
H	-6.55971600	-10.83186900	2.19142900
H	-5.05801900	0.88757100	2.37442000
H	-7.74793000	-2.44107000	1.96221500
H	7.77399500	-4.70369800	0.97247200
H	5.68085800	-0.95435900	0.73339600
H	5.14602800	-12.77155400	1.04470400
H	7.63195700	-9.27756600	0.70710200
H	-0.51750200	-10.27477100	1.41411600
H	-4.07975800	-7.34282400	1.74295200
H	-3.52631500	-3.14198400	2.31023300
H	3.50691100	-4.65618400	0.44072400
H	3.35317800	-8.88024700	0.79542400
C	0.75722700	2.70809900	2.96312600
C	-1.73313800	-0.04496600	2.73544300

C	-2.82786200	-0.53908400	2.56934900
C	1.93053200	2.00634200	3.22024700
C	1.90304600	0.60801800	3.34274600
C	-0.48216400	0.62836600	2.90985800
C	-0.44555400	2.02918400	2.81482300
H	0.77955500	3.79065100	2.88327100
C	0.69489900	-0.07955700	3.17983600
H	2.87157800	2.53134100	3.34738000
H	-1.36791300	2.56852400	2.62354800
H	0.67028100	-1.16145800	3.26513500
C	3.10675800	-0.09760900	3.67617900
C	4.13544000	-0.65970500	4.00633200
Si	5.66142900	-1.48709100	4.65246200
C	7.16796300	-0.66779600	3.88968000
C	5.53523400	-3.31335200	4.25564200
C	5.69333800	-1.23867500	6.51416900
H	7.27561800	0.35260500	4.26871800
H	7.10445100	-0.62230200	2.80066900
H	8.07144500	-1.22528000	4.15611300
H	5.36398900	-3.48511300	3.18921800
H	4.70102000	-3.75265500	4.81136500
H	6.45009000	-3.84006200	4.54543700
H	4.81486300	-1.68622400	6.98696700
H	5.71778200	-0.17589200	6.77022600
H	6.58521400	-1.71060500	6.93863500
C	0.06460400	-14.23981200	-1.94569700
C	1.25322100	-13.53327800	-2.08453300
C	1.23830200	-12.12965800	-2.09109700
C	-1.17168100	-12.16468200	-1.80952200
C	-1.14518200	-13.56665700	-1.81040800
H	0.08049700	-15.32457400	-1.93817000
C	2.45497200	-11.38760700	-2.23099900
C	3.47583800	-10.74426800	-2.34242500
C	7.07021900	-9.77366200	-2.62563200
C	6.97303600	-8.38789500	-2.66359100
C	5.71326100	-7.77099600	-2.60404900
C	4.66409600	-9.95398700	-2.46145600
C	5.92677600	-10.55985600	-2.52387300
H	8.04592300	-10.24621000	-2.66869700
C	5.60042700	-6.34384000	-2.63088600
C	5.49770300	-5.13658100	-2.64270500
C	6.44710600	-1.53379700	-2.52094200
C	5.21311500	-0.91930600	-2.68996600
C	4.05513000	-1.69845800	-2.84931800
C	5.39468000	-3.70858200	-2.65659600
C	6.54516100	-2.92100700	-2.50558500
H	7.33926500	-0.92912500	-2.39603800
C	-2.40633300	-0.75119000	-0.66974600
C	-3.48580900	-1.26889400	-0.85721500

C	-7.13085600	-1.88772800	-1.34878700
C	-7.16338700	-3.27804900	-1.34594700
C	-5.97603700	-4.01262500	-1.19810900
C	-4.73627300	-1.93741600	-1.04947000
C	-5.92382600	-1.20950500	-1.20753400
H	-8.05431300	-1.32857900	-1.45912700
C	-5.98986400	-5.44480500	-1.21032900
C	-5.96877100	-6.65644300	-1.22327300
C	-7.11194000	-10.20783100	-1.22776800
C	-5.90291300	-10.88165700	-1.34808700
C	-4.69987000	-10.16120000	-1.41743500
C	-5.94645400	-8.08875900	-1.25511400
C	-7.14223800	-8.81768200	-1.18704000
H	-8.03857100	-10.76896000	-1.16761800
C	-2.41085800	-11.46090800	-1.66861200
C	-3.45459600	-10.85669500	-1.54955500
C	0.02430100	-11.45061300	-1.94887000
C	4.56293800	-8.55821000	-2.50157400
C	4.14807900	-3.09261300	-2.82473500
C	-4.76100200	-3.33753500	-1.03790200
C	-4.72372000	-8.76415900	-1.35656400
H	2.19825200	-14.05546400	-2.18906700
H	-2.07338900	-14.11576400	-1.69377500
H	7.86391100	-7.77342800	-2.73713100
H	6.00161300	-11.64114300	-2.48188500
H	5.13074400	0.16219500	-2.70612800
H	7.50608100	-3.40517500	-2.36843800
H	-8.10474100	-3.80469500	-1.46224500
H	-5.89248600	-0.12466000	-1.20012200
H	-5.87631600	-11.96541500	-1.38917300
H	-8.08453200	-8.28819800	-1.09493500
H	0.00872500	-10.36604600	-1.94132000
H	3.58806600	-8.08614200	-2.44154300
H	3.25502900	-3.69836700	-2.93620200
H	-3.84896000	-3.89625300	-0.85158600
H	-3.79535400	-8.20143200	-1.35764200
C	-0.31902000	2.62603000	-3.58139500
C	1.76681100	-0.42900000	-3.21600700
C	2.79635300	-1.04449500	-3.04267200
C	-1.58036700	2.08481500	-3.80825600
C	-1.75080500	0.69228400	-3.85673400
C	0.61528700	0.39842400	-3.41507300
C	0.77612700	1.79326200	-3.39077100
H	-0.18628200	3.70319000	-3.56521400
C	-0.65090600	-0.14944400	-3.65160200
H	-2.43686700	2.73066300	-3.97061800
H	1.76515800	2.20903600	-3.22553200
H	-0.78004700	-1.22626200	-3.68763900
C	-3.03891900	0.14871900	-4.17935400

	C	-4.13134500	-0.27377400	-4.51346000
	Si	-5.74399400	-0.89637400	-5.17948400
	C	-7.13803000	0.14200600	-4.47302600
	C	-5.89901200	-2.70885300	-4.73284900
	C	-5.70015300	-0.68577800	-7.04606200
	H	-7.02439400	1.18964500	-4.76597000
	H	-7.17239500	0.09107400	-3.38280400
	H	-8.09718900	-0.21601200	-4.86064600
	H	-5.70623500	-2.86989600	-3.66927000
	H	-5.18122800	-3.30362000	-5.30526200
	H	-6.90446600	-3.07762300	-4.95867000
	H	-4.87764200	-1.25390200	-7.48912700
	H	-5.58018700	0.36518600	-7.32317700
	H	-6.63663400	-1.04723000	-7.48299800
	H	-5.14687900	-6.36316400	6.33300400
	H	-5.37035700	-5.54017600	4.77867600
	H	-4.29583600	-4.84817900	6.00011800
	H	4.42716900	-5.75275700	3.61987000
	H	4.86449700	-7.45924000	3.74443400
	H	3.71676200	-6.75496100	4.89779300
3a'	O	0.32920800	-4.89419600	-0.86788900
	C	0.11025400	-3.48126000	-0.61941200
	H	0.38429300	-3.21910000	0.40421500
	H	0.77442600	-2.96548900	-1.30883800
	H	-0.92916800	-3.21737100	-0.81325400
	N	-0.07623400	-0.62224800	-0.17065200
	S	-0.51918200	-5.93114300	0.00869300
	O	-0.43613600	-7.19065700	-0.70576000
	O	-1.82246200	-5.35233500	0.29943900
	C	0.42342600	-6.03784900	1.50632500
	H	0.46592200	-5.05297700	1.97176600
	H	1.42035000	-6.39871300	1.25525800
	H	-0.08949300	-6.74258200	2.16125900
	C	1.09786400	0.01053100	-0.01806500
	C	1.25985500	1.39168100	-0.04596800
	H	2.24915100	1.80780000	0.08780100
	C	0.12849300	2.21339900	-0.25235700
	N	0.22704600	3.56635400	-0.29411900
	C	-1.10961900	1.55173300	-0.41539500
	H	-2.02935600	2.09651600	-0.57997100
	C	-1.14807000	0.16136200	-0.36555700
	C	1.52363400	4.20246100	-0.13504600
	C	-0.96158100	4.37218700	-0.51476000
	H	1.40034600	5.28112600	-0.21135700
	H	2.22378300	3.88040100	-0.91418000
	H	1.96313300	3.97443600	0.84260600
	H	-1.42665800	4.14238400	-1.48024400
	H	-0.68166300	5.42393400	-0.51191100
	H	-1.70424100	4.21218100	0.27482000

	C	2.23154100	-0.85637300	0.17997100
	C	3.12799600	-1.65460800	0.34231300
	C	6.40040400	-3.26086400	1.15166500
	C	6.10827700	-4.59878900	0.89050600
	C	4.83780100	-4.96123700	0.44440300
	C	4.14831700	-2.64370100	0.52540000
	C	5.42777100	-2.28385100	0.97136000
	H	7.38885300	-2.97688500	1.49707500
	H	4.60908700	-6.00167600	0.23758400
	C	3.85913600	-3.99180000	0.26073400
	H	6.87005300	-5.35808600	1.03288400
	H	5.64754600	-1.24107500	1.17457500
	H	2.86934800	-4.26770400	-0.09200200
	C	-2.39601400	-0.53977900	-0.52634200
	C	-3.41323900	-1.18561600	-0.65130400
	C	-6.96179700	-2.18006100	-1.24310500
	C	-6.88108800	-3.56077500	-1.06768500
	C	-5.65889900	-4.15367100	-0.75382200
	C	-4.59482900	-1.98404800	-0.79187800
	C	-5.82585800	-1.39078600	-1.10668700
	H	-7.91228300	-1.71668100	-1.48610600
	H	-5.59430900	-5.22808900	-0.61622600
	C	-4.51652800	-3.37432100	-0.61459200
	H	-7.77026200	-4.17361600	-1.17425500
	H	-5.88030400	-0.31577500	-1.24230600
	H	-3.56364200	-3.83309800	-0.36610600
TS-a'	O	0.34213800	-4.65181300	-0.62934700
	C	0.12698400	-2.80341800	-0.41347300
	H	0.59224400	-2.81092500	0.56010300
	H	0.74504400	-2.67160400	-1.28727100
	H	-0.94810900	-2.85337200	-0.50035600
	N	0.03997800	-0.78293100	-0.26682100
	S	-0.55351500	-5.56124400	0.20999200
	O	-0.62867700	-6.89269200	-0.39665600
	O	-1.83831600	-4.90467300	0.49947200
	C	0.30815300	-5.72441600	1.75870500
	H	0.41830200	-4.73553500	2.20498500
	H	1.28549000	-6.16756700	1.56738200
	H	-0.28168100	-6.36743100	2.41184300
	C	1.19433600	-0.11183400	-0.08037900
	C	1.27727400	1.27108500	-0.04381200
	H	2.24546900	1.72573100	0.11289000
	C	0.10367700	2.04533100	-0.20909700
	N	0.13357900	3.39497500	-0.18624000
	C	-1.10219500	1.32932800	-0.39725900
	H	-2.04992400	1.83278000	-0.52790000
	C	-1.08427500	-0.05888100	-0.41813900
	C	1.39851400	4.09101300	-0.00354500
	C	-1.09928600	4.15163400	-0.34510000

	H	1.21888200	5.16334900	-0.04044900
	H	2.10871800	3.83304600	-0.79613800
	H	1.84918900	3.84881100	0.96494800
	H	-1.56178900	3.95697900	-1.31868300
	H	-0.87207900	5.21356000	-0.27886700
	H	-1.81918800	3.90312400	0.44181400
	C	2.36591700	-0.92426300	0.08896800
	C	3.28580600	-1.69879400	0.23052400
	C	6.58989200	-3.31966200	0.85738900
	C	6.24650200	-4.66307000	0.71341800
	C	4.93396800	-5.02270200	0.40769900
	C	4.30595700	-2.69001300	0.39226300
	C	5.62564800	-2.33096600	0.69823400
	H	7.61134200	-3.04186700	1.09478700
	H	4.66836500	-6.06860800	0.29464300
	C	3.96138700	-4.04342600	0.24606700
	H	7.00265900	-5.43086700	0.83964100
	H	5.88249800	-1.28293800	0.80963000
	H	2.93547300	-4.31046600	0.00414100
	C	-2.31119500	-0.78162500	-0.60282500
	C	-3.35292200	-1.38232200	-0.74816300
	C	-6.93088000	-2.10122400	-1.49453200
	C	-6.97941600	-3.47577200	-1.26490800
	C	-5.83178100	-4.15872600	-0.86413600
	C	-4.58326500	-2.09442000	-0.92295900
	C	-5.73882700	-1.40812200	-1.32489600
	H	-7.82332500	-1.56846600	-1.80555700
	H	-5.87131200	-5.22810900	-0.68480900
	C	-4.63196700	-3.47763900	-0.69129800
	H	-7.91235600	-4.01370900	-1.39824800
	H	-5.69072700	-0.33872200	-1.50101400
	H	-3.73318100	-4.00040700	-0.37496500
4a'	O	0.81587600	-4.96048500	-1.03948800
	C	-0.12122000	-2.16091200	-0.17770000
	H	0.15239200	-2.50174600	0.82214800
	H	0.57414400	-2.58443200	-0.89939600
	H	-1.12559200	-2.49572500	-0.40636800
	N	-0.06015600	-0.68917800	-0.22034900
	S	-0.21071100	-5.66408600	-0.22903500
	O	-0.48139600	-7.03909000	-0.69954400
	O	-1.44258500	-4.86022900	-0.03410900
	C	0.51239900	-5.83596800	1.39634700
	H	0.74416700	-4.84426800	1.78730800
	H	1.42771600	-6.42312000	1.31177300
	H	-0.19858300	-6.33998200	2.05126300
	C	1.14911500	-0.06939800	-0.05236000
	C	1.26995300	1.30130600	-0.07605500
	H	2.25602200	1.71954100	0.06410000
	C	0.12859500	2.12090900	-0.27903100



	N	0.21709200	3.45653400	-0.31188700
	C	-1.11129900	1.45034100	-0.44418700
	H	-2.03354800	1.99014600	-0.60190700
	C	-1.17947300	0.07448400	-0.40922100
	C	1.51238500	4.10873900	-0.14919700
	C	-0.98106600	4.26447500	-0.51409300
	H	1.37524700	5.18440100	-0.22856400
	H	2.20955200	3.78955800	-0.92949700
	H	1.94342200	3.88394000	0.83107300
	H	-1.44230900	4.04454900	-1.48168400
	H	-0.70249700	5.31523800	-0.49485200
	H	-1.71163500	4.08447600	0.28003000
	C	2.27166800	-0.92029900	0.15136400
	C	3.15814700	-1.72794900	0.32170500
	C	6.38027000	-3.40560300	1.15326800
	C	6.04556200	-4.73615800	0.90383200
	C	4.76630700	-5.06769800	0.45778500
	C	4.15202500	-2.73677600	0.51548600
	C	5.43841900	-2.40223500	0.96087000
	H	7.37643800	-3.14992300	1.49803000
	H	4.51054200	-6.10364200	0.26067900
	C	3.81278300	-4.07571800	0.25996300
	H	6.78486600	-5.51579600	1.05557800
	H	5.68599000	-1.36394900	1.15379900
	H	2.81377700	-4.32242600	-0.09638000
	C	-2.42443100	-0.60007300	-0.56473300
	C	-3.45628200	-1.22253600	-0.68531400
	C	-7.00376800	-2.26316100	-1.15713000
	C	-6.87645500	-3.64883500	-1.06868100
	C	-5.62571200	-4.22769800	-0.85411800
	C	-4.62607900	-2.03372700	-0.81674400
	C	-5.88323100	-1.45142900	-1.03224900
	H	-7.97752000	-1.81483500	-1.32283700
	H	-5.53059300	-5.30613500	-0.78530200
	C	-4.49542000	-3.42941000	-0.72667500
	H	-7.75448400	-4.27909700	-1.16559800
	H	-5.96954900	-0.37228900	-1.09968100
	H	-3.51617700	-3.87242100	-0.55733600
3b'	N	-0.13740000	-0.75535000	-0.24130200
	C	-0.02791700	-3.60008800	-0.79272200
	H	0.24850600	-3.35596600	0.23471100
	H	0.65790300	-3.10085200	-1.47408600
	H	-1.05731400	-3.30019700	-0.99007900
	O	0.14433000	-5.01813000	-1.05258400
	S	-0.75284300	-6.03053800	-0.19130400
	O	-0.73036000	-7.28346100	-0.92593100
	O	-2.03235500	-5.39871000	0.10586300
	C	0.18238900	-6.20844800	1.31582500
	H	0.30381200	-5.20539800	1.73561300

H	1.16144300	-6.59414800	1.01752300
C	-0.53766400	-7.14232200	2.28719500
H	-1.52864400	-6.73296700	2.50565200
C	0.26590100	-7.30128300	3.57467700
H	-0.68203500	-8.11498200	1.80666300
H	1.25349200	-7.72406600	3.36964600
H	-0.25227200	-7.96754300	4.26803500
H	0.40534500	-6.33632800	4.07037700
C	1.04604100	-0.16169900	-0.01880000
C	1.23365800	1.21312200	0.08031900
H	2.22898500	1.59674000	0.25956800
C	0.11942800	2.07169600	-0.05795500
N	0.24184400	3.42048600	0.03178600
C	-1.12861400	1.45143300	-0.29275300
H	-2.03762600	2.02638800	-0.40772200
C	-1.19274000	0.06329300	-0.37207300
C	1.54177900	4.01286800	0.29686500
C	-0.93021100	4.26527800	-0.12147400
H	1.43218500	5.09391200	0.35823300
H	2.25607100	3.78336500	-0.50194300
H	1.95572800	3.65469300	1.24609600
H	-1.39721100	4.12247400	-1.10233800
H	-0.62858400	5.30764300	-0.03589400
H	-1.67781900	4.05739600	0.65259100
C	2.15954100	-1.06496800	0.12137900
C	3.03860500	-1.89045100	0.23611800
C	6.29130300	-3.58408400	0.93600300
C	5.97248900	-4.90560700	0.62725300
C	4.69010700	-5.22912000	0.18498200
C	4.04199700	-2.90524000	0.36487000
C	5.33327500	-2.58470900	0.80696800
H	7.28899300	-3.33088900	1.27902700
H	4.44080000	-6.25699300	-0.05752800
C	3.72557100	-4.23692900	0.05229900
H	6.72296200	-5.68246500	0.73121700
H	5.57326200	-1.55432500	1.04702700
H	2.72603600	-4.48212900	-0.29602600
C	-2.45286400	-0.59554300	-0.60225900
C	-3.48411100	-1.20413900	-0.78528300
C	-7.03751000	-2.03772700	-1.56135400
C	-7.02417400	-3.42313400	-1.40496100
C	-5.84450400	-4.07308300	-1.04368600
C	-4.68839700	-1.95150300	-0.99558400
C	-5.87693500	-1.30078100	-1.35799100
H	-7.95442100	-1.52997100	-1.84226800
H	-5.83269400	-5.15122600	-0.92117500
C	-4.67755600	-3.34641500	-0.83828600
H	-7.93234200	-3.99494400	-1.56535200
H	-5.87883700	-0.22253100	-1.47817900

