

## 1. Cartesian Coordinates

The numbers 0 and -1 represent the unfrozen and frozen atoms, respectively, during the geometry optimization in the present study.

### E:MPSs

H -1 17.45618800 55.72343100 15.73990800  
H -1 14.36501800 66.87378700 19.12447800  
H -1 8.60699800 62.77680500 18.32924200  
H -1 10.42810100 62.61781200 -1.01093800  
H -1 10.37420800 60.99319800 -0.26589700  
C 0 14.54346000 60.49433600 6.58461200  
C 0 14.85718700 61.64565100 7.30660100  
C 0 14.13311900 62.00121400 8.44095600  
C 0 13.09156900 61.17779300 8.88267500  
C 0 12.76729700 60.02317600 8.16154900  
C 0 13.48791500 59.68917700 7.01609600  
H 0 15.12568300 60.23061100 5.70799000  
H 0 15.67149000 62.28536000 6.99388600  
H 0 11.95149200 59.39084500 8.49159800  
H 0 13.21871800 58.78615700 6.48200000  
O 0 16.11937200 59.21140800 12.61092400  
O 0 15.20723100 60.21429000 12.07291600  
H 0 17.92626200 66.52449600 13.99312600  
C -1 10.91655200 57.40606200 14.32228000  
C 0 11.13452000 56.24359400 13.35522000  
O 0 10.23756400 55.89262400 12.59004500  
C 0 10.66664800 58.75406700 13.63313900  
O 0 11.81260500 59.36734900 13.04515000  
H 0 9.97416500 57.15880700 14.82852700  
H 0 9.87922200 58.61957200 12.88422500  
H 0 10.30421400 59.46846600 14.37574300  
H 0 12.00622000 59.00192900 12.16508200  
N 0 12.34448800 55.62150100 13.39447400  
C 0 12.50170400 54.30334300 12.78893100  
C 0 12.31329400 54.15422400 11.27204700  
O 0 12.04349700 53.04280100 10.82750900  
H 0 12.96089900 55.83168900 14.17790400  
H 0 13.51428500 53.96123600 13.02255600

N 0 12.53858300 55.23264600 10.48680000  
C -1 12.35116400 55.13832100 9.03907000  
C 0 12.25675500 56.53560700 8.43094000  
S 0 11.62144800 56.52107200 6.70560300  
H 0 12.66535500 56.14751200 10.90115500  
H 0 11.45285900 54.55079900 8.83515200  
H 0 11.59844400 57.17081200 9.02280600  
H 0 13.23462900 57.02204400 8.39560400  
H 0 10.31875000 56.58206600 7.05190400  
C -1 14.81301500 65.87507700 19.15135200  
C 0 16.29836400 65.92498400 18.76173500  
C 0 16.98482900 64.58149000 19.03450300  
C 0 16.47614200 66.34587900 17.29905600  
H 0 14.67642500 65.48008200 20.16502700  
H 0 14.25168900 65.23165600 18.46245600  
H 0 16.78745500 66.67911600 19.39514300  
H 0 18.03675000 64.60859000 18.73294700  
H 0 16.93612800 64.31110700 20.09570600  
H 0 16.49865400 63.78082600 18.46562300  
H 0 17.52775300 66.41491900 17.00474000  
H 0 15.99265400 65.61985600 16.63287300  
H 0 16.01381400 67.32064500 17.11051900  
C -1 8.77939900 61.70512500 18.47229000  
C 0 10.21673100 61.31882600 18.09896600  
C 0 10.52555000 59.86500700 18.47487400  
C 0 10.39625600 61.53729200 16.59645300  
H 0 8.53534800 61.45263700 19.50932600  
H -1 8.12205400 61.13711100 17.80595500  
H 0 10.91715100 61.97058700 18.63848800  
H 0 11.54283900 59.58699300 18.18021700  
H 0 10.42461600 59.69671500 19.55253000  
H 0 9.83672700 59.17989500 17.96503600  
H 0 11.39018200 61.25725900 16.24392000  
H 0 9.67139900 60.92952600 16.04248100  
H 0 10.22311500 62.58050900 16.32198600  
C -1 6.93641800 59.40342200 7.02366000  
C 0 7.80850100 58.79902500 8.09305800  
C 0 7.83523900 57.41281400 8.29446900  
C 0 8.60868700 59.60751200 8.91097500  
C 0 8.61940600 56.84966800 9.30146200  
C 0 9.39104700 59.04958900 9.92255100  
C 0 9.39437300 57.66818100 10.12480400  
H 0 6.66641900 58.65973300 6.26809900  
H 0 7.45257100 60.21948900 6.51112500  
H 0 7.22980800 56.77260400 7.65756700  
H 0 8.62072500 60.68306700 8.75404900  
H 0 8.62706800 55.77473600 9.45519500  
H 0 10.00622100 59.69589700 10.54028000  
H 0 9.97458000 57.21320100 10.91775500  
C -1 17.74272200 56.74907900 15.48496700  
N 0 16.90150400 56.23663300 13.04964700  
C 0 16.61833900 55.98856600 11.72061000  
O 0 17.28424700 55.23376100 11.03870500  
N 0 15.46171300 56.59471500 11.16246600  
C 0 14.65645000 57.50729000 11.76965400  
C 0 15.27417400 58.12363000 13.03090000  
O 0 13.57976500 57.87623500 11.31121900  
C 0 14.73158000 58.98532800 15.17821700  
N 0 14.27665800 58.46876100 13.97194600  
C 0 14.04977900 59.99003000 15.87277400  
C 0 14.50415500 60.46251700 17.10438000  
C 0 13.82454100 61.61985000 17.78951600  
C 0 15.64916400 59.87430200 17.68226400  
C 0 16.16696100 60.34320200 19.01787200  
C 0 16.34116700 58.89036900 16.97856600  
C 0 15.92126800 58.45864100 15.71514700  
C 0 16.28652900 57.19899300 13.66529700  
N 0 16.61516000 57.48941500 14.95041300  
H 0 15.29695500 56.37652700 10.18420200  
H 0 13.29821100 61.30421100 18.69783200  
H 0 14.55204000 62.37859500 18.09436100  
H 0 13.10217300 62.10242500 17.13182800  
H 0 15.38842400 60.31532900 19.78803300  
H 0 16.99920400 59.72180800 19.35799400  
H 0 16.52557400 61.37809700 18.96683300  
H 0 13.18065300 60.43287200 15.39831300  
H 0 17.23413600 58.48038900 17.43123500  
H 0 18.14026600 57.24691900 16.36336500  
H 0 18.51632700 56.68916400 14.72032900  
C -1 21.24030000 63.62153100 14.93454400  
C 0 20.23257400 62.86966700 14.06510400  
O 0 20.57029400 62.34295000 13.00239700  
C 0 21.31251600 65.09832600 14.47626700  
C 0 19.97745100 65.80555200 14.75119900  
O 0 19.16048700 65.85365600 13.74390300  
O 0 19.74317200 66.20339000 15.89676600  
H 0 20.98177700 63.59659100 15.99564600  
H 0 22.09778900 65.60540100 15.04355500  
H 0 21.55757200 65.13173900 13.41132600  
N 0 18.91960500 62.87215100 14.45046600

C 0 17.92248600 62.18283700 13.63206100	H 0 20.79267500 64.16066500 8.36782700	H 0 11.63462000 60.48513900 2.19574100
C 0 17.55980000 62.82430700 12.30626200	N 0 17.29042500 60.68533400 9.18533700	C -1 8.85004200 61.71563700 4.23794900
O 0 16.74820800 62.20346900 11.56646400	C 0 16.54906900 59.43947000 9.20967400	C 0 10.27252700 61.37334900 4.69858800
C 0 16.64339800 62.16123600 14.51314500	C 0 17.41150900 58.18301600 9.19539400	C 0 10.71755700 62.27747100 5.85638600
C 0 17.17758300 62.38145800 15.92855600	O 0 16.92924900 57.13197600 8.76090800	C 0 10.39996400 59.89243700 5.06943900
C 0 18.32323300 63.36374800 15.70501800	H 0 17.17698000 61.34284900 9.95479700	H 0 8.15656700 61.67679900 5.08823200
H 0 18.26972600 61.17131500 13.39624100	H 0 15.91250400 59.44607100 10.09449300	H -1 8.80504700 62.73710500 3.84512800
H 0 15.99738100 62.99816500 14.23284100	H 0 15.90403700 59.36913900 8.33414100	H 0 10.94755800 61.56964700 3.85828400
H 0 16.09020900 61.23341900 14.38831900	N 0 18.66593800 58.29382300 9.70203200	H 0 11.75200100 62.07376500 6.14455600
H 0 16.41412800 62.77714800 16.59918100	C -1 19.68171800 57.26469900 9.50387800	H 0 10.65398100 63.33653400 5.58485500
H 0 17.55512900 61.44491600 16.34963000	C 0 20.92796100 57.79685200 8.79629600	H 0 10.08866800 62.11343100 6.74108300
H 0 17.95218700 64.38156700 15.57260700	C 0 20.61283200 58.34777500 7.39680500	H 0 11.43238800 59.63248800 5.30849900
H 0 19.05396500 63.37544500 16.51216000	C 0 19.88729700 57.29310100 6.56021300	H 0 9.79666000 59.64994400 5.95187600
N 0 18.03230200 64.01416600 11.95911900	N 0 18.71976700 57.70207400 6.00064500	H 0 10.07048400 59.24386400 4.24946100
C 0 17.37317000 64.75337700 10.87693300	O 0 20.34723300 56.16098400 6.42346100	C 0 14.93819500 68.89437200 14.27434800
C 0 17.40048900 64.01908700 9.53960200	H 0 18.97351100 59.23172700 9.92974000	C 0 14.70448100 67.37786700 14.27821400
O 0 16.52277800 64.21675100 8.69971100	H 0 19.20892200 56.51892600 8.85932600	C 0 15.91144300 66.51739900 13.92088500
C 0 17.95717600 66.18159900 10.76363000	H 0 21.41309000 58.57486000 9.39964000	O 0 17.05671900 67.12754400 14.11159500
C 0 17.14919800 67.02797700 9.76177500	H 0 21.63248600 56.96510900 8.70032600	O 0 15.77823200 65.35243700 13.54229200
C 0 19.45715200 66.18909000 10.45068800	H 0 20.02584000 59.26354000 7.46546600	H 0 14.90329000 69.26798500 13.24279300
C 0 17.25369100 68.52768700 10.04610200	H 0 21.55046400 58.58897500 6.88247700	H 0 15.94869800 69.09101200 14.63944400
H 0 18.56463300 64.56371000 12.65421100	H 0 18.27131800 58.55221500 6.32656500	H 0 14.41752500 67.05603100 15.28843400
H 0 16.31445400 64.84148000 11.13023200	H 0 18.13830200 56.99173300 5.57637100	H 0 13.87689700 67.08953600 13.62344200
H 0 17.82268100 66.62178500 11.75510800	C -1 19.48694800 53.29109200 7.88410200	C -1 18.60108700 58.32705800 1.75354900
H 0 17.48252400 66.81136200 8.74018000	C 0 18.07602600 53.45561800 7.34243000	C 0 17.29818600 58.70041700 2.48221300
H 0 16.09833000 66.73012400 9.79318800	N 0 17.21907800 54.15671700 8.12805800	C 0 17.08123300 60.18645100 2.62926600
H 0 19.84096100 67.21287500 10.46658700	O 0 17.72391100 52.95721600 6.27218800	C 0 16.63372100 60.96469200 1.55442600
H 0 20.02389100 65.62090800 11.19178200	H 0 19.89197700 54.24386600 8.23234100	C 0 17.34931400 60.82588900 3.84664100
H 0 19.65311400 65.77304900 9.45702800	H 0 20.11727700 52.91897200 7.07742700	C 0 16.44669700 62.34035500 1.69279900
H 0 16.64958400 69.10379700 9.33769600	H 0 16.30075700 54.34004200 7.75356400	C 0 17.15774100 62.19993800 3.98960600
H 0 16.89846600 68.75631200 11.05764300	H 0 17.49373600 54.69212800 8.94147300	C 0 16.70148600 62.96458900 2.91499000
H 0 18.28505500 68.88916100 9.97403600	C -1 10.76499000 62.01128100 -0.16372500	H 0 18.56250700 58.56987800 0.68718700
N 0 18.45261500 63.19192400 9.29976700	C 0 12.30892100 62.01822700 -0.19475200	H 0 19.45658300 58.84810700 2.19439600
C -1 18.55248900 62.47021500 8.05097900	C 0 12.96993600 60.81383300 0.50373000	H 0 16.44872400 58.24860600 1.95873500
C 0 17.87596100 61.09112400 8.04748000	C 0 12.83239700 63.36654800 0.31385000	H 0 17.31057900 58.24519000 3.47571300
O 0 17.92922300 60.39753300 7.02352200	C 0 12.69643400 60.65539400 1.99855000	H 0 16.42617200 60.48423500 0.60128900
C 0 20.02436600 62.25440200 7.67916800	H 0 10.36913500 62.43276300 0.76558100	H 0 17.70954600 60.25408900 4.69383900
C 0 20.79535200 63.54871900 7.46309200	H 0 12.60280400 61.93460100 -1.25152600	H 0 16.09935400 62.92565600 0.84650200
O 0 20.55691900 61.49720500 8.77833800	H 0 12.64657300 59.90054200 -0.01424000	H 0 17.35853700 62.66824300 4.94862200
H 0 19.12577700 62.99642900 10.03038900	H 0 14.05300900 60.88474700 0.35069700	H 0 16.52857100 64.02900400 3.03463800
H -1 18.05384300 63.07807200 7.28934600	H 0 13.92574400 63.40489100 0.31459400	C -1 15.09104100 52.38697200 3.66511100
H 0 20.03149500 61.64934800 6.76472100	H 0 12.46421800 64.18969100 -0.30878600	C 0 16.11928500 53.48447600 3.33421300
H 0 21.49933600 61.35434600 8.62651600	H 0 12.49156700 63.55747100 1.33520000	C 0 15.61685400 54.86463900 3.70428600
H 0 21.83525500 63.33271700 7.19336800	H 0 13.25005600 59.80215400 2.40290000	C 0 14.76518000 55.56976600 2.84465400
H 0 20.35356300 64.12829500 6.64660300	H 0 13.00931400 61.53353500 2.56988200	C 0 15.94977400 55.44816600 4.93563800

C 0 14.25836300 56.81919300 3.20105100  
C 0 15.44082000 56.69829700 5.30218800  
C 0 14.59601700 57.38853900 4.42891100  
H 0 14.12170800 52.60471800 3.20326500  
H 0 17.04472900 53.27517000 3.87701900  
H 0 16.34526600 53.46001300 2.26039900  
H 0 14.49668700 55.13148300 1.88596800  
H 0 16.61268100 54.90035300 5.59666000  
H 0 13.59927100 57.35216600 2.52134100  
H 0 15.70471500 57.12319200 6.26801100  
H 0 14.20528800 58.36395900 4.69142400  
C -1 9.36801700 64.78906800 13.86241500  
C 0 10.50888100 63.94658300 13.27896000  
C 0 11.76760600 64.15297200 14.13727700  
C 0 10.09528000 62.47288300 13.17124600  
H 0 9.26692900 64.56815900 14.93431200  
H 0 10.73172200 64.31037600 12.26690600  
H 0 12.61063100 63.55030000 13.79468700  
H 0 12.08755200 65.20003600 14.11949200  
H 0 11.57466800 63.88553300 15.18236000  
H 0 10.93664200 61.81497800 12.94281300  
H 0 9.65227000 62.12433900 14.10854900  
H 0 9.34464300 62.33765000 12.38533800  
H -1 15.41792100 51.40123500 3.31799500  
H -1 8.46279400 61.01894600 3.48752500  
H -1 18.76091400 57.25115300 1.87951100  
H -1 19.49903000 52.57368200 8.71124400  
H -1 22.21787300 63.14345900 14.80755900  
H -1 19.93336800 56.70798700 10.41261200  
H -1 6.00260500 59.81679800 7.41868700  
H -1 11.67888500 57.43269000 15.10812500  
H 0 11.79825300 53.58578100 13.22323600  
H -1 9.59030600 65.85831800 13.78351100  
H -1 8.38402000 64.58740000 13.42591800  
H 0 14.94493600 52.33131700 4.74771100  
H -1 13.20190600 54.61272600 8.59414200  
C -1 13.92188500 69.63624900 15.14353400  
H -1 14.06738700 70.72214200 15.13401900  
H -1 12.89126300 69.40645800 14.84957000  
H 0 14.02436700 69.31371800 16.18766900  
H 0 13.41967300 58.88752400 13.59302300  
C -1 9.09322200 66.03195300 8.85530900  
C 0 10.47216600 65.45326600 8.41481500  
C 0 11.61571100 66.08788100 9.17841600  
C 0 11.85943500 67.46664100 9.08569000