	H	-3.75722600	-3.84920200	-0.55428800
TS-b'	N	-0.04761600	-0.87613600	-0.29370700
	C	-0.01903300	-2.88642800	-0.56749900
	H	0.42951900	-2.97021800	0.41013500
	H	0.61560000	-2.71948600	-1.42336500
	H	-1.09332900	-2.89532400	-0.67027200
	O	0.13753100	-4.72464800	-0.89957200
	S	-0.76068300	-5.65851700	-0.08789600
	O	-0.97457400	-6.91499100	-0.81481700
	O	-1.97720200	-4.95642500	0.35714700
	C	0.19800400	-6.03467200	1.37324100
	H	0.44926200	-5.07580400	1.83859300
	H	1.12294400	-6.50032500	1.01898100
	C	-0.56279300	-6.94185600	2.33321000
	H	-1.49316800	-6.44497500	2.62527400
	C	0.27439700	-7.26841100	3.56688600
	H	-0.83794000	-7.86114900	1.80644300
	H	1.19952800	-7.78078500	3.28723600
	H	-0.27830000	-7.91708600	4.25042100
	H	0.54461600	-6.35732800	4.10878200
	C	1.12240200	-0.25355100	-0.04665500
	C	1.24352700	1.12038200	0.08750600
	H	2.22210000	1.53598100	0.28355900
	C	0.09428800	1.93781400	-0.03638100
	N	0.16173200	3.28090700	0.08540100
	C	-1.12846600	1.27232800	-0.29056100
	H	-2.06015900	1.81126200	-0.39279000
	C	-1.14900800	-0.11086000	-0.40807700
	C	1.43840800	3.92135900	0.36418100
	C	-1.04459300	4.08369900	-0.04901200
	H	1.28462000	4.99557200	0.44112100
	H	2.16037400	3.73186200	-0.43716700
	H	1.86097000	3.56435400	1.30933900
	H	-1.49891900	3.95130000	-1.03649900
	H	-0.78507300	5.13342000	0.07129400
	H	-1.78320700	3.82002000	0.71566400
	C	2.26664400	-1.11108500	0.08182700
C	3.15705100	-1.92505800	0.18646200	
C	6.38815400	-3.69683200	0.78288600	
C	6.00761300	-5.01420300	0.53113000	
C	4.69456100	-5.30635500	0.16230400	
C	4.14055600	-2.95878200	0.30102500	
C	5.46074000	-2.66753000	0.66990400	
H	7.41016300	-3.47079200	1.06807400	
H	4.39975300	-6.33179100	-0.03518100	
C	3.75862800	-4.28584900	0.04549200	
H	6.73541900	-5.81378100	0.62232700	
H	5.74659100	-1.63962300	0.86616500	
H	2.73258300	-4.50050100	-0.24416600	

	C	-2.39114400	-0.78795200	-0.65368100
	C	-3.43883700	-1.36409500	-0.84737800
	C	-6.99699200	-2.04333400	-1.72228200
	C	-7.06086300	-3.42115000	-1.51748600
	C	-5.93083000	-4.11815100	-1.09165700
	C	-4.66936200	-2.06082600	-1.07559800
	C	-5.80699500	-1.36043100	-1.50291300
	H	-7.87604600	-1.50000100	-2.05259100
	H	-5.98235800	-5.19013200	-0.93187800
	C	-4.73336000	-3.44756100	-0.86899600
	H	-7.99209700	-3.95088400	-1.68983400
	H	-5.74701600	-0.28856900	-1.65940600
	H	-3.84801800	-3.98122000	-0.53249000v
4b'	N	0.00585300	-0.92935700	-0.28399500
	C	-0.00734400	-2.38857600	-0.49025200
	H	0.51782900	-2.87089300	0.33226500
	H	0.50841300	-2.63275500	-1.41844100
	H	-1.02842500	-2.75304100	-0.52528900
	O	0.67861900	-5.18919500	-0.96750100
	S	-0.44609200	-5.84317300	-0.25005600
	O	-0.67974200	-7.23924000	-0.68300500
	O	-1.68461300	-5.02068000	-0.24503900
	C	0.08469800	-5.93306600	1.46202000
	H	0.30232100	-4.90647700	1.77582500
	H	1.02483600	-6.49443300	1.46230900
	C	-0.95473700	-6.58111900	2.36641600
	H	-1.88404800	-6.00535300	2.30200900
	C	-0.47593300	-6.65526600	3.81422900
	H	-1.17215600	-7.58442700	1.98554900
	H	0.44452200	-7.24212300	3.89195300
	H	-1.22926400	-7.12088600	4.45473900
	H	-0.26956900	-5.65599500	4.21044000
	C	1.20208100	-0.30554800	-0.04801700
	C	1.28652200	1.05573400	0.13317800
	H	2.26430500	1.47670600	0.31641600
	C	0.11974800	1.86273700	0.07718000
	N	0.17248800	3.18926900	0.25063200
	C	-1.10425000	1.18867400	-0.17117700
	H	-2.04340900	1.71935700	-0.23032000
	C	-1.13523300	-0.17852200	-0.34518600
	C	1.45133300	3.84291800	0.50880100
	C	-1.04986200	3.98391300	0.18767300
	H	1.28390800	4.91203600	0.61241500
	H	2.14773300	3.67770500	-0.31737700
	H	1.89963500	3.47032600	1.43574700
	H	-1.51986000	3.89824500	-0.79688100
	H	-0.79905100	5.02786400	0.36395400
	H	-1.76249400	3.66356100	0.95430300
	C	2.35074200	-1.14419100	0.00671600

	C	3.25239300	-1.95151600	0.05438600
	C	6.54207500	-3.66758300	0.41216100
	C	6.15682900	-4.99382600	0.21976400
	C	4.82132800	-5.30963300	-0.02930800
	C	4.25287100	-2.97084900	0.10825900
	C	5.59491500	-2.65244100	0.35819600
	H	7.58144200	-3.42535600	0.60572400
	H	4.52626800	-6.34271000	-0.18003600
	C	3.86163000	-4.30589100	-0.08745300
	H	6.90021600	-5.78327900	0.26463400
	H	5.88161300	-1.61693900	0.50794800
	H	2.81720700	-4.54062900	-0.28728600
	C	-2.36743600	-0.84879000	-0.59478000
	C	-3.40939600	-1.42939800	-0.80504200
	C	-6.97268900	-2.24051900	-1.52869600
	C	-6.91730400	-3.63350300	-1.56231700
	C	-5.70936000	-4.29418900	-1.34174300
	C	-4.60764600	-2.16844500	-1.05817800
	C	-5.82226900	-1.50320900	-1.27736100
	H	-7.91371800	-1.72863200	-1.69952100
	H	-5.67064400	-5.37801000	-1.36725500
	C	-4.54963200	-3.57121100	-1.08878100
	H	-7.81822300	-4.20471300	-1.76113200
	H	-5.85259700	-0.41927400	-1.24996400
	H	-3.60307900	-4.07578600	-0.91004800
3c'	N	-0.21143700	-0.73986800	-0.16732900
	C	-0.19059400	-3.52948600	-0.89554700
	H	0.08453700	-3.36802500	0.14818600
	H	0.50473800	-2.98992900	-1.53433600
	H	-1.21370800	-3.19740600	-1.07115600
	O	-0.04219500	-4.92564700	-1.26427200
	S	-0.90671700	-5.99152600	-0.43534900
	O	-0.95222500	-7.18099400	-1.26647000
	O	-2.15350400	-5.36643000	-0.01285300
	C	0.11823200	-6.30222200	0.99007800
	H	0.28945200	-5.33721700	1.47630400
	H	1.06684200	-6.67745600	0.59534800
	C	-0.55026600	-7.30108900	1.93071800
	H	-1.50477400	-6.88873600	2.27506000
	C	0.34715300	-7.61424400	3.12652200
	H	-0.76989400	-8.22260800	1.38008500
	H	1.30404400	-8.01524200	2.76783100
	C	-0.29401800	-8.61260300	4.08782800
	H	0.57836800	-6.68566000	3.66430100
	H	-1.24617100	-8.20460400	4.44837500
	C	0.61127200	-8.93822700	5.27233900
	H	-0.53689400	-9.53221200	3.54162300
	H	1.55675800	-9.37167300	4.93122300
	H	0.13965800	-9.65224800	5.95217100

	H	0.84645800	-8.03447700	5.84311000
	C	0.97888400	-0.19014300	0.12019900
	C	1.19746400	1.17260500	0.29263900
	H	2.19553600	1.52076400	0.52205900
	C	0.10947500	2.06575500	0.16061700
	N	0.26150100	3.40534600	0.31734600
	C	-1.14572800	1.49086100	-0.14205100
	H	-2.03612000	2.09413800	-0.25650900
	C	-1.24159600	0.11084600	-0.29101400
	C	1.56691500	3.95258300	0.64478700
	C	-0.88390100	4.28629500	0.16472000
	H	1.48149200	5.03264700	0.74835300
	H	2.29912000	3.73853200	-0.14192500
	H	1.94371600	3.54569900	1.58985700
	H	-1.32362000	4.19707000	-0.83480100
	H	-0.55929800	5.31564100	0.30454300
	H	-1.66018900	4.06558200	0.90625500
	C	2.06023100	-1.13465800	0.24416600
	C	2.89820300	-2.00539700	0.32807500
	C	6.00042300	-3.96080700	1.04241400
	C	5.62969000	-5.21988000	0.57307900
	C	4.36435400	-5.41332200	0.01970900
	C	3.83777800	-3.08419800	0.41071800
	C	5.11193200	-2.89421100	0.96374000
	H	6.98485800	-3.80905000	1.47251500
	H	4.07388000	-6.39183900	-0.34911100
	C	3.46963700	-4.35351700	-0.06362600
	H	6.32635700	-6.04926900	0.63727800
	H	5.39388100	-1.91219200	1.32861700
	H	2.48494100	-4.49718500	-0.49983800
	C	-2.50758100	-0.50658900	-0.59296700
	C	-3.53954300	-1.09002600	-0.84281900
	C	-7.05957200	-1.84541300	-1.82498800
	C	-7.07576100	-3.23407900	-1.70379800
	C	-5.92699300	-3.91225300	-1.29748200
	C	-4.74271800	-1.81172200	-1.13383000
	C	-5.90004000	-1.13294200	-1.54177000
	H	-7.95226100	-1.31550900	-2.14058600
	H	-5.93821400	-4.99312700	-1.20240300
	C	-4.76155500	-3.21038000	-1.01238300
	H	-7.98235200	-3.78722800	-1.92632600
	H	-5.87917500	-0.05219000	-1.63445400
	H	-3.86546800	-3.73591200	-0.69359800
TS-c'	N	-0.08274700	-0.88316600	-0.24953900
	C	-0.07060400	-2.86679000	-0.67306600
	H	0.37057100	-3.02631000	0.29829800
	H	0.57087700	-2.64253600	-1.51048400
	H	-1.14400900	-2.85894800	-0.78329100
	O	0.07179900	-4.67667700	-1.14194000

S	-0.81528500	-5.66167700	-0.37912300
O	-1.02761300	-6.87484400	-1.17614900
O	-2.03102000	-4.99217700	0.11531700
C	0.16063900	-6.11586000	1.04753400
H	0.39647000	-5.18480400	1.57338900
H	1.09194300	-6.53620200	0.65546800
C	-0.56807800	-7.10123100	1.95209500
H	-1.50942200	-6.65110500	2.28695500
C	0.28373800	-7.48884800	3.15892900
H	-0.82465900	-7.99534900	1.37276900
H	1.23017000	-7.92462500	2.81187000
C	-0.41996700	-8.47881400	4.08449100
H	0.54720200	-6.58544400	3.72492500
H	-1.36430400	-8.04004000	4.42966600
C	0.44065600	-8.86358800	5.28466700
H	-0.68609400	-9.37750600	3.51456200
H	1.37642400	-9.32873000	4.95873500
H	-0.07608000	-9.57004000	5.93937100
H	0.69782400	-7.98049600	5.87802900
C	1.08925800	-0.29299200	0.06039100
C	1.22307600	1.06761400	0.28666400
H	2.20164900	1.45684000	0.53088500
C	0.08554300	1.90557300	0.19350000
N	0.16575000	3.23768500	0.39817900
C	-1.14043300	1.27256600	-0.12118700
H	-2.06459000	1.82814900	-0.19988100
C	-1.17413700	-0.09931600	-0.32994400
C	1.44396900	3.84527200	0.73660600
C	-1.03068700	4.06026300	0.29880200
H	1.30262400	4.91669000	0.86199200
H	2.18079900	3.68474000	-0.05735900
H	1.84127500	3.43753800	1.67226400
H	-1.47627100	3.98866700	-0.69887500
H	-0.76155000	5.09851800	0.48100400
H	-1.77970500	3.76138000	1.04008300
C	2.21747100	-1.17617900	0.15443100
C	3.08004200	-2.02358800	0.22064400
C	6.19969300	-3.99720100	0.78816200
C	5.77777500	-5.26174800	0.37992100
C	4.47528200	-5.45060900	-0.08225000
C	4.01564500	-3.10567900	0.27506100
C	5.32485200	-2.91798800	0.73783600
H	7.21270400	-3.85165100	1.14795400
H	4.14757400	-6.43453700	-0.40148400
C	3.59169100	-4.37980700	-0.13726200
H	6.46435200	-6.10092500	0.42132100
H	5.64398600	-1.93111800	1.05541400
H	2.57478500	-4.51482800	-0.49928800
C	-2.41876000	-0.74627200	-0.63650000

	C	-3.46674800	-1.30208600	-0.88114900
	C	-7.01722500	-1.90590000	-1.83866000
	C	-7.08742100	-3.29430200	-1.73034900
	C	-5.96421100	-4.02339000	-1.34137400
	C	-4.69682500	-1.97685900	-1.16937700
	C	-5.82762200	-1.24432600	-1.55961700
	H	-7.89088000	-1.33778200	-2.14014100
	H	-6.02104000	-5.10364100	-1.25636400
	C	-4.76732700	-3.37437700	-1.05963800
	H	-8.01805100	-3.80798900	-1.94841500
	H	-5.76246400	-0.16444300	-1.64122200
	H	-3.88776400	-3.93364900	-0.75085900
4c'	N	-0.02835800	-0.94577500	-0.15950100
	C	-0.05421300	-2.39413100	-0.43195600
	H	0.47505900	-2.91365000	0.36554800
	H	0.44822500	-2.60309200	-1.37546700
	H	-1.07816800	-2.74897700	-0.47514900
	O	0.67980900	-5.07409600	-1.40895600
	S	-0.38723700	-5.85928300	-0.73637500
	O	-0.61924100	-7.18106400	-1.35957300
	O	-1.63784300	-5.08096000	-0.53973800
	C	0.24949000	-6.18581800	0.90860300
	H	0.43963400	-5.20859900	1.36482700
	H	1.21225600	-6.68818400	0.77113900
	C	-0.70189600	-7.01914200	1.75461700
	H	-1.66671900	-6.50258900	1.81682200
	C	-0.15596800	-7.27011000	3.15813000
	H	-0.88247600	-7.97386200	1.24752400
	H	0.81991800	-7.76894300	3.08629000
	C	-1.09351000	-8.11632400	4.01654900
	H	0.02504100	-6.30834300	3.65709000
	H	-2.06816300	-7.61690700	4.08498000
	C	-0.53903100	-8.36157600	5.41731500
	H	-1.27235200	-9.07551700	3.51467700
	H	0.42389800	-8.88045000	5.36817800
	H	-1.21837100	-8.97051800	6.01937100
	H	-0.37920600	-7.41480100	5.94346000
	C	1.17452100	-0.34007700	0.09010900
	C	1.27032500	1.01249700	0.32405100
	H	2.25285000	1.41915900	0.51427200
	C	0.10926300	1.82968100	0.30759400
	N	0.17345000	3.14919100	0.52530200
	C	-1.12219900	1.17394300	0.04734600
	H	-2.05789900	1.71314300	0.01851900
	C	-1.16468100	-0.18499500	-0.17958100
	C	1.45995100	3.78563600	0.78895500
	C	-1.04288500	3.95494000	0.49454400
	H	1.30125500	4.85223900	0.92823400
	H	2.14562400	3.64286200	-0.05156300



	H	1.91643200	3.38000700	1.69690500
	H	-1.52110900	3.90064800	-0.48810800
	H	-0.78290300	4.99105000	0.69704300
	H	-1.75207800	3.61917100	1.25708400
	C	2.31771800	-1.18816400	0.09801900
	C	3.21173100	-2.00530500	0.09318300
	C	6.45994900	-3.80835100	0.40252400
	C	6.06684800	-5.09751400	0.04437500
	C	4.74071600	-5.35838700	-0.30048700
	C	4.19764000	-3.03959300	0.07397400
	C	5.53037100	-2.77599700	0.41937900
	H	7.49218800	-3.60775700	0.66868600
	H	4.43896800	-6.36231800	-0.58041100
	C	3.79884200	-4.33677700	-0.28946300
	H	6.79650800	-5.90065300	0.03267500
	H	5.82336700	-1.76938400	0.69762200
	H	2.76247900	-4.52853800	-0.56343500
	C	-2.40245500	-0.83871700	-0.44384300
	C	-3.44230200	-1.41631600	-0.67207600
	C	-7.01270700	-2.24493200	-1.34284400
	C	-6.92641100	-3.62644400	-1.51469200
	C	-5.69612400	-4.27362700	-1.40144000
	C	-4.63286900	-2.15704300	-0.95160400
	C	-5.87033000	-1.50570900	-1.06190300
	H	-7.97117000	-1.74376800	-1.43004900
	H	-5.63363100	-5.34866700	-1.53333600
	C	-4.54431400	-3.54857300	-1.11945400
	H	-7.82072400	-4.19935600	-1.73717000
	H	-5.92447700	-0.43037500	-0.92795300
	H	-3.58080900	-4.04391500	-1.02288500
3d'	N	-0.26496100	-0.87536200	-0.08380300
	C	-0.27895200	-3.59687000	-1.04777400
	H	-0.01276600	-3.51929300	0.00771800
	H	0.44711500	-3.04408500	-1.63964800
	H	-1.28455300	-3.21064000	-1.21058100
	O	-0.18099700	-4.96947200	-1.50940000
	S	-1.08009700	-6.05465700	-0.74351400
	O	-1.16950600	-7.18872100	-1.64613400
	O	-2.30268800	-5.41373600	-0.27673700
	C	-0.05884100	-6.48417500	0.65233300
	H	0.15168600	-5.55410500	1.18924700
	H	0.87231300	-6.87030700	0.22780000
	C	-0.74885200	-7.50926200	1.54783700
	H	-1.69020600	-7.09005500	1.91888400
	C	0.15338000	-7.89456000	2.71910200
	H	-0.99451700	-8.39821700	0.95644600
	H	1.09917600	-8.29487400	2.33154800
	C	-0.49232100	-8.92329400	3.64423200
	H	0.40682400	-6.99435900	3.29374800

H	-1.43726500	-8.52087600	4.03286100
C	0.41181900	-9.31355000	4.81060600
H	-0.75099000	-9.82071600	3.06653500
H	1.35705600	-9.71391700	4.41911500
C	-0.22163400	-10.34179800	5.74486200
H	0.67295400	-8.41421200	5.38502900
H	-0.48492300	-11.23749300	5.16867000
H	-1.16386900	-9.93917400	6.13716800
C	0.69686300	-10.72474200	6.90156000
H	1.63255000	-11.15411000	6.52942200
H	0.22902700	-11.45953500	7.56148400
H	0.95125800	-9.84632600	7.50291200
C	0.92240800	-0.38814500	0.30936300
C	1.16927300	0.95004100	0.59846800
H	2.16172700	1.24631200	0.91023600
C	0.11624500	1.88577400	0.47643000
N	0.29708200	3.20395000	0.74451000
C	-1.13581200	1.37651300	0.06223200
H	-2.00045000	2.01586200	-0.05475700
C	-1.26242400	0.01513200	-0.19628600
C	1.59647400	3.68095600	1.18703200
C	-0.81947100	4.12661300	0.62546600
H	1.54111100	4.75531500	1.35268100
H	2.36879300	3.48947100	0.43363600
H	1.89990400	3.20228500	2.12528400
H	-1.20998700	4.14950400	-0.39813600
H	-0.47984100	5.12804800	0.88307100
H	-1.63714900	3.85464400	1.30317900
C	1.96757600	-1.37417500	0.41977200
C	2.77370300	-2.27610800	0.48347200
C	5.76933800	-4.38411900	1.21404200
C	5.39485100	-5.58721800	0.61781100
C	4.16222400	-5.69286100	-0.02486500
C	3.67548700	-3.38854700	0.53061900
C	4.91672300	-3.28676400	1.17371600
H	6.72930100	-4.29933600	1.71186900
H	3.87000400	-6.62738400	-0.49307100
C	3.30402500	-4.60121500	-0.07153500
H	6.06276500	-6.44141700	0.65171900
H	5.20144500	-2.34818500	1.63745300
H	2.34609000	-4.67570700	-0.57854100
C	-2.52746700	-0.53822100	-0.60718400
C	-3.56157800	-1.07150000	-0.94430100
C	-7.06182300	-1.64564800	-2.10287700
C	-7.11835000	-3.03862700	-2.09408800
C	-6.00268300	-3.77971300	-1.70606600
C	-4.77051600	-1.73386700	-1.33542300
C	-5.89481300	-0.99167500	-1.72579000
H	-7.92920300	-1.06729100	-2.40324600