C 0 12.42326900 65.32858500 10.03003500  
C 0 12.87430600 68.06630700 9.82951000  
C 0 13.43210500 65.92434700 10.79285100  
C 0 13.65755300 67.29774400 10.69426900  
H -1 9.29287800 66.79649200 9.61304300  
H -1 8.44501900 65.25544500 9.27465000  
H 0 8.55799400 66.50271300 8.02530900  
H 0 10.50283300 64.37052700 8.56479200  
H 0 10.63022100 65.61019300 7.34258400  
H 0 11.24421700 68.07348900 8.42561700  
H 0 12.24394600 64.26117000 10.08680000  
H 0 13.05213800 69.13442300 9.74096000  
H 0 14.03490300 65.33236400 11.47540400  
H 0 14.44033200 67.76509000 11.28221700  
C -1 12.60585400 56.71573500 17.61675200  
C 0 13.44352100 55.53959100 17.13826200  
O 0 14.00163600 55.78553400 15.84289800  
H -1 12.18864200 56.58079700 18.62027100  
H -1 11.78064300 56.90578100 16.92283000  
H 0 13.21982300 57.62448800 17.64709100  
H 0 14.24581100 55.31776300 17.85661400  
H 0 12.83747800 54.63534300 17.03263100  
H 0 14.45479900 56.63975200 15.87983900  
H 0 10.16269600 66.90278300 4.04552500  
C -1 10.41973700 67.50462800 4.92181600  
C 0 11.94073800 67.61439900 5.11466900  
C 0 12.69822000 66.30863000 5.13582000  
C 0 13.51275500 65.97394100 6.22315200  
C 0 12.65476100 65.44110600 4.03561200  
C 0 14.26913500 64.80208200 6.22168400  
C 0 13.41312500 64.27368400 4.02705600  
C 0 14.21810000 63.95155100 5.11859400  
H 0 9.92643600 67.06692400 5.79378400  
H 0 12.34040200 68.23740600 4.30222100  
H 0 12.14517700 68.16083700 6.04178900  
H 0 13.55972400 66.63933800 7.07919500  
H 0 12.04076000 65.69226400 3.17369400  
H 0 14.90147700 64.57308800 7.07189300  
H 0 13.40021300 63.61807200 3.16452600  
H 0 14.79827900 63.04019900 5.09455800  
H -1 10.04563500 68.52173700 4.76349500  
S 0 12.09038900 61.57047600 10.30703500  
C 0 13.30446000 62.27509200 11.48137300  
H 0 12.98799300 63.27080500 11.77895800  
H 0 13.36969300 61.62556400 12.35234100

H 0 14.28274500 62.34476500 11.01093000  
H 0 14.39046200 62.91760400 8.95838800  
H 0 15.85018500 60.98437100 11.98456500  
**E:MPS<sub>R</sub>**  
H -1 17.45639400 55.72340500 15.74003400  
H -1 14.36514200 66.87383900 19.12436400  
H -1 8.60697000 62.77679100 18.32916600  
H -1 10.42811600 62.61773400 -1.01100000  
H -1 10.37418900 60.99323100 -0.26615500  
C 0 14.64251100 60.59691800 6.44743400  
C 0 14.91817800 61.60075100 7.37661700  
C 0 14.19780900 61.69854600 8.56218700  
C 0 13.15844700 60.79386900 8.82759700  
C 0 12.85514700 59.81054500 7.88181000  
C 0 13.60268200 59.70784800 6.71055100  
H 0 15.23130100 60.51405100 5.54015700  
H 0 15.70217600 62.32438300 7.19679400  
H 0 12.03919300 59.12039400 8.03753900  
H 0 13.35481500 58.91277100 6.02063200  
O 0 16.01311100 59.27092400 12.65899700  
O 0 15.06255100 60.24139000 12.11081700  
H 0 18.02850200 66.60785000 13.99609900  
C -1 10.91671200 57.40597400 14.32208500  
C 0 11.09329900 56.32110700 13.26590000  
O 0 10.25810300 56.20128100 12.36885100  
C 0 10.64781400 58.78814200 13.72054400  
O 0 11.78787700 59.42876600 13.16158000  
H 0 9.98731200 57.11855100 14.83544300  
H 0 9.85624500 58.69119600 12.96939700  
H 0 10.29126200 59.45968400 14.50485600  
H 0 12.06149700 58.99907500 12.33029400  
N 0 12.16068400 55.49391400 13.39914200  
C 0 12.18074100 54.19014500 12.74931700  
C 0 12.09309100 54.11083400 11.22109600  
O 0 11.73886600 53.04729900 10.72022300  
H 0 12.75097000 55.60364200 14.22348600  
H 0 13.11435400 53.69934500 13.03932000  
N 0 12.48820500 55.18110300 10.49217600  
C -1 12.35095400 55.13834700 9.03911800  
C 0 12.24802500 56.53770600 8.45428300  
S 0 11.95932100 56.50261700 6.63796800  
H 0 12.60187600 56.08215200 10.94148500  
H 0 11.46159000 54.55136400 8.79378100  
H 0 11.43140500 57.08736800 8.92647600

H 0 13.16615900 57.11023700 8.60577300	O 0 17.21916300 55.29640000 11.03828600	H 0 15.95622500 62.90801500 14.24627700
H 0 10.61972000 56.38220700 6.72771300	N 0 15.40126200 56.66120400 11.20393400	H 0 16.15494600 61.15890300 14.45493300
C -1 14.81281200 65.87499300 19.15156500	C 0 14.57280400 57.51678000 11.86054200	H 0 16.42054400 62.81569000 16.59938400
C 0 16.31527700 65.92393700 18.83268600	C 0 15.21793300 58.16117800 13.09827800	H 0 17.60901900 61.51630800 16.39788600
C 0 16.97697000 64.56783600 19.10533600	O 0 13.44977300 57.81223000 11.46286100	H 0 17.88699800 64.42364500 15.47486500
C 0 16.56216400 66.37312700 17.38864800	C 0 14.73780100 58.99662800 15.27437900	H 0 19.03392200 63.51847800 16.46414000
H 0 14.62838000 65.46017600 20.14976000	N 0 14.24113900 58.46923300 14.08219500	N 0 17.98623000 64.00356000 11.94791700
H 0 14.28312400 65.24635300 18.42507600	C 0 14.06659600 59.99091900 15.99112600	C 0 17.29343200 64.72459000 10.87375100
H 0 16.77960400 66.65932500 19.50566000	C 0 14.55280500 60.46103800 17.21170500	C 0 17.36716100 64.01207300 9.52476800
H 0 18.04410300 64.59347900 18.86261400	C 0 13.86855400 61.59428700 17.93149100	O 0 16.50751100 64.20942400 8.66630600
H 0 16.86836300 64.26844500 20.15432700	C 0 15.72672000 59.88894300 17.74537900	C 0 17.79336200 66.18444900 10.79092800
H 0 16.51830300 63.78802600 18.48718100	C 0 16.28475100 60.36310500 19.06280500	C 0 16.85809000 67.03801700 9.91556800
H 0 17.62509100 66.42531300 17.13399000	C 0 16.40593500 58.91341900 17.01696200	C 0 19.26174800 66.27826200 10.36274600
H 0 16.09238900 65.67187200 16.68822000	C 0 15.94413800 58.47493300 15.77169100	C 0 17.02359800 68.53784700 10.17357800
H 0 16.12840400 67.36179600 17.20443300	C 0 16.26826000 57.24909300 13.69574700	H 0 18.52844500 64.55861300 12.62754700
C -1 8.77931700 61.70516800 18.47268300	N 0 16.61443500 57.51054800 14.98142400	H 0 16.22867800 64.74172700 11.11463800
C 0 10.21919100 61.34700900 18.07792000	H 0 15.19067400 56.41082500 10.24311000	H 0 17.72099100 66.56820000 11.81106400
C 0 10.53505100 59.87323000 18.35753600	H 0 13.39210400 61.25765600 18.86005300	H 0 17.02284200 66.80918300 8.85685300
C 0 10.40401600 61.66812600 16.59337100	H 0 14.58342400 62.37540100 18.20871700	H 0 15.82078700 66.75486400 10.12017900
H 0 8.54812700 61.44454000 19.51020100	H 0 13.10265900 62.05487000 17.30827000	H 0 19.61373100 67.31090000 10.42839700
H -1 8.12219700 61.13714200 17.80578800	H 0 15.53723000 60.31264400 19.86218000	H 0 19.90280100 65.67976000 11.01526500
H 0 10.91521200 61.96438500 18.66195100	H 0 17.14400000 59.76012400 19.36696800	H 0 19.39466600 65.94139500 9.32879700
H 0 11.55734200 59.62275400 18.05607000	H 0 16.61597000 61.40647100 19.00382100	H 0 16.30522100 69.11709000 9.58426400
H 0 10.42451500 59.63133200 19.42021000	H 0 13.17876300 60.42557100 15.54463300	H 0 16.85887800 68.76851300 11.23236700
H 0 9.85598600 59.21971900 17.79540900	H 0 17.32073600 58.51581300 17.43606100	H 0 18.02579600 68.89322000 9.91194400
H 0 11.39949400 61.41216200 16.22568000	H 0 18.16093000 57.23362000 16.36123600	N 0 18.43122700 63.19398400 9.30009700
H 0 9.68140700 61.10101800 15.99528700	H 0 18.50184800 56.69061800 14.70634400	C -1 18.55345700 62.47061200 8.05076500
H 0 10.23419300 62.72826000 16.38726800	C -1 21.24038800 63.62201200 14.93284000	C 0 17.89634200 61.08123600 8.06364600
C -1 6.93673800 59.40335500 7.02372200	C 0 20.22934500 62.86826900 14.06635500	O 0 17.96677800 60.36720300 7.05495400
C 0 7.54194600 58.32316500 7.88868100	O 0 20.57389600 62.30975600 13.02196800	C 0 20.03151900 62.27739200 7.69373900
C 0 7.90464400 57.08683800 7.34066500	C 0 21.33292300 65.09134400 14.45542400	C 0 20.78108400 63.58711200 7.49385100
C 0 7.79723700 58.54074500 9.25055900	C 0 20.01546000 65.82894200 14.72563300	O 0 20.56380100 61.52252400 8.79412700
C 0 8.51058300 56.09935200 8.12339900	O 0 19.20736800 65.90477900 13.71244900	H 0 19.09223100 63.00109000 10.04243900
C 0 8.40909500 57.56169000 10.03321100	O 0 19.78586200 66.22950800 15.87129300	H -1 18.05278000 63.07757500 7.28960500
C 0 8.77613800 56.33589800 9.47269500	H 0 20.98067200 63.61006300 15.99383100	H 0 20.05955900 61.67735500 6.77612500
H 0 6.73438700 59.03155800 6.01564700	H 0 22.13034300 65.59193600 15.01179300	H 0 21.51263900 61.40796700 8.65949300
H 0 7.62988600 60.24591800 6.91945600	H 0 21.57318700 65.10618100 13.38895600	H 0 21.83142500 63.39284600 7.24913600
H 0 7.71244500 56.89703900 6.28785500	N 0 18.91067000 62.90210100 14.43164500	H 0 20.34656400 64.15577700 6.66579800
H 0 7.52189500 59.49334200 9.69694100	C 0 17.91661000 62.18266300 13.63373100	H 0 20.74220600 64.20063600 8.39685200
H 0 8.77123000 55.14304400 7.67848000	C 0 17.51559900 62.81486700 12.31339500	N 0 17.30482300 60.68840100 9.20410900
H 0 8.61482100 57.73405400 11.08385900	O 0 16.68869800 62.19712300 11.59004200	C 0 16.55671300 59.44623600 9.23980100
H 0 9.26105100 55.59051800 10.09341200	C 0 16.65477800 62.12061600 14.53989400	C 0 17.41272700 58.18722100 9.20682700
C -1 17.74232200 56.74927200 15.48466300	C 0 17.19403200 62.41962500 15.94004000	O 0 16.92333300 57.14245600 8.76824500
N 0 16.88620800 56.30609600 13.05286800	C 0 18.30141400 63.43231900 15.66398500	H 0 17.17565900 61.35558800 9.96303700
C 0 16.57304700 56.05500500 11.73397000	H 0 18.29292400 61.18379600 13.39056300	H 0 15.94209100 59.45342300 10.14035700