	H	-6.04589000	-4.86389700	-1.69813200
	C	-4.83002400	-3.13640500	-1.32718400
	H	-8.03104900	-3.54651300	-2.38833700
	H	-5.84248500	0.09195500	-1.72986700
	H	-3.96021500	-3.71074300	-1.02010200
TS-d'	N	-0.06402300	-0.98492500	-0.16198000
	C	-0.03619400	-2.94386300	-0.69324100
	H	0.40751400	-3.15311500	0.26760600
	H	0.60255800	-2.66732500	-1.51683400
	H	-1.11000500	-2.93919400	-0.80272900
	O	0.12788100	-4.72296200	-1.25952900
	S	-0.80638000	-5.74762100	-0.61457700
	O	-0.98643800	-6.90136200	-1.50246500
	O	-2.04151200	-5.09935700	-0.14045000
	C	0.08507500	-6.31156400	0.82894500
	H	0.30910100	-5.42116900	1.42523900
	H	1.02745600	-6.72805700	0.46016900
	C	-0.71910900	-7.33502400	1.62041900
	H	-1.66312700	-6.87758700	1.93735900
	C	0.04508400	-7.84810500	2.83915400
	H	-0.97234000	-8.17386800	0.96190600
	H	0.99089300	-8.30061200	2.51305100
	C	-0.75948100	-8.86981500	3.63844400
	H	0.31116400	-7.00270200	3.48735400
	H	-1.70290100	-8.41196900	3.96555400
	C	-0.01012000	-9.40740700	4.85488000
	H	-1.03437700	-9.70696100	2.98242700
	H	0.93227000	-9.86811600	4.52778300
	C	-0.81974100	-10.42675800	5.65281000
	H	0.26794500	-8.57099500	5.51098700
	H	-1.09936400	-11.25874300	4.99421900
	H	-1.75943200	-9.96345900	5.97904300
	C	-0.06115400	-10.96190600	6.86419000
	H	0.86752900	-11.45260800	6.55560900
	H	-0.65576300	-11.68915800	7.42333700
	H	0.20484900	-10.14869800	7.54713700
	C	1.10501700	-0.40444700	0.17602100
	C	1.23237900	0.94416500	0.46832900
	H	2.20885500	1.32506200	0.73303200
	C	0.09116200	1.78052500	0.41392800
	N	0.16537000	3.10237500	0.67904800
	C	-1.13173000	1.15724600	0.06954300
	H	-2.05827500	1.71186000	0.01651100
	C	-1.15912500	-0.20333800	-0.20480600
	C	1.44045700	3.69983500	1.04608800
	C	-1.03599300	3.92182700	0.62292700
	H	1.29653800	4.76615300	1.20695400
	H	2.18162300	3.56799200	0.25101000
	H	1.83390200	3.26097300	1.96934000

	H	-1.48691500	3.89138100	-0.37450000
	H	-0.77125200	4.95273600	0.84808500
	H	-1.77911900	3.58694900	1.35465600
	C	2.23915000	-1.28381600	0.22307800
	C	3.11031100	-2.12475200	0.23890700
	C	6.26690500	-4.07722800	0.65151600
	C	5.84973700	-5.33158400	0.20835000
	C	4.53765700	-5.52068500	-0.22553500
	C	4.05879600	-3.19691800	0.22996000
	C	5.37765000	-3.00888600	0.66434100
	H	7.28755300	-3.93111000	0.98883300
	H	4.21348700	-6.49661700	-0.57166600
	C	3.63953900	-4.46070200	-0.21760800
	H	6.54741100	-6.16252900	0.20021100
	H	5.69335100	-2.02998500	1.00891000
	H	2.61512000	-4.59638900	-0.55756700
	C	-2.40199200	-0.83681800	-0.54503400
	C	-3.45397500	-1.37044100	-0.82018900
	C	-7.01632500	-1.86578200	-1.79355400
	C	-7.10318000	-3.25738700	-1.78129500
	C	-5.98677100	-4.02505400	-1.45151200
	C	-4.69300400	-2.01095900	-1.14615200
	C	-5.81705200	-1.23955500	-1.47708900
	H	-7.88443400	-1.26809700	-2.05048500
	H	-6.05645500	-5.10779900	-1.44156300
	C	-4.78025700	-3.41154100	-1.13371700
	H	-8.04136900	-3.74368900	-2.02805700
	H	-5.73888700	-0.15752500	-1.48383500
	H	-3.90552300	-4.00054600	-0.87132500
4d'	N	-0.10566900	-1.03391400	0.04841300
	C	-0.17909400	-2.49365100	-0.14311000
	H	0.16851700	-2.98772700	0.76544800
	H	0.45299800	-2.79489900	-0.97749300
	H	-1.20151200	-2.78845100	-0.34701100
	O	0.73047800	-5.02162400	-1.75914900
	S	-0.31653000	-5.87141700	-1.13419000
	O	-0.59124700	-7.10867300	-1.89817400
	O	-1.54643300	-5.11269000	-0.78828200
	C	0.38785800	-6.39810900	0.42974100
	H	0.66074900	-5.48742200	0.97330200
	H	1.31114200	-6.93264500	0.18299100
	C	-0.56246900	-7.26812600	1.23922800
	H	-1.47729600	-6.69955500	1.44243000
	C	0.06092300	-7.73998500	2.55090600
	H	-0.85138100	-8.13468900	0.63314900
	H	0.98341000	-8.29594400	2.33585900
	C	-0.88052700	-8.62101600	3.36867200
	H	0.35731200	-6.86866900	3.15026700
	H	-1.79967800	-8.06204800	3.59141700

C	-0.25767400	-9.11315500	4.67273400
H	-1.18455400	-9.48517200	2.76241900
H	0.66327200	-9.66908900	4.44810700
C	-1.19378800	-10.00047000	5.49058000
H	0.04543000	-8.24952700	5.28068800
H	-1.49836200	-10.85978600	4.87998000
H	-2.11145700	-9.44289100	5.71738000
C	-0.55407000	-10.49077700	6.78708100
H	0.35017900	-11.07190700	6.57866600
H	-1.23626800	-11.12473400	7.35982000
H	-0.26655000	-9.64670300	7.42225200
C	1.11301700	-0.45443000	0.28282200
C	1.24475400	0.90060100	0.48365200
H	2.23807300	1.28675900	0.66083400
C	0.10545100	1.74736300	0.45019700
N	0.20448900	3.06898900	0.64112100
C	-1.14259900	1.11923000	0.20064700
H	-2.06304100	1.68276900	0.15416200
C	-1.22129000	-0.24290600	0.00587000
C	1.50748800	3.67628700	0.89289700
C	-0.99022500	3.90589400	0.59593900
H	1.37696200	4.74904300	1.01300500
H	2.18833300	3.50046200	0.05475400
H	1.95368600	3.27515100	1.80787900
H	-1.47129300	3.84539100	-0.38491900
H	-0.70242600	4.93848700	0.77793300
H	-1.70677800	3.60392900	1.36573000
C	2.23303400	-1.33264400	0.30424900
C	3.10673000	-2.17161300	0.30077600
C	6.26047700	-4.10858700	0.75703200
C	5.88098900	-5.33676800	0.21575300
C	4.59687000	-5.51124500	-0.30081900
C	4.06784900	-3.22921500	0.27047100
C	5.35918200	-3.05153300	0.78675400
H	7.25978800	-3.97500100	1.15764200
H	4.30495700	-6.46688200	-0.72482600
C	3.68349200	-4.46409800	-0.27857700
H	6.58864700	-6.15919800	0.19492200
H	5.64272100	-2.09239400	1.20723800
H	2.68175300	-4.58785000	-0.68806000
C	-2.47317800	-0.87127500	-0.25333200
C	-3.51302100	-1.44661900	-0.48766100
C	-7.07894000	-2.33350900	-1.11445500
C	-6.96290000	-3.70406800	-1.34438900
C	-5.71440300	-4.32361000	-1.28932800
C	-4.69337300	-2.20074000	-0.77508700
C	-5.94835300	-1.57753700	-0.82980500
H	-8.05123200	-1.85345100	-1.15921000
H	-5.62774100	-5.39034400	-1.46870800

	C	-4.57404500	-3.58131400	-1.00579000
	H	-7.84828600	-4.29006200	-1.56871600
	H	-6.02608700	-0.51037500	-0.65013000
	H	-3.59544300	-4.05592300	-0.96078900
3e'	N	-0.11628600	-0.70669500	-0.06331900
	C	-0.22331800	-3.55188400	-0.72819900
	H	0.21690900	-3.47656500	0.26962400
	H	0.43098300	-3.07010000	-1.45006400
	H	-1.21118400	-3.09107200	-0.73601800
	O	-0.30938600	-4.93495500	-1.16045700
	S	-1.15690600	-5.94079200	-0.24170100
	O	-1.60640000	-6.99786100	-1.13353400
	O	-2.14299900	-5.17477400	0.51123900
	C	0.08296800	-6.58632700	0.88962700
	H	0.47424400	-5.69126000	1.39136000
	C	-0.62335000	-7.49170100	1.89524300
	H	0.11303700	-7.86397900	2.60905400
	H	-1.07314900	-8.34613100	1.38582000
	H	-1.39906600	-6.95375000	2.44202200
	C	1.17980400	-7.29849000	0.10653800
	H	1.64631900	-6.63893900	-0.62780000
	H	0.76968700	-8.16832400	-0.41081600
	H	1.94549100	-7.63899200	0.80643600
	C	1.07417300	-0.10217300	0.08192400
	C	1.27129800	1.27510300	0.04976500
	H	2.27196800	1.66564400	0.17664900
	C	0.16193400	2.12607600	-0.15361500
	N	0.29339100	3.47605400	-0.19693900
	C	-1.09190300	1.49524400	-0.31335500
	H	-1.99828200	2.06166100	-0.47957300
	C	-1.16621100	0.10615600	-0.25965000
	C	1.60634900	4.08060800	-0.04855100
	C	-0.87392800	4.30908900	-0.43052600
	H	1.50699000	5.16258300	-0.11285900
	H	2.29040600	3.74967100	-0.83830400
	H	2.05080800	3.83324200	0.92209800
	H	-1.33819100	4.08540700	-1.39797400
	H	-0.56914200	5.35397200	-0.43082000
	H	-1.62523500	4.17094100	0.35477900
	C	2.19522400	-0.98616800	0.27296000
	C	3.11296400	-1.76292000	0.42185500
	C	6.47551900	-3.25070300	1.06996900
	C	6.19981100	-4.60759400	0.90429100
	C	4.90844100	-5.02282500	0.57941000
	C	4.16671300	-2.71935000	0.58723000
	C	5.46693200	-2.30678200	0.91302000
	H	7.48003500	-2.92683200	1.32227700
	H	4.69154700	-6.07846700	0.44842900
	C	3.89457400	-4.08619200	0.42101100

	H	6.98994800	-5.34103300	1.02799400
	H	5.67401300	-1.24920600	1.04065900
	H	2.88648300	-4.39757400	0.16484500
	C	-2.43972500	-0.54549200	-0.42650600
	C	-3.50079200	-1.11364300	-0.56538600
	C	-7.10483400	-1.75720500	-1.27332200
	C	-7.17558100	-3.13411300	-1.06558100
	C	-6.03408000	-3.84288000	-0.69195800
	C	-4.74822600	-1.79804800	-0.73336600
	C	-5.89844300	-1.08779700	-1.10868300
	H	-7.99160400	-1.20342000	-1.56358500
	H	-6.08833100	-4.91444400	-0.52994700
	C	-4.82154800	-3.18390000	-0.52451800
	H	-8.11942000	-3.65330900	-1.19514900
	H	-5.83452900	-0.01663300	-1.26860800
	H	-3.93011500	-3.73156200	-0.23044400
TS-e'	N	-0.05234400	-0.59145300	-0.27475100
	C	-0.08313500	-2.61511400	-0.47026100
	H	0.16288000	-2.68834800	0.57677500
	H	0.69997100	-2.51621400	-1.20476100
	H	-1.11703600	-2.56030200	-0.77140200
	O	0.01817600	-4.47152500	-0.71417200
	S	-0.91289900	-5.32833300	0.14978800
	O	-1.81832300	-6.13298800	-0.68383000
	O	-1.57025100	-4.50183700	1.17822700
	C	0.21112900	-6.45250500	0.99728900
	H	0.86229400	-5.78413000	1.57282800
	C	-0.59491000	-7.34746400	1.93214200
	H	0.08492800	-7.98879200	2.49795800
	H	-1.27019800	-7.98304500	1.35267900
	H	-1.18424500	-6.75515500	2.63471700
	C	1.02357400	-7.24390300	-0.02050100
	H	1.59396000	-6.58243100	-0.67731800
	H	0.36124100	-7.85958000	-0.63567600
	H	1.71777400	-7.90451700	0.50620200
	C	1.13531500	0.01363100	-0.07340400
	C	1.29127500	1.38985700	-0.02779700
	H	2.28042300	1.79369100	0.13727300
	C	0.16049400	2.22577600	-0.19484500
	N	0.26305900	3.57194400	-0.16813000
	C	-1.08410200	1.57781500	-0.38288200
	H	-2.00446800	2.13304200	-0.49900500
	C	-1.13885700	0.19192000	-0.41256700
	C	1.56127100	4.19774100	0.03398200
	C	-0.92416400	4.39447300	-0.34548400
	H	1.43616700	5.27832100	0.02868500
	H	2.25989200	3.92636000	-0.76463500
	H	1.99588500	3.90509500	0.99559600
	H	-1.39546300	4.20410200	-1.31559200

	H	-0.63612000	5.44279800	-0.30426000
	H	-1.65877000	4.20636200	0.44462900
	C	2.24835600	-0.87510900	0.11032200
	C	3.08191400	-1.73944700	0.26819400
	C	6.14910200	-3.76536000	0.93931700
	C	5.63500600	-5.05434700	0.80823900
	C	4.28907700	-5.24229600	0.49375700
	C	3.97121200	-2.84713500	0.44695200
	C	5.32371200	-2.66089600	0.76091900
	H	7.19622600	-3.61946100	1.18230200
	H	3.88944000	-6.24599000	0.38968200
	C	3.45462300	-4.14687400	0.31087300
	H	6.28329400	-5.91268700	0.95048000
	H	5.71595000	-1.65496600	0.86427600
	H	2.40425100	-4.28222600	0.05927500
	C	-2.39193200	-0.49024400	-0.57663800
	C	-3.40876200	-1.13830700	-0.69103500
	C	-6.87280300	-2.32319900	-1.42091400
	C	-6.75756900	-3.67269000	-1.08905100
	C	-5.54548000	-4.17687800	-0.61810200
	C	-4.55975800	-1.98140400	-0.81813900
	C	-5.77941500	-1.47515300	-1.28884500
	H	-7.81623800	-1.93120600	-1.78602900
	H	-5.45410000	-5.22684300	-0.35922900
	C	-4.44584000	-3.33897200	-0.47816200
	H	-7.61315300	-4.33154600	-1.19602000
	H	-5.85812400	-0.42495300	-1.54950100
	H	-3.50191200	-3.72170300	-0.09832400
4e'	N	-0.08959500	-0.51368600	-0.55721300
	C	-0.21040600	-1.96224900	-0.81690500
	H	-0.41281800	-2.50574400	0.10823700
	H	0.71485500	-2.31919800	-1.25666300
	H	-1.02768600	-2.12505800	-1.51553600
	O	0.10807900	-4.84125100	-0.91894500
	S	-0.78882600	-5.37466100	0.14111100
	O	-1.84443200	-6.27087600	-0.38807100
	O	-1.32826800	-4.31065600	1.02912000
	C	0.27284500	-6.39007600	1.19290400
	H	1.03838800	-5.68963600	1.54931800
	C	-0.52702600	-6.93833100	2.36717900
	H	0.12494400	-7.52016800	3.02428700
	H	-1.32367900	-7.59285600	2.00080200
	H	-0.97767300	-6.12950600	2.94461700
	C	0.91904700	-7.49036400	0.36140400
	H	1.46319300	-7.07021400	-0.48805600
	H	0.15156600	-8.16889900	-0.02276200
	H	1.61428000	-8.06680900	0.97847100
	C	1.12520600	0.03111900	-0.23926500
	C	1.27488700	1.38363500	-0.02920100



	H	2.26271400	1.74494100	0.21717100
	C	0.15785400	2.25569400	-0.11570200
	N	0.28092600	3.57731800	0.06262600
	C	-1.10153400	1.64955100	-0.36705700
	H	-2.01686000	2.22299600	-0.38233600
	C	-1.19709400	0.29070500	-0.56713700
	C	1.58271000	4.15471000	0.38068400
	C	-0.89325400	4.43986600	-0.02050900
	H	1.47123800	5.23078600	0.48925500
	H	2.30199000	3.95825000	-0.41959500
	H	1.97172900	3.74929200	1.31975400
	H	-1.38652400	4.32717200	-0.99008600
	H	-0.57569300	5.47446100	0.08575300
	H	-1.60879800	4.20951300	0.77504500
	C	2.20922400	-0.88067600	-0.09058800
	C	3.02288600	-1.76628700	0.05470000
	C	6.04490100	-3.84930700	0.72363200
	C	5.50189700	-5.12716100	0.59552500
	C	4.15247900	-5.28915100	0.28084600
	C	3.88686300	-2.89186200	0.22955700
	C	5.24278900	-2.72892600	0.54340100
	H	7.09489000	-3.72561900	0.96604800
	H	3.73367400	-6.28538700	0.17963400
	C	3.33793800	-4.17914000	0.09308700
	H	6.13197400	-5.99868000	0.74032500
	H	5.65407500	-1.73043100	0.64512700
	H	2.28474600	-4.29693200	-0.16129100
	C	-2.45018200	-0.36281400	-0.74558200
	C	-3.43720900	-1.05630600	-0.85587000
	C	-6.79335800	-2.53729800	-1.54757900
	C	-6.54333700	-3.87412400	-1.23737300
	C	-5.28162600	-4.26803800	-0.79172700
	C	-4.51591300	-1.98723400	-0.97602900
	C	-5.78440200	-1.58979600	-1.41986000
	H	-7.77583000	-2.23294100	-1.89232300
	H	-5.08443000	-5.30731300	-0.54993300
	C	-4.26356600	-3.33228200	-0.65663900
	H	-7.33393700	-4.60992600	-1.34330500
	H	-5.96703400	-0.54865200	-1.66363800
	H	-3.28099800	-3.62889000	-0.29504600
3f'	N	-0.10655400	-0.81862300	-0.38941500
	C	-0.14426000	-3.71364000	-0.68311800
	H	0.52486800	-3.34476300	0.09921700
	H	0.23259400	-3.39720100	-1.65497500
	H	-1.15792600	-3.33808300	-0.53075800
	O	-0.13598800	-5.16270600	-0.71500000
	S	-0.89145200	-5.91170500	0.48790000
	O	-0.77323900	-7.32587300	0.16848700
	O	-2.21892500	-5.32448400	0.63632800

C	0.11029100	-5.53127100	1.93740700
H	-0.02794300	-4.45243500	2.08755000
C	-0.45078000	-6.30678900	3.14067000
H	0.34240900	-6.31656100	3.89581100
H	-0.60083800	-7.35166800	2.84194500
C	-1.72446500	-5.72278800	3.74912100
H	-1.55644500	-4.68830000	4.06628500
H	-2.02025600	-6.30203600	4.62731400
H	-2.55320900	-5.72905900	3.03785500
C	1.58629700	-5.84757500	1.65748000
H	1.84083600	-5.57587400	0.62879000
H	1.73466600	-6.92978000	1.74974900
C	2.50953700	-5.08526300	2.60677100
H	2.38486000	-4.00440900	2.47727200
H	3.55464600	-5.32561700	2.39020600
H	2.31450000	-5.32962600	3.65474200
C	1.06849600	-0.22485200	-0.12868200
C	1.24523100	1.14685700	0.01830000
H	2.23504800	1.53022800	0.22595000
C	0.12710900	2.00241900	-0.10851100
N	0.23922100	3.34851900	0.02283100
C	-1.11420100	1.38110100	-0.37318800
H	-2.02724800	1.95265600	-0.47180200
C	-1.16750800	-0.00398700	-0.49832200
C	1.53078300	3.94067000	0.32615200
C	-0.93610600	4.19019300	-0.12302700
H	1.41321700	5.01889100	0.41669900
H	2.25941100	3.73859800	-0.46710200
H	1.93172800	3.55805800	1.27151600
H	-1.39426300	4.06347400	-1.11015100
H	-0.64055900	5.23213500	-0.01541700
H	-1.68883800	3.96383800	0.64079500
C	2.18560900	-1.12533900	0.01276600
C	3.06549800	-1.94733700	0.14582900
C	6.07388700	-3.78138100	1.37357000
C	5.96605600	-4.97646800	0.66159000
C	4.91476400	-5.16218700	-0.23686300
C	4.06991800	-2.95844600	0.30022100
C	5.13248500	-2.77396800	1.19610600
H	6.89219700	-3.63490700	2.07108700
H	4.82868500	-6.09149300	-0.79296200
C	3.96923300	-4.15904400	-0.42061000
H	6.70147900	-5.76116100	0.80535200
H	5.20657500	-1.84393100	1.75019300
H	3.14747800	-4.29551600	-1.11798200
C	-2.42461200	-0.66349400	-0.74478900
C	-3.45528600	-1.27114700	-0.93477700
C	-6.96222400	-2.11598600	-1.88912600
C	-6.99621800	-3.47857600	-1.59688200

	C	-5.86436300	-4.10931700	-1.08310200
	C	-4.66023800	-2.01500200	-1.15718200
	C	-5.80148100	-1.38320900	-1.67132700
	H	-7.84210600	-1.62352500	-2.28899700
	H	-5.88948200	-5.16930100	-0.85323500
	C	-4.69746900	-3.38670700	-0.86210300
	H	-7.90417500	-4.04731900	-1.76964500
	H	-5.76703700	-0.32289000	-1.89744100
	H	-3.81561800	-3.87462000	-0.45676900
TS-f'	N	-0.02460000	-0.79888300	-0.29747800
	C	0.04392900	-2.82437900	-0.40658100
	H	0.49263700	-2.81451900	0.57459100
	H	0.67874400	-2.72344100	-1.27271000
	H	-1.02979900	-2.86347900	-0.51092800
	O	0.23238200	-4.68756100	-0.56613700
	S	-0.69420700	-5.54228200	0.30349500
	O	-0.82499800	-6.88941400	-0.26534100
	O	-1.95831100	-4.82621100	0.55494600
	C	0.18332300	-5.70104400	1.87151700
	H	0.41178200	-4.66624200	2.16192300
	C	-0.71464200	-6.36315000	2.92623800
	H	-0.05467900	-6.81231400	3.67623000
	H	-1.24493100	-7.19864100	2.45272700
	C	-1.69350700	-5.42100500	3.62140700
	H	-1.15474600	-4.60700500	4.11688000
	H	-2.26381400	-5.95752200	4.38420300
	H	-2.39132800	-4.98398000	2.90611500
	C	1.48740600	-6.47482000	1.64115400
	H	1.91967500	-6.18527600	0.67792300
	H	1.24833200	-7.54177700	1.57482200
	C	2.50777600	-6.21457200	2.74676900
	H	2.79028600	-5.15727600	2.76756500
	H	3.41672700	-6.79767100	2.57713900
	H	2.11703600	-6.48222000	3.73276100
	C	1.12573600	-0.13449200	-0.06597600
	C	1.21119800	1.24694000	0.00166000
	H	2.17639900	1.69551200	0.19113200
	C	0.04410400	2.02791500	-0.17752000
	N	0.07569000	3.37652800	-0.11912800
	C	-1.15701500	1.31942800	-0.41769400
	H	-2.09968900	1.82812100	-0.56370500
	C	-1.14207800	-0.06817200	-0.46637000
	C	1.33350700	4.06358300	0.13387400
	C	-1.15053000	4.14001100	-0.29565600
	H	1.15342500	5.13645500	0.14251500
	H	2.06861000	3.84339200	-0.64743400
	H	1.75395700	3.77555800	1.10336100
	H	-1.58803400	3.96403700	-1.28407700
	H	-0.92227800	5.19995600	-0.20523800

	H	-1.89154100	3.87994400	0.46782000
	C	2.28853200	-0.95609500	0.11727600
	C	3.19203300	-1.74829800	0.26570000
	C	6.39616000	-3.51666900	1.01373800
	C	6.03537800	-4.83028900	0.71586300
	C	4.74669200	-5.11844900	0.26725400
	C	4.17772600	-2.77468200	0.41966200
	C	5.47377100	-2.48689900	0.86738200
	H	7.39933000	-3.29435100	1.36171600
	H	4.46619600	-6.14132100	0.03482300
	C	3.81563100	-4.09735300	0.11783800
	H	6.75993100	-5.62934900	0.83297500
	H	5.74501900	-1.46235400	1.09854300
	H	2.80564400	-4.30710000	-0.22818000
	C	-2.36538800	-0.78300100	-0.69931700
	C	-3.40373300	-1.37875200	-0.88386700
	C	-6.94237000	-2.10667600	-1.79476300
	C	-7.00654800	-3.47540200	-1.53588400
	C	-5.88314500	-4.15068200	-1.06060300
	C	-4.62709900	-2.09045400	-1.10464400
	C	-5.75839300	-1.41173700	-1.58109900
	H	-7.81639700	-1.58021600	-2.16366200
	H	-5.93498800	-5.21540900	-0.85810700
	C	-4.69174400	-3.46775700	-0.84288900
	H	-7.93302400	-4.01465900	-1.70441000
	H	-5.69819500	-0.34689000	-1.77977200
	H	-3.81185100	-3.98349000	-0.46696600
4f'	N	-0.18544000	-0.80961900	-0.12439500
	C	-0.30970300	-2.27442500	-0.03277800
	H	-0.30988900	-2.57090800	1.02082000
	H	0.52315100	-2.75061200	-0.55068000
	H	-1.23612700	-2.59634000	-0.49454300
	O	0.96713900	-5.07785900	-1.22043000
	S	-0.13793600	-5.72264100	-0.46070000
	O	-0.30869500	-7.15864000	-0.78454600
	O	-1.41042600	-4.95834300	-0.54613900
	C	0.38913900	-5.66608500	1.27082600
	H	0.72031500	-4.62877700	1.42477500
	C	-0.77402100	-6.00096800	2.21254400
	H	-0.35359400	-6.41034000	3.13807600
	H	-1.35958700	-6.81191300	1.76182600
	C	-1.67028900	-4.81291900	2.55474000
	H	-1.09109000	-4.03074400	3.05858900
	H	-2.47820900	-5.11383900	3.22776300
	H	-2.10925700	-4.38758000	1.64900500
	C	1.58921100	-6.60188200	1.45420900
	H	2.24904800	-6.51019200	0.58452600
	H	1.22603800	-7.63593000	1.46592600
	C	2.38198400	-6.29517400	2.72311100

	H	2.75486400	-5.26561300	2.70618800
	H	3.24614100	-6.96042300	2.80932700
	H	1.77452900	-6.42002100	3.62454000
	C	1.03271200	-0.21744200	0.07260700
	C	1.19076500	1.14823400	0.01134700
	H	2.18255400	1.54520800	0.17205600
	C	0.08063000	1.99220700	-0.25708000
	N	0.20977600	3.32284000	-0.33057000
	C	-1.17284700	1.35075600	-0.43711400
	H	-2.07604300	1.90984700	-0.63433200
	C	-1.27888400	-0.02032400	-0.36002900
	C	1.51687100	3.94305900	-0.13793800
	C	-0.95536700	4.15761300	-0.60593500
	H	1.41170100	5.02054600	-0.23954500
	H	2.22983200	3.59122400	-0.88931900
	H	1.91031300	3.72411800	0.85943200
	H	-1.39099000	3.91055100	-1.57885100
	H	-0.64504800	5.19990000	-0.62008000
	H	-1.71650800	4.03217000	0.16996800
	C	2.13082200	-1.08224900	0.34885900
	C	3.01906100	-1.87682700	0.56004000
	C	6.16908800	-3.51252000	1.69592800
	C	5.98496500	-4.80028600	1.18982700
	C	4.82887800	-5.11659900	0.47700000
	C	4.03594000	-2.85906200	0.77694800
	C	5.20052800	-2.53831100	1.49047900
	H	7.06884700	-3.26769700	2.25061500
	H	4.68979000	-6.11983400	0.08477600
	C	3.84700000	-4.15433000	0.26721400
	H	6.74485800	-5.55771500	1.35070500
	H	5.33253000	-1.53383500	1.87968400
	H	2.93513200	-4.39300600	-0.27921600
	C	-2.53744200	-0.67179400	-0.50531400
	C	-3.57233900	-1.29281900	-0.59659200
	C	-7.14225400	-2.33577900	-0.84115900
	C	-7.00328400	-3.72310800	-0.83001800
	C	-5.73713500	-4.30290300	-0.74994300
	C	-4.74565200	-2.10529900	-0.68601100
	C	-6.01776600	-1.52252100	-0.76960500
	H	-8.12799800	-1.88761500	-0.90566700
	H	-5.63324400	-5.38263000	-0.74310200
	C	-4.60278500	-3.50277900	-0.67786800
	H	-7.88465400	-4.35420400	-0.88295800
	H	-6.11277800	-0.44215000	-0.77543300
	H	-3.61037700	-3.94524800	-0.61889000
3g'	N	-0.11972300	-1.01715500	-0.08761100
	C	-0.15178900	-3.89520700	-0.57975200
	H	0.44905700	-3.52971200	0.25361300
	H	0.27565400	-3.54036100	-1.51530100

H	-1.18389800	-3.55316600	-0.48933000
O	-0.09071100	-5.34232800	-0.63836700
S	-1.02260100	-6.13728300	0.40158600
O	-0.71085700	-7.53915200	0.17653900
O	-2.39808800	-5.68185100	0.23228000
C	-0.40431600	-5.62392000	2.01217200
H	-0.60168100	-4.54391400	2.05033300
C	-1.21193200	-6.34272200	3.10531000
H	-0.58289200	-6.34900700	4.00439000
H	-1.33861900	-7.39615300	2.82004900
C	-2.56054800	-5.70987000	3.44522100
H	-2.39105900	-4.67287800	3.76014400
C	-3.27360500	-6.48027600	4.55385200
H	-3.18986400	-5.66987800	2.55108200
H	-3.49075800	-7.50620500	4.23807000
H	-4.22044900	-6.00376000	4.81968500
H	-2.65573900	-6.53287400	5.45693000
C	1.10250000	-5.89863100	2.10888500
H	1.58962800	-5.76607300	1.13658600
H	1.24638400	-6.94755100	2.39681700
C	1.77163600	-4.96367300	3.11907900
H	1.73994700	-3.94110500	2.72037400
C	3.21484600	-5.36825400	3.39866900
H	1.20090400	-4.95057200	4.05573400
H	3.25755600	-6.36524700	3.85188500
H	3.69881700	-4.66538000	4.08485400
H	3.79550400	-5.39386700	2.47178100
C	1.08116400	-0.45912400	0.13385800
C	1.31392900	0.90956100	0.21299800
H	2.32062800	1.26293800	0.39070100
C	0.22951400	1.80202400	0.05123700
N	0.39641700	3.14718900	0.11584000
C	-1.03731200	1.21928200	-0.17914200
H	-1.92621900	1.82145700	-0.31000400
C	-1.14725900	-0.16693500	-0.23540200
C	1.72056800	3.70191200	0.34038900
C	-0.73981300	4.02821400	-0.09395600
H	1.64654700	4.78680300	0.38529200
H	2.41032700	3.43458600	-0.46860900
H	2.14217000	3.34790500	1.28743800
H	-1.18497100	3.87752000	-1.08399400
H	-0.40384300	5.06098500	-0.02305300
H	-1.51470400	3.86587600	0.66341800
C	2.16363300	-1.39955200	0.28322200
C	3.00803100	-2.26311100	0.37726500
C	6.07863300	-4.24579000	1.15797600
C	5.79356900	-5.43899300	0.49495000
C	4.59019900	-5.58383800	-0.19516300
C	3.96019100	-3.33294500	0.43527300

	C	5.16937400	-3.19398800	1.13092800
	H	7.01358900	-4.13370800	1.69712500
	H	4.36410200	-6.51189000	-0.70987800
	C	3.67543000	-4.53779100	-0.22754600
	H	6.50660200	-6.25645100	0.51883900
	H	5.38574400	-2.26300300	1.64438000
	H	2.73755000	-4.64249600	-0.76592000
	C	-2.43004500	-0.78464500	-0.45493100
	C	-3.48984300	-1.33713700	-0.65354100
	C	-7.07606400	-1.98030000	-1.45953100
	C	-7.14427300	-3.36171900	-1.28310400
	C	-6.00721100	-4.07273500	-0.90096100
	C	-4.73121600	-2.02011200	-0.86963000
	C	-5.87697800	-1.30800800	-1.25417400
	H	-7.95950400	-1.42493400	-1.75676600
	H	-6.05809000	-5.14799500	-0.76331700
	C	-4.80224100	-3.41100800	-0.69387900
	H	-8.08242300	-3.88286300	-1.44382600
	H	-5.81616400	-0.23311600	-1.38884100
	H	-3.91584700	-3.96344200	-0.39552100
TS-g'	N	-0.08619200	-1.14684300	-0.17710500
	C	-0.17363700	-3.15995400	-0.32938700
	H	0.44405600	-3.19567600	0.55347800
	H	0.30111600	-3.09023000	-1.29573400
	H	-1.25146700	-3.12511700	-0.25272700
	O	-0.12470100	-5.03172400	-0.48843200
	S	-1.03675600	-5.79537500	0.47515500
	O	-0.90580800	-7.23994000	0.24916100
	O	-2.40589400	-5.25069400	0.41537800
	C	-0.37750200	-5.43291500	2.11598800
	H	-0.51737300	-4.34911600	2.22828800
	C	-1.17447000	-6.16840600	3.20016700
	H	-0.54978900	-6.17398900	4.10283400
	H	-1.28208600	-7.21837800	2.89787500
	C	-2.53675000	-5.57325600	3.55224300
	H	-2.40297300	-4.51870100	3.82513300
	C	-3.19432800	-6.32512700	4.70647400
	H	-3.18462400	-5.58859500	2.67208500
	H	-3.35136200	-7.37700600	4.44710700
	H	-4.16628400	-5.89416600	4.95999200
	H	-2.56769600	-6.29452400	5.60367000
	C	1.11664200	-5.77727300	2.17134000
	H	1.57947900	-5.63433100	1.18924300
	H	1.22137600	-6.84034500	2.42221800
	C	1.86376100	-4.91508100	3.19023400
	H	1.87000900	-3.87626800	2.83300100
	C	3.29580500	-5.39424500	3.40852500
	H	1.32507500	-4.91046200	4.14620700
	H	3.30468500	-6.40144800	3.83719500

	H	3.83797600	-4.73255400	4.08939700
	H	3.84415400	-5.42741000	2.46165900
	C	1.10601500	-0.57542500	0.08900600
	C	1.28217800	0.79102700	0.23591100
	H	2.27485400	1.16465300	0.44527300
	C	0.16959400	1.65654500	0.10285500
	N	0.29058600	2.99447600	0.23623000
	C	-1.07538300	1.04472500	-0.17589800
	H	-1.98208800	1.62271500	-0.28864200
	C	-1.15278200	-0.33530300	-0.30365600
	C	1.58770300	3.58001000	0.54039800
	C	-0.87676200	3.84885700	0.07703100
	H	1.47436300	4.65798800	0.63360600
	H	2.31213300	3.37546000	-0.25512200
	H	1.98375100	3.19222800	1.48474700
	H	-1.31922400	3.73078500	-0.91756900
	H	-0.57263800	4.88664200	0.19604200
	H	-1.63948000	3.62285200	0.82994200
	C	2.21480900	-1.48017000	0.21198800
	C	3.07111100	-2.33280500	0.29359900
	C	6.14594400	-4.34112300	0.97777700
	C	5.80000200	-5.54976300	0.37441800
	C	4.55845300	-5.69348700	-0.24526000
	C	4.01183600	-3.41142900	0.33671900
	C	5.25864800	-3.27086900	0.96118600
	H	7.11088500	-4.23120200	1.46116100
	H	4.28669800	-6.63487600	-0.71105000
	C	3.66299500	-4.63091700	-0.26608500
	H	6.49699000	-6.38116600	0.38889900
	H	5.52062100	-2.32690600	1.42703900
	H	2.68867900	-4.73398500	-0.73680000
	C	-2.41887800	-0.95455100	-0.57799600
	C	-3.49141300	-1.47105100	-0.80251600
	C	-7.06938900	-1.93065600	-1.73775800
	C	-7.20201700	-3.31228400	-1.60481400
	C	-6.11219200	-4.08423900	-1.20440000
	C	-4.75261600	-2.09471600	-1.07188400
	C	-5.85028000	-1.31865600	-1.47284800
	H	-7.91743200	-1.32926300	-2.04762200
	H	-6.21773600	-5.15907600	-1.09921400
	C	-4.88660900	-3.48508400	-0.93615600
	H	-8.15570200	-3.78702200	-1.81142100
	H	-5.73637900	-0.24446000	-1.57418000
	H	-4.03457900	-4.07873600	-0.61650200
4g'	N	-0.27779400	-0.93805200	0.06275700
	C	-0.40658900	-2.39747600	0.20323900
	H	-0.21555300	-2.66592500	1.24511800
	H	0.31318900	-2.90158000	-0.44326200
	H	-1.40622000	-2.70985700	-0.07581200



O	0.68666400	-5.34201500	-0.97739200
S	-0.44454000	-5.88298800	-0.17620800
O	-0.67865800	-7.32865300	-0.39630400
O	-1.68104300	-5.07015100	-0.31885200
C	0.08350700	-5.72561700	1.54910700
H	0.47532800	-4.70242000	1.62376100
C	-1.10521700	-5.91271800	2.49891400
H	-0.73242100	-6.32200700	3.44653500
H	-1.77185900	-6.67823300	2.08084500
C	-1.89227100	-4.63626500	2.79302100
H	-1.21849200	-3.90694700	3.26244800
C	-3.08540200	-4.89790500	3.70881800
H	-2.23037000	-4.19987600	1.84710800
H	-3.79032300	-5.59336500	3.23985900
H	-3.62685400	-3.97444800	3.93652200
H	-2.76184800	-5.34235000	4.65596100
C	1.22756700	-6.70599000	1.82147100
H	1.88932300	-6.74352700	0.94784400
H	0.80809300	-7.71140700	1.94460100
C	2.05202000	-6.32020400	3.04876700
H	2.51201900	-5.33969200	2.87113400
C	3.13796400	-7.34698300	3.35887100
H	1.39772000	-6.20451500	3.92191500
H	2.69984000	-8.32888800	3.56272900
H	3.72875000	-7.05340600	4.23010300
H	3.82228300	-7.45642700	2.51079000
C	0.95452700	-0.35872400	0.20862000
C	1.12641700	1.00404300	0.12615600
H	2.12745300	1.39172400	0.24675600
C	0.01665200	1.85691900	-0.11511600
N	0.15615700	3.18566900	-0.20095600
C	-1.24762700	1.22713000	-0.25923300
H	-2.14863900	1.79354400	-0.44426500
C	-1.36780100	-0.14165800	-0.16307500
C	1.47296200	3.79562000	-0.04456200
C	-1.00690600	4.02866000	-0.45836700
H	1.37264400	4.87462900	-0.13713400
H	2.16148800	3.44232600	-0.81832600
H	1.89256600	3.56890300	0.94029800
H	-1.46484000	3.77805800	-1.42020300
H	-0.68755800	5.06779000	-0.48735300
H	-1.75304300	3.91630600	0.33404000
C	2.04396100	-1.24418800	0.44706300
C	2.90164400	-2.07867600	0.63581200
C	6.00543800	-3.88429300	1.63969600
C	5.70799300	-5.17023900	1.18702300
C	4.49255200	-5.42837400	0.55253700
C	3.86639100	-3.11618400	0.82858200
C	5.09164200	-2.85319600	1.45944600