H 0 15.89260700 59.37747300 8.37805100	H 0 10.95094400 61.52835300 3.88339600	H 0 16.52731400 54.94943500 5.58199700
N 0 18.67057200 58.29435800 9.70571200	H 0 11.73227400 62.00088300 6.18855000	H 0 13.78752500 57.34930300 2.21973800
C -1 19.68170600 57.26453300 9.50367000	H 0 10.68931800 63.29811500 5.60275900	H 0 15.65403300 57.23177000 6.09428900
C 0 20.93507500 57.79546500 8.80710100	H 0 10.05595700 62.09956900 6.74856300	H 0 14.31816800 58.44838600 4.36683900
C 0 20.63716900 58.33451100 7.39902400	H 0 11.35747200 59.56996600 5.34081400	C -1 9.36858400 64.78778100 13.86295400
C 0 19.91222400 57.26928400 6.57700100	H 0 9.70248700 59.62573100 5.93693800	C 0 10.47237200 63.96578100 13.17882100
N 0 18.71852200 57.65322400 6.05795400	H 0 10.01551000 59.22859200 4.24211500	C 0 11.79937800 64.09689400 13.93662500
O 0 20.38879400 56.14562700 6.42635700	C 0 14.95818500 68.89574100 14.29944700	C 0 10.05844500 62.49764400 13.02577600
H 0 18.98066400 59.23035100 9.93735800	C 0 14.79341300 67.37535000 14.39455000	H 0 9.30292600 64.53690500 14.92960600
H 0 19.20950100 56.52081800 8.85658900	C 0 16.02867300 66.54758000 14.05969500	H 0 10.62927900 64.37258200 12.17225000
H 0 21.40977100 58.57893800 9.41155900	O 0 17.15059900 67.21753300 14.12750400	H 0 12.59681900 63.54004400 13.43826100
H 0 21.64334700 56.96519700 8.72642400	O 0 15.93660900 65.34478800 13.80052100	H 0 12.12114100 65.14106000 13.99827800
H 0 20.05350400 59.25356300 7.45272200	H 0 14.90141300 69.20990700 13.24928400	H 0 11.70767900 63.71283000 14.95927700
H 0 21.58062400 58.56253300 6.89010800	H 0 15.96201200 69.15627200 14.64318200	H 0 10.88419900 61.88966900 12.64983200
H 0 18.27097100 58.50601800 6.37828300	H 0 14.54150900 67.09971300 15.42704400	H 0 9.74893200 62.07385400 13.98654000
H 0 18.13806800 56.93472500 5.64681400	H 0 13.96091500 67.01460800 13.78370700	H 0 9.21255900 62.39866300 12.33510100
C -1 19.48707300 53.29100800 7.88397000	C -1 18.60133600 58.32716700 1.75399000	H -1 15.41792800 51.40124100 3.31798500
C 0 18.07545100 53.48418800 7.35139400	C 0 17.55171500 58.78822800 2.77340100	H -1 8.46289700 61.01901400 3.48740900
N 0 17.23500400 54.19903700 8.14220400	C 0 17.24157500 60.26687100 2.75341000	H -1 18.76068200 57.25108500 1.87922800
O 0 17.70799500 52.99631200 6.28139300	C 0 16.72727900 60.88369800 1.60468600	H -1 19.49894700 52.57379300 8.71134100
H 0 19.91270900 54.23691300 8.22666900	C 0 17.44066500 61.05427300 3.89545900	H -1 22.21776000 63.14285800 14.80895200
H 0 20.10335800 52.90865000 7.07115800	C 0 16.41760000 62.24342000 1.59643900	H -1 19.93332200 56.70816200 10.41273200
H 0 16.32325300 54.41046600 7.76636500	C 0 17.11911500 62.41292700 3.89313400	H -1 6.00266200 59.81695100 7.41866400
H 0 17.52134900 54.73729700 8.94931900	C 0 16.60465300 63.01526300 2.74493300	H -1 11.67879000 57.43291000 15.10821500
C -1 10.76511800 62.01133000 -0.16330100	H 0 18.28041100 58.51008700 0.72317000	H 0 11.35536200 53.56358200 13.10383500
C 0 12.30900800 62.03615500 -0.16606200	H 0 19.55745400 58.83829900 1.90585200	H -1 9.58983200 65.85840000 13.78328800
C 0 12.97026500 60.82984700 0.52931100	H 0 16.62912900 58.22559300 2.60096700	H -1 8.38398700 64.58828600 13.42558200
C 0 12.80377600 63.38139100 0.38019900	H 0 17.89211400 58.51172400 3.77432500	H 0 14.92618700 52.33467400 4.74492900
C 0 12.67288500 60.65998100 2.01836800	H 0 16.56336300 60.29031400 0.70861700	H -1 13.20197700 54.61279200 8.59420500
H 0 10.35327800 62.43051400 0.76058600	H 0 17.83704800 60.60706300 4.80081300	C -1 13.92153800 69.63673200 15.14269900
H 0 12.62602500 61.97495100 -1.21749700	H 0 16.02751100 62.70091200 0.69197900	H -1 14.06766200 70.72210900 15.13459900
H 0 12.66125200 59.91879800 -0.00113900	H 0 17.26423600 63.00159300 4.79468200	H -1 12.89127200 69.40612900 14.84979100
H 0 14.05531300 60.90945600 0.39487700	H 0 16.34097100 64.06784200 2.75045300	H 0 14.01590600 69.32378900 16.19102400
H 0 13.89610600 63.44197000 0.38408000	C -1 15.09103700 52.38696400 3.66513000	H 0 13.39233700 58.92681900 13.72981300
H 0 12.42045900 64.21335600 -0.22117100	C 0 16.14503700 53.46168700 3.34211400	C -1 9.09313800 66.03194900 8.85506800
H 0 12.45708900 63.53646500 1.40622100	C 0 15.64901700 54.86083900 3.63354800	C 0 10.44770700 65.49358100 8.34529200
H 0 13.21460700 59.80002100 2.42441100	C 0 14.86865900 55.54701900 2.69503800	C 0 11.54536600 65.52586600 9.38770600
H 0 12.97949500 61.53309400 2.60152000	C 0 15.92244100 55.48672200 4.85869900	C 0 11.94490100 66.74053100 9.96755800
H 0 11.60709400 60.49186900 2.19547600	C 0 14.38170600 56.82565400 2.96380300	C 0 12.20148200 64.35824400 9.78274800
C -1 8.84960900 61.71550400 4.23805400	C 0 15.43536700 56.76690300 5.13596600	C 0 12.95533900 66.78042800 10.92781100
C 0 10.25956400 61.34738800 4.71285200	C 0 14.67104000 57.44147900 4.18098600	C 0 13.20937600 64.39400700 10.74686900
C 0 10.71167600 62.23831000 5.87800300	H 0 14.13386900 52.61595500 3.18388700	C 0 13.58867700 65.60126200 11.32891900
C 0 10.34051100 59.86066600 5.07666500	H 0 17.04398800 53.26080500 3.93051000	H -1 9.29288100 66.79647800 9.61305600
H 0 8.14825800 61.67447900 5.08260800	H 0 16.41534900 53.39427400 2.28050100	H -1 8.44514500 65.25543900 9.27483700
H -1 8.80518800 62.73712600 3.84516700	H 0 14.64654300 55.07289100 1.74159900	H 0 8.52802300 66.50122200 8.04197700

H 0 10.34301000 64.47784600 7.95298800	H -1 14.36500600 66.87378000 19.12441500	H 0 14.69580000 65.48787100 20.17053800
H 0 10.77311700 66.10355500 7.49687600	H -1 8.60683600 62.77683100 18.32963200	H 0 14.23746000 65.22656000 18.47919800
H 0 11.46107800 67.66500400 9.66013600	H -1 10.42842100 62.61807800 -1.01087500	H 0 16.79746100 66.66274000 19.36259100
H 0 11.91726800 63.41074700 9.34144000	H -1 10.37412700 60.99333000 -0.26687400	H 0 18.02160300 64.59667500 18.65790900
H 0 13.25032100 67.73081000 11.36482800	C 0 14.19072100 60.63717500 6.70872000	H 0 16.93838700 64.27878100 20.03054600
H 0 13.69151400 63.47532500 11.06310900	C 0 14.78883900 61.78790700 7.21632800	H 0 16.47748500 63.77865600 18.39637400
H 0 14.35633300 65.60687500 12.09466700	C 0 14.52340200 62.21722100 8.51483300	H 0 17.49176800 66.42343000 16.96399600
C -1 12.60594100 56.71578800 17.61681500	C 0 13.65303600 61.47412900 9.31927200	H 0 15.95304500 65.62807700 16.60606000
C 0 13.44373000 55.54734600 17.12122400	C 0 13.04326400 60.31610000 8.81437500	H 0 15.97672900 67.32671700 17.09533100
O 0 13.86886100 55.74108100 15.76661900	C 0 13.30752900 59.90780900 7.50882800	C -1 8.77987700 61.70537700 18.47134800
H -1 12.18857800 56.58079200 18.62024400	H 0 14.42175500 60.31328100 5.69947400	C 0 10.22174900 61.34476900 18.08858300
H -1 11.78065200 56.90564100 16.92280900	H 0 15.48759600 62.34806900 6.60910000	C 0 10.53806900 59.87386200 18.38195200
H 0 13.21495800 57.62772500 17.64361800	H 0 12.37241000 59.73726900 9.43638500	C 0 10.41594800 61.65409400 16.60348500
H 0 14.31783800 55.39445000 17.76982300	H 0 12.82094200 59.01996100 7.12001200	H 0 8.54391100 61.44635200 19.50845500
H 0 12.86865800 54.61680900 17.11801800	O 0 16.00822700 59.34333100 12.67518300	H -1 8.12185500 61.13695500 17.80628500
H 0 14.19628200 56.64732600 15.67091700	O 0 14.77280300 60.50967800 11.98517800	H 0 10.91295900 61.96797500 18.67214800
H 0 10.22055000 66.91985000 4.01912600	H 0 17.92201100 66.50539300 14.03883000	H 0 11.56046400 59.62105700 18.08357100
C -1 10.41966600 67.50460300 4.92198700	C -1 10.91677500 57.40612400 14.32221500	H 0 10.42671400 59.64234100 19.44682300
C 0 11.92741600 67.62013500 5.19837100	C 0 11.12686200 56.32184300 13.26527900	H 0 9.85979800 59.21507600 17.82527900
C 0 12.68341300 66.31454000 5.22083400	O 0 10.30785400 56.17841800 12.35682500	H 0 11.42417400 61.42717600 16.25168400
C 0 13.34615800 65.88998300 6.37661800	C 0 10.63169600 58.77450400 13.69712700	H 0 9.71978500 61.05753400 16.00297900
C 0 12.77523900 65.52760500 4.06428700	O 0 11.74744400 59.39411900 13.06404300	H 0 10.21283600 62.70609800 16.38646100
C 0 14.08484900 64.70716600 6.38980300	H 0 9.98681600 57.10781100 14.82742400	C -1 6.93658200 59.40319300 7.02401300
C 0 13.52003600 64.35102000 4.06800900	H 0 9.80792700 58.65589500 12.98403700	C 0 7.99333900 59.47341100 8.10505400
C 0 14.17362100 63.93952300 5.22952000	H 0 10.31168200 59.47272300 14.47379100	C 0 8.41634000 58.33208700 8.79772100
H 0 9.88115600 67.04225200 5.75292900	H 0 12.11638600 58.82035600 12.36214700	C 0 8.52397600 60.71450800 8.48636400
H 0 12.36478200 68.26787200 4.42631400	N 0 12.22099800 55.53062000 13.40735000	C 0 9.32408900 58.42406000 9.85894100
H 0 12.07866300 68.14099900 6.15076100	C 0 12.30252200 54.22467500 12.76587100	C 0 9.44628000 60.81286800 9.52547400
H 0 13.29054000 66.49186100 7.27911400	C 0 12.21494600 54.11816100 11.23868500	C 0 9.84089400 59.66911300 10.22296800
H 0 12.27790300 65.85033400 3.15219200	O 0 11.92728600 53.02781800 10.75386500	H 0 6.74656400 58.37296700 6.71193200
H 0 14.59966400 64.41074700 7.29549100	H 0 12.80272600 55.66264200 14.23467300	H 0 7.21730300 59.98403800 6.14171800
H 0 13.61622300 63.76013900 3.16399300	H 0 13.25971300 53.78352200 13.05884000	H 0 8.00841500 57.36192900 8.52416500
H 0 14.74828300 63.02464900 5.21594000	N 0 12.53371100 55.20022800 10.49000400	H 0 8.20398700 61.61149000 7.96299600
H -1 10.04574300 68.52175900 4.76338700	C -1 12.35105900 55.13829900 9.03891500	H 0 9.60697600 57.53623800 10.41862700
S 0 12.30865300 60.92856500 10.38183200	C 0 12.26849900 56.55496400 8.47060700	H 0 9.85856700 61.77983900 9.79867300
C 0 10.75758100 60.03400800 10.06166100	S 0 11.65621400 56.60370300 6.73437200	H 0 10.53851300 59.75825500 11.04807600
H 0 10.90137800 58.95272500 10.03956500	H 0 12.59814600 56.11066800 10.93052100	C -1 17.74274300 56.74891400 15.48516500
H 0 10.09177200 60.28283500 10.88886000	H 0 11.44968400 54.56246800 8.81572700	N 0 16.89904900 56.37641300 13.02953900
H 0 10.30103800 60.35769400 9.12438600	H 0 11.60644900 57.17965700 9.07321600	C 0 16.56972000 56.12903300 11.71834600
H 0 14.45354100 62.48028800 9.26627900	H 0 13.25026600 57.03584800 8.46364600	O 0 17.20088400 55.36931200 11.00588300
H 0 15.69312300 61.01614100 12.00546900	H 0 10.35851600 56.77404300 7.06024700	N 0 15.39088900 56.73771000 11.20422000
	C -1 14.81301100 65.87511000 19.15144600	C 0 14.58315900 57.60914100 11.86402400
	C 0 16.29018300 65.91832100 18.73188800	C 0 15.25008700 58.26633900 13.08914000
	C 0 16.97390900 64.56730000 18.97349700	O 0 13.46209800 57.91118700 11.44486000
	C 0 16.44376000 66.35136300 17.27018200	C 0 14.75065000 59.02477400 15.30193000
H -1 17.45623800 55.72340200 15.73984700		