	H	6.95286000	-3.68536700	2.13038500
	H	4.26656600	-6.42875100	0.19454400
	C	3.56236400	-4.41022000	0.37363400
	H	6.42667500	-5.97119700	1.32698600
	H	5.31391100	-1.84846700	1.80396900
	H	2.60602600	-4.60783500	-0.11046800
	C	-2.63571400	-0.77945800	-0.28433700
	C	-3.68501800	-1.36956800	-0.41566100
	C	-7.25962900	-2.35734400	-0.78744700
	C	-7.14027300	-3.74689100	-0.76827000
	C	-5.88662400	-4.34468600	-0.63552600
	C	-4.86831100	-2.16127700	-0.53954500
	C	-6.12799000	-1.55983700	-0.67371000
	H	-8.23554600	-1.89500600	-0.89209600
	H	-5.79756400	-5.42602000	-0.62245900
	C	-4.74518300	-3.56095000	-0.52121300
	H	-8.02705600	-4.36564700	-0.85602000
	H	-6.20803000	-0.47797700	-0.68650800
	H	-3.76235400	-4.01870300	-0.42420800
3h'	N	-0.18873400	-1.23975900	-0.18511100
	C	-0.50196800	-4.14326400	-0.62671900
	H	0.33531600	-3.85511500	0.01188200
	H	-0.27243000	-3.90411100	-1.66320000
	H	-1.41272000	-3.62613500	-0.32131200
	O	-0.68727300	-5.58137100	-0.58280600
	S	-1.55437700	-6.15727300	0.63947800
	O	-1.57850800	-7.59589000	0.42880000
	O	-2.81785600	-5.43078600	0.70159500
	C	-0.55143500	-5.76638700	2.08052100
	H	-0.44796500	-4.67286500	2.05410400
	C	-1.30106800	-6.19171800	3.35380400
	H	-0.54023800	-6.31729000	4.13350600
	H	-1.73605500	-7.18797100	3.19534500
	C	-2.36180800	-5.20947100	3.84710800
	H	-1.89278200	-4.22921400	4.00734600
	C	-3.01530300	-5.67669500	5.14658300
	H	-3.12940000	-5.06964600	3.07920600
	H	-3.47380600	-6.66030400	4.98531200
	C	-4.06838500	-4.69384300	5.65245800
	H	-2.24170300	-5.81777300	5.91148500
	C	0.82048700	-6.43875600	1.94493900
	H	1.13797600	-6.46274700	0.89619000
	H	0.72943700	-7.48089600	2.27399600
	C	1.88574300	-5.70638300	2.76125500
	H	2.08596800	-4.73255000	2.29111800
	C	3.18565600	-6.50114600	2.85588500
	H	1.51570000	-5.49370800	3.77339200
	H	3.00037600	-7.42500900	3.41761900
	C	4.30532000	-5.70059200	3.51140500

H	3.49378400	-6.80556600	1.84809000
C	0.98235300	-0.69316300	0.17773900
C	1.17835000	0.66079000	0.43620600
H	2.16416600	1.00219000	0.72151700
C	0.08804400	1.55110700	0.31661300
N	0.22079000	2.88168100	0.54882100
C	-1.14903200	0.97952100	-0.05571500
H	-2.04394600	1.57791700	-0.16113100
C	-1.22442800	-0.39106200	-0.28611600
C	1.51167600	3.42388500	0.93727900
C	-0.92916800	3.75864900	0.40655800
H	1.41525300	4.49873400	1.08055100
H	2.26812700	3.24632100	0.16447900
H	1.86409700	2.98228100	1.87651300
H	-1.33966100	3.71386400	-0.60862200
H	-0.62021600	4.78343700	0.60534900
H	-1.72340300	3.49435700	1.11431000
C	2.09469700	-1.60248800	0.28933500
C	3.02717800	-2.37018100	0.38598800
C	6.45668800	-3.67903900	1.05132700
C	6.33760600	-4.98906500	0.58840300
C	5.12411600	-5.43721400	0.06861200
C	4.14518400	-3.26240700	0.47212800
C	5.36928600	-2.81534600	0.99381500
H	7.40033200	-3.32805200	1.45591000
H	5.02938700	-6.45565300	-0.29396500
C	4.02857600	-4.58262000	0.01236800
H	7.18965800	-5.65936800	0.63206700
H	5.45565500	-1.79339100	1.34728200
H	3.07997700	-4.92420300	-0.39222800
C	-2.48624600	-0.98152200	-0.65393300
C	-3.53983200	-1.49609800	-0.95848300
C	-7.02011400	-1.98276000	-2.21144500
C	-7.18362900	-3.35332600	-2.01509700
C	-6.14679400	-4.10831000	-1.46846100
C	-4.77831400	-2.12297800	-1.31615700
C	-5.82399200	-1.36566100	-1.86438600
H	-7.82624400	-1.39347700	-2.63608800
H	-6.27438700	-5.17461500	-1.31274900
C	-4.94573000	-3.50211000	-1.11810500
H	-8.11870800	-3.83235600	-2.28670100
H	-5.68803000	-0.29977500	-2.01448600
H	-4.13861900	-4.08425700	-0.68248700
H	-4.52986500	-5.04372700	6.57993500
H	-4.86157600	-4.55879400	4.91070700
H	-3.62362200	-3.71223200	5.84600300
H	4.50179700	-4.78264900	2.94682100
H	5.23619200	-6.27275300	3.55190800
H	4.03592600	-5.41794800	4.53453600

TS-h'	N	-0.17514200	-1.28021500	-0.13125600
	C	-0.43236700	-3.28090500	-0.29803300
	H	0.46644000	-3.41461900	0.28538800
	H	-0.35652500	-3.18911400	-1.37064600
	H	-1.39697300	-3.16548300	0.17569400
	O	-0.63680000	-5.13896500	-0.49367400
	S	-1.50460700	-5.81737500	0.56790300
	O	-1.65003600	-7.24584400	0.26174600
	O	-2.75966000	-5.06536300	0.75742300
	C	-0.54451200	-5.67777400	2.08706700
	H	-0.42490900	-4.59548400	2.23416500
	C	-1.29829200	-6.28748200	3.27494500
	H	-0.55219700	-6.47911900	4.05702700
	H	-1.67917800	-7.27153800	2.97103900
	C	-2.42344000	-5.44218200	3.86811400
	H	-2.02570500	-4.45615300	4.14602600
	C	-3.04317200	-6.10078900	5.09877200
	H	-3.19489500	-5.26809600	3.11182400
	H	-3.42026100	-7.09418400	4.82384100
	C	-4.17447800	-5.26915600	5.69712600
	H	-2.26440300	-6.26498700	5.85448700
	C	0.82678000	-6.33610700	1.88870700
	H	1.14826300	-6.23829800	0.84618000
	H	0.72718600	-7.40929100	2.09335100
	C	1.89453000	-5.71689100	2.79044900
	H	2.12624100	-4.70691600	2.42105400
	C	3.17574200	-6.54578800	2.83387500
	H	1.50925600	-5.59203100	3.81136300
	H	2.96496200	-7.50539300	3.32221200
	C	4.30908900	-5.82390200	3.55551700
	H	3.48538800	-6.78102300	1.80825200
	C	1.01585000	-0.73018800	0.17420200
	C	1.21431100	0.63680600	0.30476000
	H	2.20563700	0.99167500	0.54991800
	C	0.13095300	1.52510700	0.10712200
	N	0.27670200	2.86240500	0.22127200
	C	-1.11288000	0.93505000	-0.21753200
	H	-2.00002200	1.52929200	-0.38688100
	C	-1.21481200	-0.44484900	-0.32137800
	C	1.57505000	3.42509900	0.56072700
	C	-0.86184100	3.73935000	-0.00876400
	H	1.48220600	4.50648700	0.63401800
	H	2.32170400	3.19261600	-0.20621500
	H	1.93058900	3.04395200	1.52355500
	H	-1.25829900	3.61536100	-1.02211100
	H	-0.54068000	4.77212600	0.11007500
	H	-1.66472100	3.54198600	0.70962000
	C	2.12829400	-1.62118000	0.35454500
	C	3.08711600	-2.34984500	0.48445100

	C	6.51423100	-3.61047200	1.24118400
	C	6.43118700	-4.91259500	0.74875700
	C	5.24275100	-5.37165700	0.18316800
	C	4.21731700	-3.22245800	0.59717600
	C	5.41495200	-2.76337300	1.16635300
	H	7.43903900	-3.25280900	1.68132100
	H	5.17664000	-6.38471800	-0.19991400
	C	4.13493800	-4.53486600	0.10914400
	H	7.29295400	-5.56938100	0.80531900
	H	5.47287300	-1.74698000	1.54086400
	H	3.20418800	-4.88325000	-0.32923100
	C	-2.48424600	-1.03401200	-0.64375700
	C	-3.56674400	-1.50921300	-0.90770400
	C	-7.08068400	-1.81084000	-2.10646900
	C	-7.33161300	-3.15991000	-1.85823800
	C	-6.34198800	-3.96271400	-1.29258600
	C	-4.84549800	-2.07095800	-1.22641400
	C	-5.84299500	-1.26321300	-1.79251000
	H	-7.85046000	-1.18463100	-2.54502200
	H	-6.54020700	-5.01146200	-1.09699500
	C	-5.09867400	-3.42802800	-0.97418800
	H	-8.29953500	-3.58477100	-2.10381600
	H	-5.63722300	-0.21510800	-1.98272500
	H	-4.32336800	-4.04313200	-0.52518800
	H	-4.61267300	-5.75559000	6.57253000
	H	-4.97182500	-5.11408300	4.96344700
	H	-3.81150500	-4.28371400	6.00612100
	H	4.53636600	-4.87495200	3.05653200
	H	5.22453200	-6.42203000	3.56768400
	H	4.03439400	-5.60326300	4.59263100
4h'	N	-0.28427400	-1.35555100	-0.04809900
	C	-0.44717100	-2.79518000	-0.32233700
	H	0.46440100	-3.31736700	-0.04899700
	H	-0.64108200	-2.94076400	-1.38596200
	H	-1.28936400	-3.18653700	0.24943100
	O	-0.53078100	-5.69319200	-0.71711100
	S	-1.41698700	-6.04887700	0.42053900
	O	-1.76428200	-7.48726300	0.47210400
	O	-2.60695000	-5.15660900	0.50600200
	C	-0.43901100	-5.72669800	1.90946100
	H	-0.19555900	-4.65667800	1.85311700
	C	-1.24327000	-6.01130000	3.18331900
	H	-0.52854600	-6.21075500	3.99261900
	H	-1.80289400	-6.94508200	3.03551200
	C	-2.18599900	-4.89530100	3.63299000
	H	-1.60780600	-3.96967100	3.77105000
	C	-2.90458000	-5.23737300	4.93666600
	H	-2.91736700	-4.69505900	2.84329600
	H	-3.46833200	-6.16963800	4.80141800

C	-3.84820000	-4.12805200	5.39657600
H	-2.16111000	-5.43848200	5.71896400
C	0.85735500	-6.54043200	1.84865800
H	1.21130700	-6.58202600	0.81235000
H	0.64197400	-7.57212200	2.15689800
C	1.96141200	-5.94219200	2.71756100
H	2.21287500	-4.94358400	2.33027500
C	3.22447900	-6.79858000	2.74345600
H	1.60599200	-5.79262000	3.74602100
H	2.99429100	-7.77106500	3.19665000
C	4.36339000	-6.12187100	3.49963800
H	3.53806400	-7.00374500	1.71205400
C	0.91733800	-0.82069800	0.32514000
C	1.06849700	0.53381700	0.53085100
H	2.04719600	0.88609700	0.82215800
C	-0.02295900	1.42314300	0.35219800
N	0.10733300	2.74462900	0.52119800
C	-1.26129300	0.83481900	-0.01327600
H	-2.15605000	1.42462900	-0.15046500
C	-1.36145900	-0.52527500	-0.20329900
C	1.39690200	3.31001100	0.90396400
C	-1.03673900	3.62550900	0.30758800
H	1.28951800	4.38662900	1.01018200
H	2.15377700	3.10891300	0.13996800
H	1.73463800	2.89938000	1.85991400
H	-1.42305900	3.52110200	-0.71050600
H	-0.71820500	4.65505100	0.45166100
H	-1.83788700	3.40554600	1.01953700
C	2.03299300	-1.69278000	0.49459400
C	3.02417300	-2.37953900	0.61180800
C	6.45933100	-3.64422400	1.31466800
C	6.39128900	-4.91428600	0.74359100
C	5.20892900	-5.35396100	0.14920400
C	4.16189200	-3.24466900	0.68542900
C	5.35135100	-2.80562300	1.28620000
H	7.37877700	-3.30448900	1.77950100
H	5.15537400	-6.34311700	-0.29287000
C	4.09134700	-4.52781300	0.12177800
H	7.26067800	-5.56309300	0.76391500
H	5.39730400	-1.81268800	1.72002800
H	3.16446900	-4.86070500	-0.33653100
C	-2.60148900	-1.12287700	-0.56552600
C	-3.65392900	-1.63483800	-0.87829700
C	-7.17131300	-2.10573100	-2.00280300
C	-7.27805600	-3.49488600	-1.94671800
C	-6.19247400	-4.26663900	-1.53407200
C	-4.88674800	-2.26240300	-1.23955300
C	-5.97938700	-1.48480100	-1.65130400
H	-8.01811100	-1.50675900	-2.31994700

	H	-6.28133200	-5.34666100	-1.48766200
	C	-4.99319800	-3.66060500	-1.17770800
	H	-8.21066800	-3.97660000	-2.22255400
	H	-5.88345700	-0.40529400	-1.69114000
	H	-4.14466600	-4.24891200	-0.83664500
	H	-4.35651500	-4.39135300	6.32845200
	H	-4.61410500	-3.93132800	4.63947700
	H	-3.30033200	-3.19443400	5.56404200
	H	4.59681200	-5.15087400	3.04867900
	H	5.27511900	-6.72567500	3.48468700
	H	4.08842200	-5.94977700	4.54554200
15-3a	O	-0.16278800	-5.23541400	-0.76160200
	C	-0.15453900	-3.80106500	-0.53163100
	H	0.22606400	-3.57190000	0.46584100
	H	0.52647300	-3.39486900	-1.27669400
	H	-1.15353400	-3.38536000	-0.66248400
	N	-0.00216500	-0.85649700	-0.23747200
	S	-1.17148900	-6.12883800	0.09779400
	O	-1.20365300	-7.41766800	-0.57328600
	O	-2.41348800	-5.39520800	0.29928000
	C	-0.34017900	-6.29668900	1.65475600
	H	-0.23744900	-5.31144600	2.10978100
	H	0.63216700	-6.75401000	1.47678900
	H	-0.96209700	-6.93775500	2.28029000
	C	1.16333700	-0.20386400	-0.10610500
	C	1.31073900	1.17884800	-0.15412900
	H	2.29922700	1.60253800	-0.03851600
	C	0.16761300	1.98759700	-0.31324400
	N	0.24938700	3.34397100	-0.34245800
	C	-1.06388100	1.31315400	-0.43956900
	H	-1.99488900	1.84448200	-0.58423400
	C	-1.08257100	-0.07814400	-0.41197300
	C	1.54777000	3.98924100	-0.26770500
	C	-0.96012600	4.13558500	-0.47571100
	H	1.41127500	5.06852600	-0.31018700
	H	2.19098700	3.68893800	-1.10372100
	H	2.06307400	3.74316800	0.66835300
	H	-1.48180800	3.91614500	-1.41497300
	H	-0.69686800	5.19187100	-0.46793500
	H	-1.65166100	3.94614200	0.35364800
	C	-6.89839100	-10.22836700	-1.81355100
	C	6.40798500	-1.51890900	-2.73938700
	C	5.14632400	-0.97348600	-2.94189200
	C	4.01142700	-1.80119700	-2.93951800
	C	5.43220600	-3.72099700	-2.51470700
	C	6.55787400	-2.88496300	-2.52688300
	H	7.28097500	-0.87492900	-2.74117400
	C	2.71570300	-1.22544200	-3.14616300
	C	1.63979700	-0.69323200	-3.31732800

C	-0.83160100	2.05526500	-3.78582900
C	-2.01769000	1.34280200	-3.92456700
C	-2.00775200	-0.05985800	-3.86433100
C	0.39366400	-0.01489700	-3.51788600
C	0.37050200	1.38709700	-3.58452900
H	-0.84316500	3.13911400	-3.83965800
C	-5.68488400	-10.89925600	-1.72368200
C	-4.49349700	-10.17714400	-1.54568600
C	-5.75990000	-8.10882000	-1.53828300
C	-6.94258600	-8.84036700	-1.72473200
H	-7.81724900	-10.78883800	-1.95355500
C	-3.24148800	-10.86894200	-1.48328200
C	-2.19144500	-11.47273600	-1.45000800
C	0.30390400	-14.24348300	-1.30235400
C	1.49885300	-13.53555600	-1.35112900
C	1.48094400	-12.13447800	-1.43404200
C	-0.94427500	-12.17482900	-1.41370400
C	-0.91525700	-13.57449700	-1.33410700
H	0.32186800	-15.32613800	-1.23376700
C	2.70074000	-11.38733900	-1.48629900
C	3.71787900	-10.73023500	-1.52994900
C	7.29314600	-9.65157800	-1.48188500
C	7.16336900	-8.28479300	-1.69861700
C	5.88944300	-7.71860300	-1.86553600
C	4.89229200	-9.91354200	-1.58613700
C	6.16891200	-10.46971700	-1.42647800
H	8.27934400	-10.08441700	-1.35091700
C	5.58742200	-5.12645100	-2.28774200
C	5.73602900	-6.31341200	-2.09355600
C	4.15930400	-3.17433500	-2.72142800
C	-0.79902300	-0.73387800	-3.65467300
C	-4.53467800	-8.78186900	-1.44505200
C	0.25730300	-11.45875100	-1.45976900
C	4.75837900	-8.53715700	-1.80351300
H	5.02453700	0.09192600	-3.10578800
H	7.53972300	-3.31489400	-2.36044400
H	-2.95715000	1.86036600	-4.08682300
H	1.29816900	1.93855600	-3.47020400
H	-5.64412100	-11.98070000	-1.79861300
H	-7.88782300	-8.31044000	-1.78752400
H	2.45058600	-14.05547200	-1.32610400
H	-1.84904800	-14.12463200	-1.28890600
H	8.03955300	-7.64679900	-1.74080100
H	6.26870800	-11.53550100	-1.25128900
H	3.28570200	-3.81749700	-2.70659600
H	-0.78822400	-1.81709100	-3.59406000
H	-3.61650000	-8.22236400	-1.29082900
H	0.23691200	-10.37501600	-1.50923900
H	3.77103900	-8.10392200	-1.92255600



C	-5.80731600	-6.68205100	-1.44001800
C	-5.85730800	-5.47367600	-1.36110800
C	-2.34075200	-0.75350100	-0.58575600
C	-3.41219300	-1.29709600	-0.74080300
C	-7.05583300	-1.94018700	-1.22865500
C	-7.07101500	-3.32570500	-1.33772700
C	-5.87108400	-4.04738500	-1.24530300
C	-4.65784100	-1.97393000	-0.93420900
C	-5.85854500	-1.25905500	-1.03272500
H	-7.98477000	-1.38443100	-1.30746200
C	-4.66728600	-3.36865000	-1.03875600
H	-8.00214700	-3.85665800	-1.50597600
H	-5.84430400	-0.17718000	-0.95038300
H	-3.74304800	-3.92979900	-0.94472200
C	-7.89167600	-2.04648200	-4.73288300
C	-4.25665400	-1.41201900	-4.19959500
C	-3.22627500	-0.79531500	-4.03312300
C	-7.91060300	-3.42704000	-4.89823200
C	-6.71649600	-4.16037900	-4.82655800
C	-5.49192800	-2.10542200	-4.41721100
C	-6.69288000	-1.38350900	-4.50095700
H	-8.81708900	-1.48331300	-4.79114700
C	-5.51035600	-3.49616500	-4.57434200
H	-8.84244800	-3.94671600	-5.09392100
H	-6.67291500	-0.30590000	-4.37640100
H	-4.58569700	-4.06028500	-4.51199300
C	-6.73216000	-5.57631700	-5.06498300
C	-6.76842600	-6.76784900	-5.31689500
Si	-6.83439200	-8.54455400	-5.83522900
C	-8.42955900	-9.30112500	-5.19784700
C	-5.33429600	-9.43383200	-5.15192000
C	-6.81433400	-8.58489900	-7.71351500
H	-9.30057000	-8.79952300	-5.62890100
H	-8.49559200	-9.23320000	-4.10927400
H	-8.47490100	-10.35931100	-5.47508800
H	-5.29306700	-9.35888500	-4.06214200
H	-4.41148600	-9.01386000	-5.56212700
H	-5.37362600	-10.49490800	-5.41903500
H	-5.89865800	-8.13420800	-8.10614500
H	-7.66882800	-8.04498600	-8.13074800
H	-6.86124800	-9.62005600	-8.06647400
C	6.29462000	-10.69679500	2.03626800
C	-6.36554000	-0.77810600	2.35295100
C	-5.06650700	-0.31256100	2.51459500
C	-3.99071000	-1.21528000	2.53253700
C	-5.54622700	-3.04995400	2.22611100
C	-6.61195900	-2.13931800	2.21158500
H	-7.19209500	-0.07562500	2.33438400
C	5.04075800	-11.29691100	2.03629900