## MPS-TS<sub>5</sub>

N 0 14.25134600 58.53556500 14.09989200	N 0 18.14992800 64.04099700 11.95474900	N 0 18.71157900 57.74197000 5.98335200
C 0 14.08923000 60.00581100 16.04721500	C 0 17.57066700 64.85375500 10.88441100	O 0 20.33049300 56.18830300 6.39526900
C 0 14.56171500 60.42611700 17.29101500	C 0 17.57253700 64.15858700 9.52423600	H 0 18.98797900 59.21792700 10.01125600
C 0 13.88179900 61.54465700 18.03821300	O 0 16.75146100 64.48417500 8.65830400	H 0 19.19498700 56.52687200 8.86087800
C 0 15.71750100 59.81834200 17.82148700	C 0 18.26892600 66.23497200 10.83430100	H 0 21.42739300 58.55456200 9.39372900
C 0 16.26761900 60.24425700 19.15878900	C 0 17.44777000 67.23820000 10.00989800	H 0 21.62101900 56.95149900 8.67155600
C 0 16.39013900 58.85586300 17.06821500	C 0 19.72990200 66.13070800 10.38478600	H 0 20.00532600 59.27078100 7.49082800
C 0 15.94562200 58.47051100 15.79897500	C 0 17.89512200 68.68669500 10.21937300	H 0 21.53037900 58.61870800 6.88256200
C 0 16.27368800 57.30797500 13.68852700	H 0 18.67602700 64.55247200 12.68134500	H 0 18.25020100 58.57052000 6.34530700
N 0 16.61624500 57.52424800 14.98752600	H 0 16.51952000 65.02825500 11.12586500	H 0 18.12650900 57.03192800 5.56294700
H 0 15.14572600 56.46058100 10.26003900	H 0 18.26801500 66.58999700 11.86653400	C -1 19.48696600 53.29107000 7.88404300
H 0 13.41197300 61.19118000 18.96395500	H 0 17.48614800 66.97433200 8.94681100	C 0 18.07057000 53.43591500 7.35292800
H 0 14.59783200 62.32182300 18.32557900	H 0 16.39649400 67.14973600 10.30627800	N 0 17.22369500 54.17806000 8.11047700
H 0 13.11023700 62.01634400 17.42978200	H 0 20.25287100 67.07604000 10.54897100	O 0 17.70690500 52.88392200 6.31222700
H 0 15.51389000 60.17504900 19.95135100	H 0 20.26204900 65.36190900 10.95278300	H 0 19.88671100 54.24601500 8.23197500
H 0 17.11921100 59.62425000 19.45049400	H 0 19.80157000 65.88609500 9.31918600	H 0 20.11596500 52.91854500 7.07662800
H 0 16.60867000 61.28662800 19.13716500	H 0 17.24958100 69.37960000 9.66905600	H 0 16.29420300 54.32638900 7.74843700
H 0 13.20926000 60.46493800 15.60888300	H 0 17.84847900 68.95437800 11.28067700	H 0 17.49427200 54.73551700 8.91071300
H 0 17.28915900 58.42539700 17.48925700	H 0 18.92120800 68.85336500 9.87646600	C -1 10.76462700 62.01066200 -0.16252400
H 0 18.17352100 57.23124300 16.35729000	N 0 18.51413500 63.21328200 9.29443200	C 0 12.30687700 61.92663500 -0.32834200
H 0 18.49398700 56.68707100 14.69926700	C -1 18.55260200 62.47051200 8.05098100	C 0 12.96790900 60.71359000 0.35881900
C -1 21.24029700 63.62142200 14.93447100	C 0 17.84436100 61.10790300 8.09033600	C 0 12.99045700 63.25658200 0.00751000
C 0 20.24369500 62.88932500 14.03384600	O 0 17.83193000 60.41172900 7.06673300	C 0 12.98525500 60.70320200 1.88692400
O 0 20.59007500 62.43197800 12.94142700	C 0 20.00890300 62.21386400 7.63970400	H 0 10.44033900 62.44409700 0.78682800
C 0 21.31876700 65.11277300 14.53622100	C 0 20.79646900 63.48844400 7.37201200	H 0 12.46723300 61.75507900 -1.40357700
C 0 19.97963900 65.80127800 14.83073600	O 0 20.55843400 61.47260100 8.73981300	H 0 12.46569900 59.80530400 -0.00111700
O 0 19.15938500 65.84201200 13.82580100	H 0 19.16091200 62.95534400 10.03057200	H 0 14.00394200 60.64738300 0.00214900
O 0 19.74225100 66.18651100 15.97937500	H -1 18.05377200 63.07793200 7.28928100	H 0 14.06212300 63.21475700 -0.21394300
H 0 20.97127400 63.56032400 15.99146400	H 0 19.97597900 61.58896000 6.73915800	H 0 12.55956900 64.07485800 -0.58067000
H 0 22.10004900 65.59614100 15.12900100	H 0 21.48983200 61.29547000 8.55917000	H 0 12.88537000 63.52130100 1.06209100
H 0 21.56790500 65.19118900 13.47459400	H 0 21.82601200 63.24741700 7.08460200	H 0 13.44298600 59.78176000 2.26074300
N 0 18.93721200 62.83232100 14.43199900	H 0 20.34586000 64.05436400 6.55064300	H 0 13.57583800 61.53135800 2.28460500
C 0 17.93195600 62.18498400 13.58323300	H 0 20.82443400 64.12210600 8.26127000	H 0 11.97454600 60.76180600 2.30120700
C 0 17.59878100 62.87125000 12.27249200	N 0 17.31240300 60.71777700 9.25770600	C -1 8.85004100 61.71557800 4.23796600
O 0 16.76202100 62.31056100 11.51908100	C 0 16.56621400 59.47571500 9.33379300	C 0 10.27097900 61.36072800 4.69362800
C 0 16.64781100 62.16103700 14.45287500	C 0 17.42352100 58.22079400 9.20687400	C 0 10.71677000 62.25504300 5.85747900
C 0 17.18291500 62.27949600 15.87929600	O 0 16.93992600 57.20177600 8.70715000	C 0 10.40174500 59.87750100 5.05535000
C 0 18.35242000 63.24763500 15.72056800	H 0 17.23250900 61.37915000 10.02997200	H 0 8.15969600 61.67697200 5.09081100
H 0 18.25064100 61.17005100 13.32302100	H 0 16.05332300 59.45933900 10.29613300	H -1 8.80496100 62.73712600 3.84519200
H 0 16.03934000 63.03956800 14.21899500	H 0 15.82695400 59.42370300 8.53446400	H 0 10.94246200 61.55507000 3.84981800
H 0 16.06738800 61.26134600 14.26230900	N 0 18.67838300 58.29946600 9.71904400	H 0 11.76164000 62.07424700 6.12085600
H 0 16.42820800 62.64658300 16.57601800	C -1 19.68152300 57.26470900 9.50387200	H 0 10.62201400 63.31488500 5.60267400
H 0 17.53667400 61.30926700 16.23993000	C 0 20.92630200 57.78904900 8.78728300	H 0 10.11240300 62.05336800 6.74704000
H 0 18.00932600 64.28315100 15.66572700	C 0 20.59848600 58.36097300 7.39988400	H 0 11.43674500 59.62006900 5.29293800
H 0 19.08378300 63.17720200 16.52516200	C 0 19.87317500 57.31922700 6.54759600	H 0 9.79946600 59.62982900 5.93571900