C	3.89103200	-10.52075900	1.81978500
C	5.28107200	-8.54276500	1.60105700
C	6.42220500	-9.32794600	1.82013600
H	7.18113500	-11.29945100	2.20589900
C	2.58971400	-11.11746400	1.83602900
C	1.47936300	-11.60214300	1.86339700
C	-1.30412100	-14.07842300	2.06888200
C	-2.41506800	-13.24540300	2.00399100
C	-2.24571700	-11.85663300	1.89084400
C	0.16146300	-12.16092100	1.90364700
C	-0.01998700	-13.54620000	2.02311000
H	-1.43969800	-15.15140300	2.15491200
C	-3.37880400	-10.98271800	1.84004200
C	-4.32326700	-10.22461100	1.79971800
C	-7.80222300	-8.89384200	1.57435400
C	-7.57807200	-7.52769400	1.69180000
C	-6.26967200	-7.04150400	1.84308700
C	-5.42794700	-9.31489800	1.75604600
C	-6.73854100	-9.78981900	1.60845600
H	-8.81413800	-9.26554700	1.45190900
C	-5.80010000	-4.45188500	2.08614700
C	-6.02345400	-5.63726100	1.97140100
C	-4.23449900	-2.58346200	2.37925200
C	4.01796900	-9.14584800	1.59719800
C	-0.95545800	-11.32026300	1.83352900
C	-5.19788900	-7.93821000	1.86641300
H	-4.87021300	0.74825400	2.62821400
H	-7.62339800	-2.50865500	2.08071800
H	4.93828800	-12.36292600	2.20852600
H	7.39954300	-8.85617900	1.81125000
H	-3.41763000	-13.65753200	2.04527200
H	0.84903200	-14.19362000	2.06993100
H	-8.40613000	-6.82746300	1.66684100
H	-6.91046800	-10.85633400	1.51067700
H	-3.40684900	-3.28505400	2.36479200
H	3.13280200	-8.54347000	1.42301300
H	-0.82087800	-10.24880300	1.72596000
H	-4.18454000	-7.56340900	1.96511300
C	5.39979100	-7.13201700	1.39799800
C	5.50544200	-5.93625700	1.23347800
C	2.33790900	-1.00601300	0.10935500
C	3.34564000	-1.64401600	0.31910000
C	6.92915600	-2.50779000	0.88171500
C	6.84949200	-3.87965900	1.08376500
C	5.60423100	-4.52469300	1.02609800
C	4.53420100	-2.39985600	0.56768200
C	5.78114400	-1.76388800	0.62844400
H	7.89231800	-2.01065600	0.93579300
C	4.45001200	-3.78180400	0.76539200

	H	7.74035900	-4.46048000	1.29856000
	H	5.83861400	-0.69094200	0.47746200
	H	3.48624100	-4.27838700	0.71291100
	C	-2.65527900	-0.72233900	2.69310800
	C	-1.54027500	-0.26633500	2.82792800
	C	1.14063000	2.30519900	3.10427300
	C	2.26943200	1.51321600	3.28533400
	C	2.14990000	0.11481800	3.32349900
	C	-0.24419200	0.32395700	2.98353700
	C	-0.11175100	1.72081100	2.95548700
	H	1.23666600	3.38599100	3.08205500
	C	0.89003800	-0.47505200	3.16718000
	H	3.24772700	1.96616100	3.40650100
	H	-0.99461000	2.33429400	2.80645200
	H	0.79394200	-1.55563200	3.18322000
	C	7.89839700	-2.17816300	4.29322800
	C	4.30156800	-1.36499200	3.74884300
	C	3.30993500	-0.69876700	3.54151800
	C	7.83832800	-3.54312100	4.55157900
	C	6.60282900	-4.20734300	4.54341200
	C	5.49451700	-2.11652600	4.00760300
	C	6.73695100	-1.46295300	4.02986600
	H	8.85577700	-1.66810700	4.30346200
	C	5.43341600	-3.49210700	4.25795600
	H	8.74052700	-4.10327100	4.77266800
	H	6.77766000	-0.39691600	3.83233400
	H	4.47715200	-4.00425400	4.24065200
	C	6.54829300	-5.60306800	4.87780200
	C	6.53217600	-6.77348000	5.21680600
	Si	6.52405100	-8.51233300	5.85590100
	C	8.04109000	-9.40194000	5.20191300
	C	4.94167600	-9.35728000	5.31461800
	C	6.60104000	-8.42664500	7.73110900
	H	8.95730800	-8.91373900	5.54566500
	H	8.05240900	-9.42713100	4.10992300
	H	8.05043700	-10.43487500	5.56449700
	H	4.83433900	-9.34358900	4.22685900
	H	4.06865200	-8.86599000	5.75418900
	H	4.94535200	-10.40176600	5.64295700
	H	5.74206900	-7.88568400	8.13757900
	H	7.51297200	-7.92551000	8.06711800
	H	6.59480300	-9.43784600	8.15048300
15-TS-a	O	0.19720900	-4.72576100	-0.53878300
	C	0.07621000	-2.87449300	-0.37091000
	H	0.42468800	-2.88131800	0.65157100
	H	0.80367000	-2.77782800	-1.16640100
	H	-0.98061900	-2.87349700	-0.58174800
	N	0.03524500	-0.83996100	-0.26820100
	S	-0.81954500	-5.57031200	0.22816200

O	-0.97291200	-6.88244600	-0.40925600
O	-2.06298800	-4.81570700	0.45998600
C	-0.06871600	-5.83250300	1.82021900
H	0.07369500	-4.86431600	2.30185300
H	0.88966500	-6.33119500	1.67544300
H	-0.73728000	-6.45433500	2.41583400
C	1.19606400	-0.17627600	-0.11592600
C	1.29764800	1.20576300	-0.15266200
H	2.27238300	1.65408700	-0.02035100
C	0.13023800	1.98346500	-0.31717100
N	0.17609000	3.33472400	-0.34653600
C	-1.08735700	1.27928200	-0.44719800
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C	-1.08129100	-0.10838800	-0.43652100
C	1.45798300	4.01690700	-0.26699800
C	-1.05572000	4.09751800	-0.47050900
H	1.29233000	5.09049000	-0.33062200
H	2.11508900	3.71807800	-1.09147700
H	1.96625100	3.80016900	0.67942000
H	-1.57482000	3.86449500	-1.40710200
H	-0.81756200	5.15925500	-0.46337900
H	-1.73403800	3.88856800	0.36426700
C	-6.92445700	-10.30200400	-1.79177700
C	6.38974400	-1.56001600	-2.72514700
C	5.13329900	-1.00442100	-2.93060200
C	3.99246800	-1.82417500	-2.93229300
C	5.39566300	-3.75530600	-2.50758900
C	6.52791900	-2.92777600	-2.51536200
H	7.26784700	-0.92318700	-2.72353400
C	2.70248500	-1.23713300	-3.14367200
C	1.63109000	-0.69671500	-3.31787900
C	-0.81463400	2.07796800	-3.76329900
C	-2.00630600	1.37675600	-3.91436200
C	-2.00732900	-0.02666500	-3.87548200
C	0.39288300	-0.00552100	-3.52005400
C	0.38171400	1.39760400	-3.56807200
H	-0.81700100	3.16262300	-3.80217900
C	-5.72217600	-10.99417500	-1.71363800
C	-4.51697600	-10.29325200	-1.54501200
C	-5.74712800	-8.20198300	-1.53058000
C	-6.94393400	-8.91368200	-1.70288500
H	-7.85431900	-10.84633500	-1.92266300
C	-3.27406800	-11.00130300	-1.48602300
C	-2.22184800	-11.60110100	-1.44863200
C	0.31301400	-14.33668500	-1.29009800
C	1.49727000	-13.61121400	-1.34296400
C	1.45850200	-12.21103700	-1.43298100
C	-0.96615000	-12.28801600	-1.41045900
C	-0.91617600	-13.68650800	-1.32407800

H	0.34749500	-15.41862900	-1.21629800
C	2.66721000	-11.44627800	-1.48948100
C	3.67747600	-10.77890200	-1.53694800
C	7.24791200	-9.68639200	-1.50157900
C	7.11280700	-8.31953100	-1.71383500
C	5.83627800	-7.75698100	-1.87440800
C	4.84686600	-9.95509000	-1.59696400
C	6.12609300	-10.50764100	-1.44407100
H	8.23577800	-10.11656100	-1.37490800
C	5.54094100	-5.16254400	-2.28621600
C	5.68208900	-6.35103300	-2.09661000
C	4.12726200	-3.19843700	-2.71455900
C	-0.80447600	-0.71334500	-3.67208900
C	-4.53402100	-8.89718400	-1.44622500
C	0.22473800	-11.55426500	-1.46158400
C	4.70760000	-8.57866800	-1.81072800
H	5.01985800	0.06182500	-3.09391700
H	7.50593700	-3.36589300	-2.34854000
H	-2.94113300	1.90428400	-4.07161000
H	1.31362800	1.93990300	-3.44487900
H	-5.70137100	-12.07608500	-1.78819600
H	-7.88056400	-8.36761100	-1.75601200
H	2.45671900	-14.11667900	-1.31548700
H	-1.84150700	-14.25054000	-1.27564400
H	7.98652700	-7.67836200	-1.75709600
H	6.22956000	-11.57344600	-1.27153500
H	3.24809900	-3.83476200	-2.70061600
H	-0.80203700	-1.79764100	-3.63016300
H	-3.60618200	-8.35285400	-1.30045300
H	0.18927300	-10.47145400	-1.51818600
H	3.71839700	-8.14781900	-1.92407800
C	-5.77016100	-6.77407300	-1.44424000
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C	-2.31798800	-0.81194600	-0.61626800
C	-3.38122200	-1.36811600	-0.78035600
C	-7.00898600	-2.03264600	-1.32371200
C	-7.01462800	-3.41918000	-1.41464800
C	-5.81535800	-4.13672900	-1.28368000
C	-4.61911200	-2.05625200	-0.98329100
C	-5.81830200	-1.34443900	-1.11454400
H	-7.93809000	-1.48243500	-1.43071600
C	-4.61736600	-3.45321900	-1.06015900
H	-7.93980100	-3.95612900	-1.59644700
H	-5.80692000	-0.26136500	-1.05167100
H	-3.69005300	-4.00079300	-0.91937700
C	-7.89264400	-1.98746700	-4.79569500
C	-4.26117100	-1.36338500	-4.23481200
C	-3.22847400	-0.75340600	-4.05886100
C	-7.91688000	-3.37044100	-4.93850600

C	-6.72722700	-4.10892500	-4.84695400
C	-5.49636800	-2.05415900	-4.46057300
C	-6.69248300	-1.32692300	-4.56565700
H	-8.81491200	-1.42106100	-4.87011800
C	-5.51951700	-3.44696600	-4.59609600
H	-8.84992900	-3.88877800	-5.13214400
H	-6.66735800	-0.24764300	-4.45796900
H	-4.59791500	-4.01374700	-4.51706900
C	-6.75275500	-5.52844500	-5.06314300
C	-6.80070800	-6.72257900	-5.30074700
Si	-6.88770100	-8.50204700	-5.80820900
C	-8.48568800	-9.23885400	-5.15458800
C	-5.39587700	-9.41204300	-5.13414800
C	-6.88249800	-8.54735200	-7.68647900
H	-9.35553100	-8.72068500	-5.56793700
H	-8.53389300	-9.17974100	-4.06457100
H	-8.55086900	-10.29383100	-5.43989700
H	-5.35378300	-9.35272500	-4.04337600
H	-4.46809500	-8.99807800	-5.53910400
H	-5.44783600	-10.46905200	-5.41486300
H	-5.96696600	-8.10354800	-8.08707000
H	-7.73655400	-8.00241300	-8.09820300
H	-6.93907600	-9.58288200	-8.03672200
C	6.25553100	-10.69595400	2.00249900
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C	-5.05327000	-0.39241000	2.44742100
C	-3.96737300	-1.28287300	2.47482800
C	-5.49604400	-3.13634900	2.16599000
C	-6.57301000	-2.23869700	2.13981500
H	-7.18018400	-0.18198300	2.24943900
C	5.00546800	-11.30307500	2.01246800
C	3.84896400	-10.53360600	1.80753300
C	5.22426100	-8.54727500	1.57996000
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C	-2.41589800	-13.35142800	2.01339300
C	-2.26754900	-11.96059200	1.89816900
C	0.14394800	-12.22785600	1.90876200
C	-0.01620100	-13.61568400	2.03008100
H	-1.41116700	-15.24188100	2.16666200
C	-3.41090100	-11.10047000	1.84543800
C	-4.35717100	-10.34496600	1.80382600
C	-7.81388200	-8.95017300	1.59226300
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C	-6.24023600	-7.12751000	1.82949400
C	-5.44817600	-9.41917300	1.76196300

C	-6.76912200	-9.86833600	1.62800400
H	-8.83452900	-9.30135500	1.48125700
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C	-4.19049500	-2.65473100	2.32170000
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C	-0.98562400	-11.40461800	1.83977300
C	-5.18821300	-8.04649800	1.85754300
H	-4.87016300	0.67074600	2.56098000
H	-7.57891800	-2.62167900	2.00537100
H	4.91066600	-12.37009800	2.18267600
H	7.34651000	-8.84815400	1.77034600
H	-3.41201700	-13.77874600	2.05642200
H	0.86242800	-14.24991800	2.07614700
H	-8.37272400	-6.87038600	1.66324700
H	-6.96386300	-10.93197700	1.54238200
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H	3.07345700	-8.56064900	1.42001900
H	-0.86693500	-10.33104200	1.73503000
H	-4.16591500	-7.69413500	1.94678000
C	5.34053800	-7.13602800	1.37605200
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C	3.38272700	-1.59886600	0.31912400
C	6.94317900	-2.53745200	0.89830300
C	6.83071500	-3.90823500	1.09070900
C	5.57271500	-4.52845100	1.02011400
C	4.55575900	-2.37866400	0.56973200
C	5.81350200	-1.76702000	0.64280700
H	7.91653800	-2.06259600	0.96286300
C	4.43648600	-3.75999100	0.75607000
H	7.70728300	-4.50934100	1.30813100
H	5.89387000	-0.69444500	0.50059000
H	3.46147100	-4.23278000	0.68718700
C	-2.63984500	-0.77324200	2.64720200
C	-1.53189800	-0.30347900	2.79250500
C	1.12493000	2.28971800	3.10592300
C	2.25865100	1.50532400	3.29188600
C	2.14898000	0.10601500	3.32404400
C	-0.24338800	0.29841000	2.96141400
C	-0.12171300	1.69678800	2.94253900
H	1.21269100	3.37143700	3.09377500
C	0.89492500	-0.49252400	3.15358200
H	3.23215500	1.96513300	3.42452400
H	-1.00814800	2.30455900	2.79088200
H	0.80611800	-1.57397600	3.17351100
C	7.89712600	-2.18907300	4.30642100
C	4.30322700	-1.36647200	3.75792800
C	3.31160000	-0.70091700	3.54945800

	C	7.83346500	-3.55584600	4.55502500
	C	6.59652200	-4.21733800	4.53934800
	C	5.49444600	-2.12059500	4.01654000
	C	6.73796100	-1.46930000	4.04563300
	H	8.85554200	-1.68134700	4.32282500
	C	5.42946300	-3.49754600	4.25664700
	H	8.73388700	-4.11932100	4.77425800
	H	6.78118000	-0.40191500	3.85622000
	H	4.47190300	-4.00726800	4.23360900
	C	6.53547500	-5.61493500	4.86424500
	C	6.51098100	-6.78759300	5.19440300
	Si	6.48635900	-8.52636100	5.83374900
	C	7.99448000	-9.43160300	5.18138100
	C	4.89787100	-9.35848100	5.29088600
	C	6.56101600	-8.43728700	7.70898100
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	H	7.99848600	-9.46789900	4.08945500
	H	7.99908700	-10.46087400	5.55430600
	H	4.81256600	-9.38196800	4.20125400
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	H	4.87507300	-10.39038800	5.65634800
	H	5.70453800	-7.89041800	8.11294800
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15-4a	O	-0.01652600	-5.28091300	-0.33279100
	C	-0.03852500	-2.30329100	-0.23121600
	H	0.50933000	-2.65330500	0.64316600
	H	0.44094500	-2.69484400	-1.13014200
	H	-1.06602000	-2.65148800	-0.17151200
	N	-0.00129700	-0.82975300	-0.26269200
	S	-1.24700000	-5.74981900	0.34722700
	O	-1.82901000	-6.97099400	-0.26114900
	O	-2.24666500	-4.66601200	0.54511400
	C	-0.73567500	-6.22206400	1.99573800
	H	-0.30175400	-5.34815500	2.48514000
	H	0.00702900	-7.01890800	1.92156200
	H	-1.60766500	-6.57037100	2.55178800
	C	1.20302500	-0.19079900	-0.14983300
	C	1.30825800	1.17937500	-0.21491600
	H	2.29497800	1.60838700	-0.11891400
	C	0.14910600	1.98159900	-0.36296400
	N	0.22115300	3.31918200	-0.40867600
	C	-1.08671500	1.29642900	-0.46204800
	H	-2.02147200	1.82093000	-0.59654300
	C	-1.13360600	-0.08098000	-0.43138200
	C	1.51908800	3.98228800	-0.35133800
	C	-0.99867300	4.11088400	-0.51861400
	H	1.36692200	5.05791100	-0.39959500
	H	2.14841200	3.68057100	-1.19475000



H	2.03882300	3.74550500	0.58269600
H	-1.53573100	3.87613000	-1.44317100
H	-0.73457900	5.16571000	-0.52952200
H	-1.66070600	3.92490900	0.33293600
C	-6.78609900	-10.24675700	-1.88296800
C	6.34129900	-1.58209800	-2.86427500
C	5.07566800	-1.03958900	-3.04661500
C	3.94092000	-1.86654200	-2.99743400
C	5.36801800	-3.77835500	-2.56499800
C	6.49349300	-2.94353800	-2.62535400
H	7.21496700	-0.94017600	-2.90190400
C	2.64518300	-1.28526700	-3.18813300
C	1.57706400	-0.73328500	-3.34580500
C	-0.82461300	2.08353400	-3.76664100
C	-2.03316800	1.40492100	-3.89112100
C	-2.05963800	0.00222000	-3.84660100
C	0.34706300	-0.02191700	-3.53071300
C	0.36193500	1.38153900	-3.58893600
H	-0.80588200	3.16760100	-3.81618200
C	-5.57264000	-10.91742600	-1.79982400
C	-4.38322500	-10.19823100	-1.59645200
C	-5.64839500	-8.13253300	-1.56399100
C	-6.82992700	-8.86066300	-1.76862800
H	-7.70396800	-10.80472100	-2.03856700
C	-3.13662900	-10.90000800	-1.52635600
C	-2.09665200	-11.52055900	-1.48179100
C	0.36383300	-14.32253000	-1.30415700
C	1.56827600	-13.62909700	-1.33416500
C	1.56707400	-12.22830400	-1.41710000
C	-0.85931500	-12.23957300	-1.43271800
C	-0.84713200	-13.63972800	-1.35330000
H	0.36788100	-15.40536000	-1.23596400
C	2.79026600	-11.48572500	-1.45367300
C	3.79799900	-10.81350900	-1.48407400
C	7.34373000	-9.64021500	-1.38896200
C	7.18136200	-8.28129400	-1.63197800
C	5.89543200	-7.75238000	-1.82865000
C	4.95267800	-9.96839400	-1.52695800
C	6.24081500	-10.48730000	-1.33817700
H	8.33885400	-10.04454700	-1.23571900
C	5.53585900	-5.17718400	-2.30778400
C	5.70953600	-6.35608100	-2.08684600
C	4.09001100	-3.23512000	-2.75176500
C	-0.86625500	-0.70710000	-3.66009400
C	-4.42157800	-8.80459800	-1.46904300
C	0.35133500	-11.53906400	-1.46205100
C	4.78552200	-8.59935500	-1.76889900
H	4.94987500	0.02183800	-3.23158400
H	7.47865100	-3.37144400	-2.47357000