H 0	10.07933600	59.23335200	4.22927400	C 0	11.76548600	64.01210100	14.01099300	H 0	14.91978800	68.34852200	8.66248100
C 0	14.94280500	68.90286400	14.26926000	C 0	9.98527300	62.47209100	13.05518800	C -1	12.60583400	56.71580000	17.61658500
C 0	14.70015600	67.38729500	14.22789900	H 0	9.28949800	64.54861100	14.92939300	C 0	13.45264300	55.55216000	17.12554800
C 0	15.91101200	66.52369600	13.88585600	H 0	10.65490400	64.31580500	12.20117900	O 0	13.90229600	55.75600700	15.78177200
O 0	17.05411000	67.11908900	14.12241800	H 0	12.50030000	63.28648100	13.65443000	H -1	12.18869400	56.58078200	18.62029100
O 0	15.77827700	65.36701400	13.48157900	H 0	12.21780500	65.00731700	13.94826700	H -1	11.78061000	56.90561000	16.92284900
H 0	14.92905400	69.30194800	13.24745900	H 0	11.58973200	63.79558700	15.06939300	H 0	13.21202000	57.62968500	17.64473900
H 0	15.94881000	69.08020500	14.65625700	H 0	10.78084900	61.82420000	12.67884100	H 0	14.31444400	55.39516400	17.78973900
H 0	14.38019400	67.04152200	15.22041000	H 0	9.65570200	62.06508300	14.01594300	H 0	12.87867800	54.62100600	17.10481800
H 0	13.89167600	67.11933600	13.54014100	H 0	9.13806800	62.40537000	12.36382000	H 0	14.25495700	56.65482500	15.70435300
C -1	18.60159200	58.32714900	1.75426800	H -1	15.41795000	51.40119200	3.31814700	H 0	9.83417400	66.82323300	4.29769600
C 0	17.26350900	58.68551700	2.43340600	H -1	8.46282100	61.01904100	3.48742300	C -1	10.41975800	67.50474700	4.92139600
C 0	17.05080600	60.16834900	2.62368500	H -1	18.76053900	57.25102400	1.87887600	C 0	11.90508400	67.50939100	4.53013300
C 0	16.62723700	60.98548700	1.56773600	H -1	19.49901600	52.57373300	8.71128800	C 0	12.56040700	66.15163300	4.51719500
C 0	17.30365200	60.76583800	3.86580100	H -1	22.21791000	63.14352200	14.80760900	C 0	13.69444000	65.89684400	5.29262800
C 0	16.45882300	62.35919400	1.74491200	H -1	19.93348000	56.70799000	10.41258400	C 0	12.05616800	65.12249300	3.71338400
C 0	17.13686100	62.13891400	4.04581300	H -1	6.00257000	59.81702700	7.41836400	C 0	14.30969200	64.64524700	5.27851600
C 0	16.71323600	62.94314300	2.98692600	H -1	11.67867100	57.43282400	15.10834000	C 0	12.66688300	63.87252500	3.69678800
H 0	18.60714100	58.58224700	0.69036700	H 0	11.51076800	53.56061600	13.12932200	C 0	13.79529800	63.62579700	4.47894700
H 0	19.43288000	58.84726300	2.23969500	H -1	9.59077400	65.85825900	13.78404900	H 0	10.28606100	67.22267700	5.96761300
H 0	16.43691500	58.25959000	1.85311800	H -1	8.38387600	64.58709200	13.42638600	H 0	11.99823500	67.96119800	3.53249700
H 0	17.22473000	58.19602900	3.41043200	H 0	15.01772100	52.34117400	4.75557100	H 0	12.44881900	68.16397200	5.21937300
H 0	16.42235300	60.53735600	0.59832200	H -1	13.20198800	54.61274800	8.59427300	H 0	14.08696300	66.68181200	5.92921300
H 0	17.63775600	60.16254300	4.70141700	C -1	13.92190500	69.63618900	15.14363300	H 0	11.17909000	65.29862200	3.09571100
H 0	16.12142300	62.97433100	0.91620300	H -1	14.06735500	70.72214600	15.13397000	H 0	15.17781000	64.47387400	5.90760100
H 0	17.33709400	62.57275300	5.02109900	H -1	12.89126200	69.40652000	14.84952700	H 0	12.25318500	63.08258400	3.08474500
H 0	16.56046400	64.00728800	3.13303600	H 0	14.02534300	69.31038600	16.18646100	H 0	14.26422900	62.65010300	4.46029200
C -1	15.09098700	52.38701500	3.66491700	H 0	13.43687800	59.04453600	13.75000600	H -1	10.04555000	68.52174700	4.76376300
C 0	16.06155900	53.51458600	3.26710700	C -1	9.09367100	66.03150800	8.85578700	S 0	13.32595500	61.85636500	11.02881900
C 0	15.58711500	54.86530600	3.76613000	C 0	10.40499500	65.36807700	8.39140400	C 0	13.97749500	63.54287300	11.22595700
C 0	14.66260800	55.62594500	3.03980500	C 0	11.64652100	66.23534900	8.43765900	H 0	13.31230600	64.25743500	10.74112100
C 0	16.01936600	55.35350500	5.00812700	C 0	11.59877300	67.63364900	8.40559900	H 0	14.03927800	63.75327000	12.29216700
C 0	14.17156600	56.83176900	3.54396700	C 0	12.90157700	65.61927300	8.52143700	H 0	14.98116500	63.60128600	10.81945400
C 0	15.52640200	56.55587800	5.52416100	C 0	12.77107800	68.39089100	8.47435300	H 0	15.02004600	63.10725600	8.87266100
C 0	14.59860000	57.29750800	4.78799100	C 0	14.07493900	66.36524900	8.61310400	H 0	15.52706400	61.15168200	11.91159900
H 0	14.08784500	52.57473300	3.26652000	C 0	14.00968000	67.76066700	8.59190000				
H 0	17.04496500	53.29774600	3.69405200	H -1	9.29270500	66.79679500	9.61278200				
H 0	16.16918700	53.54272400	2.17527700	H -1	8.44477800	65.25556000	9.27449100				
H 0	14.31797300	55.26536300	2.07306200	H 0	8.56510000	66.52014800	8.03142600	H -1	17.45636000	55.72341900	15.74005300
H 0	16.73826700	54.76244100	5.56378200	H 0	10.60012500	64.48652200	9.01369100	H -1	14.36514000	66.87384000	19.12432000
H 0	13.44621500	57.40376900	2.97193200	H 0	10.27982800	64.97393800	7.37416800	H -1	8.60695400	62.77678000	18.32910500
H 0	15.86273400	56.90464700	6.49810200	H 0	10.64196800	68.14139000	8.33327600	H -1	10.42811100	62.61771700	-1.01101000
H 0	14.20302200	58.22470300	5.18465200	H 0	12.95857300	64.53493400	8.49683300	H -1	10.37418400	60.99323500	-0.26617600
C -1	9.36752900	64.78935000	13.86134600	H 0	12.71092600	69.47551200	8.45039100	C 0	14.76063600	60.61785200	6.20486100
C 0	10.45833000	63.92352600	13.20990700	H 0	15.03082200	65.85698800	8.68574500	C 0	15.14717400	61.68937500	7.00803900

## MPS-TS<sub>R</sub>



C 0 14.58407500 61.88535600 8.26358700	H 0 17.61751400 66.42688900 17.12280500	C 0 16.50769800 58.93842600 17.06370200
C 0 13.61674300 60.98586300 8.72721700	H 0 16.07680600 65.69104500 16.67911300	C 0 15.98470400 58.49184800 15.84696200
C 0 13.20223600 59.92116500 7.91937500	H 0 16.12898800 67.37627100 17.21267600	C 0 16.23877200 57.31750600 13.73233700
C 0 13.77556200 59.74484000 6.66390300	C -1 8.77919700 61.70518200 18.47285700	N 0 16.62190400 57.54212700 15.01491400
H 0 15.23145700 60.46848200 5.23918500	C 0 10.22692900 61.36568600 18.08830900	H 0 14.91925500 56.27889000 10.43002900
H 0 15.90844300 62.37753800 6.66993200	C 0 10.53856600 59.87924100 18.29585000	H 0 13.54974100 61.15977500 19.11145600
H 0 12.44374200 59.22406600 8.24006300	C 0 10.45133100 61.77029500 16.62886800	H 0 14.62991000 62.34409200 18.38700900
H 0 13.44420800 58.90391800 6.07024000	H 0 8.54601800 61.44161700 19.50911300	H 0 13.10740200 61.94741600 17.59185200
O 0 15.76008500 59.32314900 12.68093100	H -1 8.12224500 61.13712200 17.80575700	H 0 15.77270000 60.29261000 19.96712700
O 0 14.45137900 60.21112500 11.66233900	H 0 10.90780900 61.94993700 18.72242000	H 0 17.36340200 59.79962000 19.36868800
H 0 18.03598500 66.59409200 14.01474500	H 0 11.57148400 59.64694800 18.01819300	H 0 16.75894900 61.42975700 19.05501200
C -1 10.91705000 57.40621600 14.32185600	H 0 10.39183700 59.57906700 19.33907600	H 0 13.16541900 60.37269000 15.79130700
C 0 11.06990000 56.33203600 13.24916600	H 0 9.88121500 59.25677700 17.67552700	H 0 17.45737900 58.56634000 17.42520300
O 0 10.26345500 56.29050900 12.31826000	H 0 11.45941200 61.54160900 16.27596100	H 0 18.18817700 57.21520100 16.35791900
C 0 10.63649900 58.79992600 13.76926400	H 0 9.75005400 61.23368100 15.97954100	H 0 18.48668200 56.68853400 14.69206900
O 0 11.78482600 59.45095000 13.24291900	H 0 10.28184300 62.84036100 16.47739800	C -1 21.24006600 63.62185500 14.93267500
H 0 9.99574400 57.10125700 14.84216400	C -1 6.93681700 59.40343600 7.02374500	C 0 20.23510300 62.87916500 14.03261800
H 0 9.84881400 58.72368600 13.00949800	C 0 7.61402800 58.38536800 7.90577000	O 0 20.60489700 62.34576000 12.98366400
H 0 10.27025600 59.44331600 14.57288500	C 0 7.72420800 57.05078500 7.49854700	C 0 21.33386300 65.10071700 14.49067500
H 0 12.18013000 58.88242500 12.54839000	C 0 8.18956800 58.75351600 9.13104300	C 0 20.00961400 65.82684100 14.75949400
N 0 12.04991400 55.41278500 13.41381600	C 0 8.37758200 56.10465700 8.29334000	O 0 19.20987900 65.90649600 13.74016200
C 0 12.00346400 54.12794400 12.72900200	C 0 8.83831400 57.81219000 9.92883300	O 0 19.76915600 66.21488800 15.90738300
C 0 12.02061900 54.06630600 11.19469800	C 0 8.93448500 56.48056900 9.51568000	H 0 20.96847200 63.58339400 15.99016200
O 0 11.68438700 53.01303600 10.66222200	H 0 6.70827500 58.97607100 6.04320800	H 0 22.12176000 65.59220300 15.06852800
H 0 12.64528300 55.48112800 14.24057000	H 0 7.59752900 60.25968000 6.85016100	H 0 21.58759600 65.14100500 13.42791200
H 0 12.86466600 53.54844100 13.07292300	H 0 7.29561300 56.75077600 6.54582700	N 0 18.90787000 62.89468300 14.37436600
N 0 12.46365600 55.14287800 10.49895300	H 0 8.12289600 59.78794300 9.46081700	C 0 17.91472100 62.16261900 13.57167700
C -1 12.35119300 55.13834700 9.03934600	H 0 8.44588500 55.07334300 7.95911300	C 0 17.45970300 62.82002100 12.27609000
C 0 12.30268800 56.56579900 8.50758600	H 0 9.27258600 58.08996900 10.88219500	O 0 16.59016800 62.24502100 11.57639700
S 0 11.87037500 56.63629200 6.72219400	H 0 9.43511900 55.76415900 10.15606100	C 0 16.67730900 62.03002500 14.50196600
H 0 12.51532100 56.03959600 10.97174800	C -1 17.74211500 56.74967400 15.48423900	C 0 17.22588600 62.33743100 15.89685200
H 0 11.45041700 54.58640300 8.75827600	N 0 16.87445100 56.40790600 13.05105200	C 0 18.28510900 63.39805000 15.61092000
H 0 11.56646900 57.15206700 9.06078300	C 0 16.47729000 56.09914300 11.77720900	H 0 18.31922900 61.18479300 13.29281600
H 0 13.27344200 57.06042700 8.60237700	O 0 17.08659500 55.33830600 11.04918500	H 0 15.93881300 62.78889900 14.23009300
H 0 10.53766000 56.54605500 6.91402100	N 0 15.23790100 56.64011800 11.32146700	H 0 16.22052000 61.04885700 14.39556500
C -1 14.81281100 65.87499900 19.15161800	C 0 14.43365600 57.48085100 12.01436700	H 0 16.44805900 62.69170800 16.57529700
C 0 16.31334300 65.91679100 18.82287300	C 0 15.13149300 58.21022800 13.17867900	H 0 17.68810000 61.44948400 16.33902200
C 0 16.96503700 64.55042300 19.06698800	O 0 13.27072500 57.72011500 11.66797200	H 0 17.82469800 64.36954200 15.42047500
C 0 16.55574400 66.38210000 17.38351400	C 0 14.74589300 58.99048000 15.41760600	H 0 19.01886900 63.52321600 16.40429900
H 0 14.63341800 65.46206500 20.15158400	N 0 14.18399000 58.43128000 14.26495500	N 0 17.98620700 63.99728200 11.92011200
H 0 14.27729500 65.24558300 18.42995700	C 0 14.09381400 59.96441700 16.17637000	C 0 17.33509800 64.76218500 10.85818300
H 0 16.78871900 66.63800300 19.50357200	C 0 14.62921500 60.43354300 17.37734900	C 0 17.40970900 64.06660600 9.50210100
H 0 18.03353400 64.57599200 18.83055900	C 0 13.94048500 61.52611100 18.15404200	O 0 16.57419800 64.30515100 8.62679000
H 0 16.84855900 64.22499000 20.10747500	C 0 15.84617900 59.89232300 17.83763200	C 0 17.88906000 66.20450500 10.80584300
H 0 16.50602200 63.79019700 18.42500600	C 0 16.46720200 60.37517100 19.12344000	C 0 17.00563200 67.10695500 9.92609400