H	-2.95999300	1.94961100	-4.03562400
H	1.30685300	1.90641500	-3.49080300
H	-5.53010000	-11.99725400	-1.89481100
H	-7.77455900	-8.32906500	-1.82696700
H	2.51317200	-14.16047900	-1.29532400
H	-1.78748300	-14.17953200	-1.32108200
H	8.04109000	-7.62111900	-1.67266200
H	6.36661700	-11.54717400	-1.14450900
H	3.21540100	-3.87519000	-2.69854800
H	-0.88456200	-1.79138800	-3.62001600
H	-3.50726400	-8.24608600	-1.28329200
H	0.34632500	-10.45552200	-1.51404500
H	3.78900100	-8.19454600	-1.90981000
C	-5.70731200	-6.70658800	-1.45221400
C	-5.78385400	-5.49992400	-1.36956400
C	-2.38028200	-0.74831200	-0.58789300
C	-3.46268600	-1.27154700	-0.73563300
C	-7.08398500	-1.99937900	-1.24671600
C	-7.05297000	-3.38440000	-1.36123400
C	-5.83519300	-4.07438900	-1.25273200
C	-4.69441800	-1.96800300	-0.93290300
C	-5.91007000	-1.28164100	-1.04023000
H	-8.02886800	-1.47345100	-1.33595100
C	-4.65398700	-3.36344200	-1.02767400
H	-7.96644000	-3.94113800	-1.54360100
H	-5.92680000	-0.19962400	-0.96100300
H	-3.71352600	-3.88788200	-0.88475000
C	-7.97002500	-1.97148400	-4.69267500
C	-4.33474200	-1.30207800	-4.18716300
C	-3.29242400	-0.70823800	-4.01330900
C	-7.97230300	-3.35224000	-4.86015800
C	-6.76840400	-4.07043300	-4.79999000
C	-5.56884600	-1.99979500	-4.39568400
C	-6.77843100	-1.29203900	-4.47031100
H	-8.90336700	-1.42082900	-4.74310200
C	-5.57000500	-3.39029900	-4.55491100
H	-8.89912200	-3.88296200	-5.05004300
H	-6.77191100	-0.21432400	-4.34549300
H	-4.63716600	-3.94155000	-4.50043500
C	-6.76111400	-5.48510600	-5.04644400
C	-6.77685400	-6.67582900	-5.30423200
Si	-6.81168200	-8.44899700	-5.83869600
C	-8.38382700	-9.24465200	-5.19232300
C	-5.28281400	-9.31286800	-5.18652200
C	-6.81480200	-8.46766600	-7.71765800
H	-9.26919800	-8.75937800	-5.61275500
H	-8.44258500	-9.18592200	-4.10297400
H	-8.40833800	-10.30169400	-5.47663900
H	-5.22233600	-9.24583700	-4.09703100

H	-4.37650400	-8.87082000	-5.61040800
H	-5.30526300	-10.37237600	-5.46178800
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H	-6.84450100	-9.49951900	-8.08204400
C	6.26927500	-10.66296000	2.12036000
C	-6.30791400	-0.87953500	2.39096000
C	-5.00773600	-0.41404900	2.54037500
C	-3.93050000	-1.31551600	2.51481400
C	-5.48287500	-3.14651700	2.20482800
C	-6.55137600	-2.23925400	2.22791700
H	-7.13716400	-0.18008700	2.40246400
C	5.01888800	-11.26927600	2.10510900
C	3.86801700	-10.50214600	1.86234200
C	5.25051500	-8.52032100	1.64389900
C	6.39235400	-9.29571600	1.89221100
H	7.15581600	-11.25921500	2.31123400
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C	1.47156600	-11.61718600	1.87286900
C	-1.26091400	-14.15221300	2.04253300
C	-2.38857600	-13.34278500	1.96477500
C	-2.24684500	-11.95099300	1.85484600
C	0.16565900	-12.20412500	1.89679500
C	0.01217000	-13.59322200	2.01266100
H	-1.37482000	-15.22792100	2.12622500
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C	-7.80054700	-8.95383000	1.53028600
C	-7.54920800	-7.59259900	1.64994500
C	-6.23111900	-7.13053900	1.79487700
C	-5.43439000	-9.41956000	1.70082100
C	-6.75391800	-9.87007800	1.55915500
H	-8.82017600	-9.30555300	1.41271500
C	-5.73734600	-4.54680600	2.05109600
C	-5.96415000	-5.73048600	1.92712400
C	-4.16737900	-2.68138900	2.33261700
C	3.98978200	-9.12880400	1.62671100
C	-0.96749100	-11.38745100	1.81408100
C	-5.17648000	-8.04729000	1.80907900
H	-4.81153200	0.64422400	2.67613300
H	-7.56428200	-2.60947200	2.11008200
H	4.91912600	-12.33407400	2.28631400
H	7.36675500	-8.81772400	1.89572200
H	-3.38266300	-13.77600600	1.99428600
H	0.89396700	-14.22234400	2.06922100
H	-8.36411600	-6.87673600	1.63141500
H	-6.94645400	-10.93330000	1.46347500
H	-3.33897300	-3.37875900	2.25096500
H	3.10463300	-8.53297000	1.42997600

H	-0.85515600	-10.31298100	1.71177100
H	-4.15386100	-7.69506400	1.88978400
C	5.37116200	-7.11369300	1.41448700
C	5.47519300	-5.92195600	1.22362500
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C	3.37948100	-1.61671500	0.25303900
C	6.95259500	-2.52891900	0.75799000
C	6.84726800	-3.89373800	0.99301600
C	5.58934400	-4.51774100	0.98009900
C	4.55860400	-2.38467000	0.49636600
C	5.81500400	-1.76647200	0.51469300
H	7.92713000	-2.05218000	0.77759900
C	4.44401600	-3.75985100	0.72643100
H	7.73147600	-4.48767900	1.19927800
H	5.88890600	-0.69893400	0.33629100
H	3.46844500	-4.23531900	0.70306200
C	-2.59536500	-0.81801400	2.66356100
C	-1.48455300	-0.34899000	2.78996200
C	1.17348500	2.25145600	3.02424000
C	2.31246900	1.47127200	3.19824000
C	2.20499600	0.07280000	3.25565600
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C	-0.07572600	1.65499300	2.89554100
H	1.25886300	3.33310000	2.99611200
C	0.94843100	-0.53045400	3.11932100
H	3.28768800	1.93413600	3.30427600
H	-0.96677000	2.25935400	2.75768900
H	0.86122600	-1.61143200	3.16211900
C	7.95643700	-2.26596600	4.16140400
C	4.36305800	-1.39701200	3.67749500
C	3.36945900	-0.73286900	3.47422900
C	7.87415300	-3.62396000	4.44930300
C	6.62565200	-4.26311800	4.48369300
C	5.54973900	-2.16144900	3.92558500
C	6.80423300	-1.53183900	3.90858300
H	8.92419200	-1.77623000	4.13955900
C	5.46557600	-3.52992800	4.20749900
H	8.76969500	-4.19748200	4.66318000
H	6.86199600	-0.47106800	3.68801100
H	4.49842300	-4.02148100	4.22324700
C	6.54633100	-5.64844100	4.85425600
C	6.50831200	-6.80968900	5.22148000
Si	6.46611500	-8.53229700	5.90280000
C	7.98183200	-9.45720700	5.29556300
C	4.87730600	-9.36424700	5.36049800
C	6.51655000	-8.40379900	7.77667500
H	8.89764500	-8.97879200	5.65417000
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	H	4.77070100	-9.35192000	4.27285900
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	H	5.66084400	-7.83881400	8.15667800
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	H	6.48523500	-9.40510300	8.21837900
17-3a	O	-0.55839800	-5.25151300	-0.53623200
	C	-0.44715200	-3.81601400	-0.34616800
	H	0.04488300	-3.58657100	0.60137000
	H	0.17417200	-3.46679700	-1.16783500
	H	-1.43106200	-3.34818400	-0.38640400
	N	-0.14113800	-0.85716200	-0.14333300
	S	-1.46728600	-6.07333400	0.48878400
	O	-1.67230600	-7.36889300	-0.13653400
	O	-2.62301300	-5.26845400	0.86221400
	C	-0.41204000	-6.26640100	1.90151500
	H	-0.18386500	-5.28317700	2.31342700
	H	0.49257500	-6.78407300	1.58350100
	H	-0.96281800	-6.86200400	2.63033500
	C	1.02386700	-0.19552400	-0.05969700
	C	1.15453300	1.19023000	-0.06841100
	H	2.14492800	1.61915900	0.00175600
	C	-0.00129600	1.99217400	-0.13901000
	N	0.06724500	3.34997300	-0.12544700
	C	-1.23067100	1.30824500	-0.22073100
	H	-2.17336800	1.83387200	-0.29395100
	C	-1.23628000	-0.08370800	-0.23029800
	C	1.36266500	4.00503000	-0.11161200
	C	-1.15215000	4.13270800	-0.21282800
	H	1.21547500	5.08354800	-0.09881500
	H	1.95348300	3.74585000	-0.99873400
	H	1.93876100	3.72601300	0.77801100
	H	-1.69414700	3.92956800	-1.14444600
	H	-0.89859600	5.19107400	-0.18620000
	H	-1.82115000	3.91753500	0.62844300
	C	6.63670900	-10.51272900	0.87704700
	C	-6.53483700	-0.55737100	2.81472300
	C	-5.24016700	-0.05647400	2.89257800
	C	-4.14526800	-0.93438900	2.86461600
	C	-5.67160000	-2.81223000	2.68185100
	C	-6.75780400	-1.92638500	2.71218500
	H	-7.37802900	0.12510500	2.83158300
	C	-2.80310400	-0.44108400	2.94446800
	C	-1.65878600	-0.04955200	3.02308400
	C	1.36324600	2.13305700	3.23972700
	C	2.37461800	1.18321900	3.33568300
	C	2.05822100	-0.18482400	3.33437200
	C	-0.29522800	0.37678900	3.12409500
	C	0.03321500	1.74064800	3.13484700

H	1.61338400	3.18906400	3.25226600
C	3.09440300	-1.16699200	3.46005400
C	3.97760300	-1.98975100	3.57358100
C	7.43046800	-3.34914500	3.89422900
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C	5.05502200	-2.92455100	3.71301300
C	6.37532100	-2.45407200	3.75685100
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C	5.37380500	-11.05569700	1.08256500
C	4.25500400	-10.21331900	1.17488400
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C	6.80591000	-9.13672200	0.76109900
H	7.49953900	-11.16814300	0.81503200
C	2.94469800	-10.75451500	1.38064600
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C	-0.94945300	-13.66761000	1.86543400
C	-2.06006700	-12.83340600	1.89756800
C	-1.89395400	-11.44053700	1.83453500
C	0.50944200	-11.74388800	1.67359900
C	0.33136900	-13.13296200	1.76236600
H	-1.08199100	-14.74353400	1.91847200
C	-3.03385700	-10.57967200	1.92572300
C	-4.00230100	-9.86014200	2.03951200
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C	-5.16472900	-9.03817700	2.19174000
C	-6.43375800	-9.62792500	2.28870300
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C	-5.87945800	-4.22489300	2.57965800
C	-6.03015100	-5.42501500	2.50779100
C	-4.36679200	-2.31068300	2.75099600
C	0.72148200	-0.58105700	3.22273500
C	4.80477200	-4.30005000	3.80951500
C	4.42154300	-8.83159400	1.04901000
C	-0.60901900	-10.90107200	1.70945500
C	-5.04041500	-7.64589000	2.25344200
H	-5.06504600	1.01083100	2.97617700
H	-7.76666900	-2.31917900	2.64421900
H	3.41207000	1.48888200	3.41994300
H	-0.75684500	2.47997700	3.05047300
H	8.00420300	-5.41604000	4.09555400
H	6.56145300	-1.38878000	3.67222600
H	5.24268400	-12.12782600	1.18553400
H	7.79086900	-8.71178900	0.59895300
H	-3.05927200	-13.24593600	1.98704400
H	1.20147600	-13.78099600	1.73358000
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H	-3.52467300	-2.99332300	2.69974800
H	0.46997100	-1.63637400	3.21073600
H	3.78504700	-4.66806800	3.77012200
H	3.56024400	-8.17466300	1.11361900
H	-0.48078800	-9.82637000	1.63299900
H	-4.06569500	-7.17895700	2.15529500
C	6.64822500	-11.36423500	4.30824300
C	5.53775300	-7.81286200	4.16160500
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C	4.25962300	-11.29322500	4.68512300
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H	7.56823400	-11.93129300	4.21235200
C	4.27991700	-9.90192800	4.53955800
H	5.42805500	-13.10194300	4.67651900
H	7.60415000	-9.46237800	3.97311100
H	3.35813600	-9.33626100	4.62487200
C	3.03439800	-11.97234200	4.99545000
C	2.01251000	-12.56255600	5.29695000
Si	0.46853000	-13.42703600	5.83818200
C	0.40967500	-15.12247900	5.03505800
C	-0.98723500	-12.35371200	5.34354400
C	0.53442500	-13.61770700	7.70643000
H	1.23960000	-15.74351000	5.38438900
H	0.46621100	-15.05472800	3.94599900
H	-0.52556900	-15.62727900	5.29731200
H	-0.92200800	-12.07031300	4.28955100
H	-1.00871700	-11.43944500	5.94462700
H	-1.93136100	-12.88579200	5.49734900
H	0.61086200	-12.64435400	8.19939700
H	1.39046000	-14.22588800	8.01208500
H	-0.37616100	-14.10884500	8.06426800
C	5.82893800	-6.86812900	0.72103300
C	5.88030200	-5.66086300	0.62734300
C	2.22754000	-0.97589600	0.05035900
C	3.29167900	-1.54482100	0.15527400
C	6.96964700	-2.09180400	0.40217300
C	7.03452600	-3.47722100	0.50932000
C	5.85530000	-4.23495600	0.51354600
C	4.55746700	-2.19983700	0.28128700
C	5.74239100	-1.44901600	0.29199400
H	7.88464200	-1.50830000	0.40295400
C	4.61915600	-3.59043800	0.39565200
H	7.99147500	-3.97980700	0.60278700
H	5.68820800	-0.36937000	0.19906600
H	3.70482200	-4.17510400	0.39088600
C	-7.05487700	-10.19648500	-1.09598700

C	6.33336700	-0.96315600	-3.07441900
C	5.05768000	-0.41814000	-3.16551800
C	3.93259400	-1.25722600	-3.14076700
C	5.39067400	-3.18581300	-2.92628600
C	6.50699100	-2.33772800	-2.95543500
H	7.20024700	-0.31115400	-3.09048100
C	2.61018400	-0.71616000	-3.23823000
C	1.48084200	-0.28343000	-3.31788900
C	-1.42647000	2.04303400	-3.58390000
C	-2.48419000	1.14468600	-3.66760500
C	-2.23843200	-0.23740300	-3.63361300
C	0.13919300	0.20645800	-3.42406500
C	-0.11885600	1.58480100	-3.46171100
H	-1.62235300	3.10989500	-3.61839800
C	-5.80283700	-10.78293500	-1.22848000
C	-4.65010600	-9.98096000	-1.23902400
C	-6.03314100	-8.00756000	-0.98751800
C	-7.17753900	-8.81566900	-0.97870000
H	-7.94407700	-10.81877000	-1.09531800
C	-3.35880800	-10.58522900	-1.37466400
C	-2.27149300	-11.11286600	-1.47017000
C	0.33056800	-13.78256600	-1.58627400
C	1.49141000	-13.03146100	-1.72197500
C	1.41790200	-11.63051300	-1.78385900
C	-0.99572500	-11.75604400	-1.56299900
C	-0.90950600	-13.15547000	-1.50891200
H	0.39040800	-14.86515800	-1.53673300
C	2.60914300	-10.85581800	-1.95550900
C	3.61230200	-10.19696800	-2.12184400
C	7.17721400	-9.22844900	-2.65060700
C	7.07247100	-7.84483500	-2.73125200
C	5.81699200	-7.22756700	-2.61546100
C	4.78779700	-9.40520400	-2.32388000
C	6.04542800	-10.01210300	-2.45126800
H	8.14976000	-9.70052200	-2.74225700
C	5.55728700	-4.60341800	-2.80752600
C	5.68848200	-5.80471600	-2.71488700
C	4.10533100	-2.63972200	-3.01780300
C	-0.92482700	-0.69996700	-3.50638500
C	-4.76740200	-8.59391200	-1.11399200
C	0.17374100	-10.99678000	-1.69534600
C	4.67939600	-8.01246300	-2.40616700
H	4.92001800	0.65387100	-3.25855000
H	7.50088700	-2.76447700	-2.87364000
H	-3.50412200	1.50096700	-3.76514600
H	0.70821000	2.28390000	-3.39039600
H	-5.70386000	-11.85789500	-1.33906200
H	-8.15422000	-8.35414800	-0.87615400
H	2.45976600	-13.51578300	-1.78816200



H	-1.81846200	-13.73703800	-1.39261300
H	7.95386300	-7.23266300	-2.89008900
H	6.12517200	-11.09162300	-2.38118600
H	3.23779300	-3.29043900	-2.98649100
H	-0.72889400	-1.76633000	-3.47150000
H	-3.87615600	-7.97326900	-1.10168800
H	0.11246200	-9.91404500	-1.72972700
H	3.70803200	-7.54046200	-2.30437300
C	-6.13895600	-6.58461200	-0.88200500
C	-6.19876200	-5.37623900	-0.80890100
C	-2.50288500	-0.75644900	-0.33894400
C	-3.59290300	-1.27691400	-0.43182000
C	-7.27852300	-1.79718200	-0.68420100
C	-7.34979500	-3.18488900	-0.75528900
C	-6.17427400	-3.94788100	-0.72875000
C	-4.86902000	-1.91409000	-0.54425600
C	-6.04853300	-1.15672700	-0.58521600
H	-8.19070100	-1.20960600	-0.70818600
C	-4.93601100	-3.30774500	-0.61471800
H	-8.30890100	-3.68439300	-0.84402300
H	-5.99042200	-0.07496000	-0.52468300
H	-4.02915200	-3.90259800	-0.56636600
C	-3.32464700	-1.16612200	-3.73814600
C	-4.25176600	-1.94114000	-3.83459600
C	-7.78474600	-3.06962600	-4.15729400
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C	-6.35336300	-5.02294000	-4.15139300
C	-5.38759200	-2.80651100	-3.95770700
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C	-5.23249300	-4.19731400	-4.01615300
H	-8.49903400	-5.09566800	-4.31790400
H	-6.78419800	-1.16909900	-3.97449800
H	-4.24166000	-4.63433900	-3.95226100
C	-7.46284800	-11.14451600	-4.50173900
C	-6.17248500	-7.65689200	-4.30604800
C	-6.22123700	-6.44797300	-4.22846500
C	-6.28782700	-11.87096000	-4.65569900
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C	-6.18982400	-9.08619500	-4.40981100
C	-7.42071300	-9.76074200	-4.38394300
H	-8.41722100	-11.65988600	-4.47640700
C	-5.00545200	-9.81655000	-4.55858900
H	-6.31530300	-12.95043000	-4.75941000
H	-8.33514300	-9.18894500	-4.26524100
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C	-3.84815000	-11.96278500	-4.90748700
C	-2.85307300	-12.62893800	-5.13177200
Si	-1.37931400	-13.65826900	-5.57239700

	C	-1.46517400	-15.27187300	-4.61709200
	C	0.17033800	-12.68992900	-5.15760000
	C	-1.45524500	-14.01119900	-7.41601600
	H	-2.36503500	-15.83423700	-4.88154800
	H	-1.47121600	-15.09840100	-3.53838800
	H	-0.59495500	-15.89151900	-4.85658100
	H	0.16815500	-12.37942000	-4.10956200
	H	0.24679800	-11.79511000	-5.78223300
	H	1.05994300	-13.30412300	-5.33030300
	H	-1.44109200	-13.08514200	-7.99706900
	H	-2.36104200	-14.56584200	-7.67589900
	H	-0.59116100	-14.61315600	-7.71511900
17-TS-a	O	-0.19680800	-4.69455700	-0.39963000
	C	-0.19560000	-2.83829800	-0.23211300
	H	0.41353400	-2.85098400	0.66077600
	H	0.29601000	-2.76778800	-1.19160500
	H	-1.27025100	-2.79152200	-0.15562400
	N	-0.15499000	-0.79840900	-0.14338400
	S	-1.12099600	-5.49428200	0.51744700
	O	-1.48318600	-6.76988100	-0.11150700
	O	-2.24438900	-4.66608800	0.98825300
	C	-0.11834300	-5.86874700	1.93991200
	H	0.19378100	-4.93241900	2.40475900
	H	0.74927200	-6.44146100	1.61226300
	H	-0.72086500	-6.45360300	2.63535100
	C	1.02381000	-0.15443900	-0.06297100
	C	1.14318900	1.22758800	-0.06671000
	H	2.13290800	1.65731700	0.00058100
	C	-0.01858700	2.02783000	-0.12600700
	N	0.04786200	3.37886300	-0.11121600
	C	-1.25200600	1.34387300	-0.19809900
	H	-2.19494500	1.86968300	-0.25858900
	C	-1.26815400	-0.04370900	-0.21780700
	C	1.34329800	4.03896200	-0.09032600
	C	-1.17493700	4.16310200	-0.17438600
	H	1.19149000	5.11635500	-0.07709700
	H	1.93467300	3.78169100	-0.97655000
	H	1.91462900	3.75971900	0.80170600
	H	-1.72900600	3.96164600	-1.09830200
	H	-0.91998100	5.22068000	-0.14900200
	H	-1.82733500	3.94377500	0.67797400
	C	6.60950900	-10.52352900	0.91666200
	C	-6.48732200	-0.69100700	2.90271700
	C	-5.19337600	-0.18771700	2.96987900
	C	-4.09617600	-1.06045000	2.89651800
	C	-5.61617300	-2.93785400	2.69619000
	C	-6.70536700	-2.05817600	2.77041500
	H	-7.33275100	-0.01305100	2.95351900
	C	-2.75790000	-0.55640200	2.97214300

C	-1.61990200	-0.14573500	3.04268600
C	1.36034700	2.09537900	3.24261000
C	2.39108900	1.16501600	3.32476000
C	2.10042900	-0.20860900	3.32168400
C	-0.26493300	0.30760800	3.13306300
C	0.03710700	1.67783800	3.14699300
H	1.58996800	3.15597700	3.25974500
C	3.15154900	-1.17507300	3.43618600
C	4.03933500	-1.99345400	3.54321700
C	7.48900900	-3.37265800	3.81646400
C	7.23468400	-4.73320700	3.92894700
C	5.91259800	-5.20828900	3.92018900
C	5.11475900	-2.93126300	3.67332200
C	6.43881600	-2.47006800	3.69023700
H	8.51229000	-3.01235700	3.82203400
C	5.35406900	-11.08225100	1.12534500
C	4.22312100	-10.25509700	1.20504900
C	5.63488100	-8.31303200	0.85237400
C	6.75886800	-9.14678700	0.78448000
H	7.48202100	-11.16685500	0.86457700
C	2.92048300	-10.81423000	1.41103200
C	1.80774900	-11.27331600	1.55721500
C	-0.93321200	-13.77957100	1.90506500
C	-2.05665000	-12.96180700	1.91837800
C	-1.91069200	-11.56783200	1.83821900
C	0.49829200	-11.83647600	1.69938700
C	0.34005600	-13.22707000	1.80383000
H	-1.04956300	-14.85659900	1.97190300
C	-3.06147600	-10.71991300	1.91074300
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C	-5.19208700	-9.17089400	2.12658600
C	-6.47606500	-9.73304100	2.15328500
H	-8.58394600	-9.34959000	2.29538300
C	-5.82835100	-4.34806200	2.57117100
C	-5.99190700	-5.54478600	2.47489700
C	-4.31078700	-2.43468200	2.74891000
C	0.77067100	-0.63046400	3.22090400
C	4.85498400	-4.30355700	3.78712200
C	4.36944000	-8.87248200	1.06337700
C	-0.63278300	-11.01022200	1.71699300
C	-5.03965700	-7.78336400	2.22682800
H	-5.01973200	0.87739000	3.08038700
H	-7.71362200	-2.45461300	2.71478000
H	3.42304100	1.49035500	3.40136800
H	-0.76811800	2.40200300	3.07510600
H	8.04997500	-5.44191500	4.02754500

H	6.63160200	-1.40699600	3.59346200
H	5.23802400	-12.15489700	1.24023500
H	7.73797100	-8.70951600	0.61980800
H	-3.05001300	-13.38833800	2.00730000
H	1.21957200	-13.86269200	1.79005800
H	-8.31109700	-6.89095600	2.48888200
H	-6.58845500	-10.80817600	2.06336600
H	-3.46799300	-3.11180000	2.64862700
H	0.53874300	-1.69057300	3.21728800
H	3.83172000	-4.66349900	3.76818000
H	3.49806700	-8.22801900	1.11696300
H	-0.52011900	-9.93423600	1.63096200
H	-4.04879800	-7.34231800	2.18495300
C	6.61177900	-11.38176500	4.36021800
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C	5.67831400	-6.61634900	4.04702400
C	5.40508400	-12.01906800	4.62110100
C	4.22347700	-11.26966600	4.73086700
C	5.48240400	-9.24059100	4.30880500
C	6.65759400	-10.00097400	4.20865000
H	7.52334600	-11.96397700	4.27541300
C	4.26475600	-9.88119400	4.56502900
H	5.36489900	-13.09534000	4.75045400
H	7.59711700	-9.49885500	4.00370500
H	3.35158400	-9.30030300	4.63980700
C	2.98971000	-11.92743900	5.05322400
C	1.96341600	-12.50088400	5.37160100
Si	0.41263700	-13.33803600	5.93597200
C	0.36662000	-15.07065100	5.21684800
C	-1.03940100	-12.29988000	5.36524000
C	0.45510500	-13.43063900	7.81184900
H	1.19904000	-15.66989500	5.59674800
H	0.42612300	-15.05184700	4.12608400
H	-0.56680100	-15.56792200	5.49919400
H	-0.96951100	-12.09027400	4.29475500
H	-1.06327500	-11.34673600	5.90164000
H	-1.98419300	-12.82035600	5.55121000
H	0.52024600	-12.43246800	8.25362500
H	1.31035300	-14.01670900	8.15959400
H	-0.45748600	-13.90751300	8.18342900
C	5.75275800	-6.89360400	0.71494600
C	5.79840500	-5.68747700	0.60629400
C	2.21930700	-0.94253300	0.03618500
C	3.27621900	-1.52596500	0.13270800
C	6.94379700	-2.14176400	0.32749600
C	6.98183300	-3.52698900	0.44609700
C	5.78870900	-4.26289400	0.47655400
C	4.53030400	-2.20524200	0.24548500
C	5.72787400	-1.47570500	0.23135700

H	7.87012300	-1.57687000	0.30895400
C	4.56321300	-3.59632900	0.37131900
H	7.93003700	-4.04771500	0.52896900
H	5.69249400	-0.39609200	0.13072300
H	3.63640400	-4.16145600	0.38423800
C	-7.02347000	-10.20491100	-1.25559900
C	6.23820700	-1.03571600	-3.14021300
C	4.95691400	-0.50242100	-3.21568100
C	3.83963600	-1.35132500	-3.16772600
C	5.31623000	-3.26531700	-2.96053100
C	6.42455600	-2.40797600	-3.01329600
H	7.09927300	-0.37673800	-3.17419400
C	2.51450600	-0.81487200	-3.25055400
C	1.39088000	-0.36614700	-3.32293600
C	-1.45680400	2.03486500	-3.55582000
C	-2.53871200	1.16504500	-3.63839300
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C	0.06136500	0.15687700	-3.42007100
C	-0.16062700	1.54204100	-3.44592800
H	-1.62480800	3.10668000	-3.58224200
C	-5.77646900	-10.80798200	-1.35218300
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C	0.34556100	-13.87288300	-1.55918800
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C	1.44067400	-11.72521900	-1.75788600
C	-0.97386800	-11.84241800	-1.54626700
C	-0.89286900	-13.24180300	-1.48647400
H	0.40138600	-14.95555300	-1.50767600
C	2.63111400	-10.94969100	-1.92894300
C	3.63290800	-10.28955400	-2.09767400
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C	7.06283700	-7.89939800	-2.72733000
C	5.79919900	-7.29788300	-2.61756000
C	4.79889900	-9.48611500	-2.30697000
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C	5.65024400	-5.87794000	-2.72910400
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C	-1.02606800	-0.72066600	-3.50278900
C	-4.71318300	-8.63876800	-1.14840400
C	0.19849500	-11.08746400	-1.67470700
C	4.67206100	-8.09577800	-2.40128600
H	4.80805100	0.56751600	-3.31481000

H	7.42306500	-2.82603600	-2.94323900
H	-3.54944000	1.54867000	-3.72666300
H	0.68500500	2.21885600	-3.37696200
H	-5.68897000	-11.88178000	-1.48138900
H	-8.10191300	-8.35008900	-1.03770200
H	2.47617200	-13.61424800	-1.75769800
H	-1.80368900	-13.82057400	-1.37107800
H	7.93603800	-7.27691800	-2.89127700
H	6.15821800	-11.15532400	-2.35005900
H	3.16328600	-3.38933100	-2.98763300
H	-0.85876700	-1.79246500	-3.48471900
H	-3.81545200	-8.03081500	-1.08627800
H	0.14140900	-10.00474300	-1.71426700
H	3.69471400	-7.63562000	-2.30241800
C	-6.06865600	-6.61314300	-0.92636200
C	-6.12764700	-5.40670500	-0.82702800
C	-2.52967400	-0.71967000	-0.31755800
C	-3.61489300	-1.25099900	-0.40216000
C	-7.28758500	-1.85936400	-0.61372200
C	-7.32161400	-3.24663400	-0.71133900
C	-6.12675200	-3.98027600	-0.71440800
C	-4.87654700	-1.91708200	-0.50826600
C	-6.07370700	-1.18812100	-0.52051900
H	-8.21532200	-1.29640700	-0.61468300
C	-4.90356300	-3.31156400	-0.60080800
H	-8.26831900	-3.76969100	-0.79786100
H	-6.04228900	-0.10650700	-0.44167400
H	-3.97634300	-3.87545600	-0.56058200
C	-3.43175500	-1.13012700	-3.72019400
C	-4.35950800	-1.90427300	-3.81530900
C	-7.88338100	-3.07668700	-4.08374500
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C	-5.48730200	-2.78020700	-3.93370400
C	-6.78052200	-2.23866200	-3.96588900
H	-8.88274500	-2.65471800	-4.10122700
C	-5.31184400	-4.16696600	-4.02433900
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H	-6.90808300	-1.16433000	-3.88710100
H	-4.31315500	-4.58906500	-3.99166600
C	-7.48035500	-11.11893000	-4.67336600
C	-6.20677100	-7.63508600	-4.36001500
C	-6.27037800	-6.42873500	-4.25678600
C	-6.29908400	-11.84084200	-4.79942600
C	-5.06281000	-11.17773200	-4.77905100
C	-6.21423400	-9.06181800	-4.49617600
C	-7.44440600	-9.73791500	-4.52815700
H	-8.43403000	-11.63563500	-4.69288400
C	-5.02384400	-9.78758700	-4.61671700

	H	-6.32086500	-12.91810700	-4.92482400
	H	-8.36321400	-9.16889000	-4.43224200
	H	-4.06954400	-9.27218300	-4.58916500
	C	-3.85478300	-11.93033900	-4.96894200
	C	-2.85764600	-12.59879600	-5.17720000
	Si	-1.38051000	-13.63180800	-5.59951700
	C	-1.49312300	-15.25388100	-4.66183300
	C	0.16985900	-12.68371100	-5.14378700
	C	-1.42466600	-13.96358000	-7.44810300
	H	-2.39459500	-15.80612000	-4.94155600
	H	-1.50942900	-15.08950400	-3.58169900
	H	-0.62530400	-15.87866800	-4.89678800
	H	0.16163000	-12.40484200	-4.08694800
	H	0.25807700	-11.77135500	-5.74072600
	H	1.05641500	-13.29916700	-5.32748600
	H	-1.39270100	-13.03115500	-8.01819600
	H	-2.32988400	-14.50799700	-7.73067900
	H	-0.55991100	-14.56894300	-7.73815800
17-4a	O	-0.31041200	-5.24655100	0.05193300
	C	-0.17956200	-2.27939100	-0.03282300
	H	0.57292100	-2.61565500	0.67871100
	H	0.03790700	-2.71161200	-1.01199900
	H	-1.16384300	-2.60267400	0.30325200
	N	-0.13180300	-0.80860800	-0.11472400
	S	-1.47742500	-5.58517800	0.90036100
	O	-2.16071900	-6.83679700	0.49127500
	O	-2.41155900	-4.44327600	1.07791100
	C	-0.81716100	-5.90873700	2.53188900
	H	-0.32003200	-5.00580700	2.88991100
	H	-0.10270700	-6.73020400	2.46745200
	H	-1.63898700	-6.17473400	3.19785900
	C	1.07151500	-0.16053900	-0.07205100
	C	1.15908900	1.21065100	-0.15500400
	H	2.14626600	1.64751100	-0.11688600
	C	-0.01122700	2.00225000	-0.26202700
	N	0.04652700	3.34061300	-0.31347900
	C	-1.24253200	1.30504500	-0.31841800
	H	-2.18583000	1.81936600	-0.43113600
	C	-1.27514300	-0.07170700	-0.26087800
	C	1.33825800	4.01668700	-0.27820500
	C	-1.18297400	4.11994400	-0.40006900
	H	1.17378900	5.09114800	-0.30607400
	H	1.95127900	3.73453700	-1.14011800
	H	1.88172100	3.77130000	0.63968900
	H	-1.73887200	3.87291500	-1.30997000
	H	-0.92938600	5.17705600	-0.42541300
	H	-1.82301500	3.93444400	0.46835100
	C	6.61302700	-10.49463700	0.88210700
	C	-6.52128600	-0.61742800	2.75427700

C	-5.22123900	-0.13280000	2.83519900
C	-4.13847700	-1.02628700	2.80879900
C	-5.68362200	-2.88388000	2.63291400
C	-6.75886100	-1.98504200	2.65792000
H	-7.35668400	0.07467800	2.76732600
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C	-1.65165800	-0.14403100	2.98070800
C	1.35320200	2.06736700	3.14113800
C	2.37178300	1.12864400	3.26734600
C	2.06425700	-0.24070800	3.31310600
C	-0.29312400	0.29609800	3.08203300
C	0.02555200	1.66253400	3.04681100
H	1.59563500	3.12510500	3.12223000
C	3.10542400	-1.21305200	3.45953000
C	3.98980000	-2.03257200	3.58417200
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C	6.38603600	-2.48267800	3.80167100
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C	5.35078100	-11.04016100	1.08345100
C	4.22914900	-10.19997000	1.16606000
C	5.66550100	-8.27234600	0.83742900
C	6.77927200	-9.11836600	0.76213400
H	7.47810500	-11.14770200	0.82721400
C	2.91900800	-10.74340500	1.36627500
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C	-0.93699800	-13.69923600	1.84004000
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C	-1.91594500	-11.48690200	1.83050000
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C	0.33427800	-13.14444300	1.72578300
H	-1.05243600	-14.77732200	1.88908400
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C	-7.47222500	-7.50855100	2.51336500
C	-6.20319500	-6.91879400	2.40032700
C	-5.21306100	-9.11918500	2.18168600
C	-6.48431400	-9.69954800	2.29902700
H	-8.58827700	-9.34197400	2.53889800
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C	-6.05109200	-5.49689000	2.47368400
C	-4.37045500	-2.40065000	2.69503700
C	0.73024500	-0.65082400	3.21766500
C	4.82484500	-4.33923000	3.81607800
C	4.39243700	-8.81832200	1.03918400
C	-0.64058900	-10.92707400	1.69697300



C	-5.07617200	-7.72645500	2.21807000
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H	-7.77264400	-2.36609800	2.59343800
H	3.40697000	1.44421000	3.33956300
H	-0.76993500	2.39331000	2.94158200
H	8.02667500	-5.43802300	4.13662800
H	6.56631100	-1.41543200	3.72982700
H	5.22197200	-12.11209500	1.19133200
H	7.76400000	-8.69128700	0.60430700
H	-3.05169400	-13.31099800	1.98721700
H	1.21412500	-13.77851100	1.68295500
H	-8.34304700	-6.87511500	2.64590000
H	-6.58300900	-10.77905600	2.25625700
H	-3.53815500	-3.09371800	2.61622200
H	0.48503900	-1.70748900	3.25586300
H	3.80782500	-4.71241600	3.75867200
H	3.52911700	-8.16374200	1.09825700
H	-0.53203500	-9.84960400	1.62606100
H	-4.09769000	-7.27693900	2.07181000
C	6.74265200	-11.38175300	4.31447700
C	5.57656300	-7.84986700	4.15750300
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C	5.55452500	-12.06152800	4.55324200
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C	6.74436200	-9.99834200	4.18157600
H	7.67369300	-11.93262300	4.23173300
C	4.34552100	-9.96066000	4.51523200
H	5.54800600	-13.14032400	4.66703400
H	7.66896800	-9.46331300	3.99220200
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C	2.11385800	-12.65900200	5.24133000
Si	0.57341400	-13.54889200	5.75121500
C	0.52738200	-15.21850200	4.89393000
C	-0.88807800	-12.46565200	5.29618400
C	0.63732300	-13.80897300	7.61112600
H	1.34794900	-15.85156200	5.24402000
H	0.60896800	-15.12076400	3.80906500
H	-0.41446900	-15.72850100	5.12028100
H	-0.81907200	-12.13071400	4.25791800
H	-0.92165500	-11.58180300	5.94038300
H	-1.82846700	-13.01267400	5.41755100
H	0.70365400	-12.85536200	8.14226500
H	1.49735000	-14.42171900	7.89547900
H	-0.26999400	-14.32173000	7.94666200
C	5.79927600	-6.85225000	0.72237500
C	5.85329300	-5.64472900	0.63630900
C	2.26351900	-0.92852800	0.05949400

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C	5.84401700	-4.21812200	0.53208800
C	4.58531900	-2.16170400	0.30588800
C	5.77723400	-1.42359000	0.34284300
H	7.91627200	-1.51835600	0.48386000
C	4.61891000	-3.55518700	0.40470600
H	7.98134000	-3.99179600	0.65297000
H	5.73923600	-0.34235500	0.26374800
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C	-7.03209700	-10.18367100	-1.11111200
C	6.32082600	-0.98462000	-3.00589300
C	5.04294900	-0.44784300	-3.10940200
C	3.92479600	-1.29682400	-3.10993100
C	5.39257400	-3.21645900	-2.89480900
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H	7.18330800	-0.32670300	-3.00244300
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C	1.47496300	-0.32573300	-3.31997700
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C	0.14121900	0.17966300	-3.44610500
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H	-1.57016100	3.10556300	-3.73355500
C	-5.77981600	-10.76875900	-1.24198600
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C	-7.15453000	-8.80312900	-0.98891500
H	-7.92142000	-10.80565400	-1.11764300
C	-3.33743900	-10.57680100	-1.37504600
C	-2.25765500	-11.11777700	-1.48046700
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C	1.42762900	-11.65621600	-1.80777100
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C	-0.90736700	-13.16913700	-1.52981500
H	0.38328600	-14.88558000	-1.56628900
C	2.62105300	-10.88333100	-1.97360100
C	3.63012500	-10.23240600	-2.13543200
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C	-0.93674000	-0.71155700	-3.51356800
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C	4.69546200	-8.04549600	-2.40505000
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H	7.49818200	-2.77981300	-2.80826400
H	-3.47912000	1.52554200	-3.83327300
H	0.74672100	2.24748600	-3.47845100
H	-5.68022700	-11.84293300	-1.35954500
H	-8.13148000	-8.34092300	-0.89194700
H	2.45965700	-13.54732100	-1.81800800
H	-1.81881600	-13.74616300	-1.41038200
H	7.96860900	-7.25893300	-2.89006800
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H	3.24104200	-3.33619000	-2.98615100
H	-0.75874600	-1.78089100	-3.46753700
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H	-8.21120200	-1.21196300	-0.82041300
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H	-4.02499300	-3.86168500	-0.50074900
C	-3.33879900	-1.14753600	-3.75439700
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H	-6.36055300	-12.93773200	-4.76003800
H	-8.35203400	-9.15967700	-4.27821800
H	-4.06573600	-9.30943900	-4.55102700
C	-3.88515200	-11.97300800	-4.88694700
C	-2.89574500	-12.64840400	-5.10880200
Si	-1.43428800	-13.69163000	-5.55783500
C	-1.52001400	-15.29938400	-4.59212100
C	0.12801300	-12.73211400	-5.17154100
C	-1.53711200	-14.05807500	-7.39775700
H	-2.42514300	-15.85837000	-4.84575900
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H	-0.65524100	-15.92479000	-4.83643800
H	0.14266300	-12.41216300	-4.12643600
H	0.20310100	-11.84361800	-5.80533100
H	1.01014400	-13.35513400	-5.35102800
H	-1.52350200	-13.13663100	-7.98615700
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