C 0 19.36804200 66.24995400 10.40754400	H 0 20.04907800 59.24274700 7.45018300	H 0 14.89632800 69.20332700 13.24763800
C 0 17.22094100 68.59473100 10.21571400	H 0 21.57187000 58.54893700 6.87628000	H 0 15.96193100 69.15702000 14.63868700
H 0 18.53550400 64.52184400 12.61376300	H 0 18.24558500 58.48298700 6.41299000	H 0 14.56622000 67.10546100 15.44263700
H 0 16.26882900 64.81758900 11.08255800	H 0 18.11338000 56.91729100 5.67482400	H 0 13.95134800 67.00955500 13.81209000
H 0 17.81094700 66.57391900 11.83058500	C -1 19.48705600 53.29100800 7.88394500	C -1 18.60132800 58.32721700 1.75415300
H 0 17.18564000 66.89078100 8.86699100	C 0 18.07586600 53.54334700 7.37612000	C 0 17.55419400 58.78274200 2.78178600
H 0 15.95397100 66.85977900 10.10310000	N 0 17.25495500 54.22676700 8.21221600	C 0 17.29336200 60.27009600 2.79379300
H 0 19.76032500 67.26510700 10.50791500	O 0 17.69433200 53.13141900 6.27870200	C 0 16.70404600 60.90699500 1.69289800
H 0 19.97177200 65.60806500 11.05402900	H 0 19.95161800 54.22304500 8.21504100	C 0 17.63433600 61.04962100 3.90778000
H 0 19.50687100 65.93589700 9.36697500	H 0 20.07259300 52.89066800 7.05708500	C 0 16.46590100 62.28084900 1.69895800
H 0 16.54191300 69.21240400 9.61867900	H 0 16.35985900 54.51013300 7.84403300	C 0 17.39270400 62.42468500 3.91716900
H 0 17.03635800 68.81198200 11.27395400	H 0 17.55620600 54.71479200 9.04516600	C 0 16.80945100 63.04826700 2.81352900
H 0 18.24300600 68.91477700 9.98768000	C -1 10.76509900 62.01133900 -0.16328200	H 0 18.27660000 58.51704100 0.72591400
N 0 18.44297500 63.20947100 9.29292000	C 0 12.30949500 62.03755100 -0.19247300	H 0 19.55751200 58.83735100 1.90824200
C -1 18.55411300 62.47065000 8.05094600	C 0 12.99524100 60.85387700 0.51724400	H 0 16.61854500 58.24906000 2.58870100
C 0 17.90079900 61.08103000 8.09697800	C 0 12.81027400 63.39793100 0.30797500	H 0 17.88445800 58.47216900 3.77608600
O 0 17.96156500 60.35155600 7.09807100	C 0 12.74207100 60.71934700 2.01807400	H 0 16.42768300 60.31630200 0.82297800
C 0 20.03002800 62.27205400 7.68395800	H 0 10.36445900 62.43255900 0.76431500	H 0 18.07192600 60.58194500 4.78336100
C 0 20.77841000 63.57954000 7.46598300	H 0 12.60496100 61.95104700 -1.24838100	H 0 16.01278300 62.75379500 0.83273900
O 0 20.56909500 61.52728300 8.78615900	H 0 12.68059900 59.92662400 0.01949000	H 0 17.65791200 63.01081400 4.79307500
H 0 19.08594600 63.00042100 10.04747800	H 0 14.07554000 60.93840400 0.34901000	H 0 16.60803300 64.11440200 2.82974900
H -1 18.05235700 63.07740100 7.28965100	H 0 13.90256600 63.46294900 0.28357600	C -1 15.09096900 52.38695800 3.66533900
H 0 20.05097000 61.66377000 6.77134200	H 0 12.41025900 64.21321400 -0.30503600	C 0 16.13410300 53.46813500 3.32729700
H 0 21.51863100 61.41839900 8.65206700	H 0 12.48671300 63.57750000 1.33750700	C 0 15.62136200 54.86469100 3.60261100
H 0 21.82623600 63.38246400 7.21292600	H 0 13.32017500 59.88719300 2.43203700	C 0 14.84733200 55.53636100 2.64835300
H 0 20.33689800 64.14248500 6.63753800	H 0 13.03615200 61.61770600 2.56906800	C 0 15.86976200 55.49975500 4.82856300
H 0 20.74834700 64.19958600 8.36477300	H 0 11.68672300 60.52404400 2.22602900	C 0 14.33543500 56.80756800 2.90509900
N 0 17.31971900 60.70797400 9.24886100	C -1 8.84958300 61.71552200 4.23807100	C 0 15.36155600 56.77462100 5.09194000
C 0 16.57576600 59.46369800 9.31760500	C 0 10.26872600 61.36323200 4.70138400	C 0 14.59635000 57.43127000 4.12472100
C 0 17.42399400 58.20635300 9.21987100	C 0 10.74740000 62.30168800 5.81828600	H 0 14.12765000 52.60863300 3.19289600
O 0 16.92855400 57.17990700 8.75094300	C 0 10.36599800 59.89545400 5.13078600	H 0 17.03625900 53.28500600 3.91650600
H 0 17.19182000 61.38029700 10.00548800	H 0 8.15432400 61.67425100 5.08713100	H 0 16.40300700 53.39120800 2.26605300
H 0 16.03439000 59.45114900 10.26426900	H -1 8.80519300 62.73712200 3.84515600	H 0 14.64677800 55.05510100 1.69373300
H 0 15.85726400 59.40029500 8.50115200	H 0 10.94192800 61.51005900 3.85059600	H 0 16.46871300 54.97004200 5.56335900
N 0 18.68421700 58.29893400 9.71608900	H 0 11.77616500 62.07335500 6.11242000	H 0 13.74158300 57.31832200 2.15179400
C -1 19.68170600 57.26437900 9.50352100	H 0 10.72179200 63.35009400 5.50283100	H 0 15.56672400 57.24857700 6.04902500
C 0 20.93551400 57.78194300 8.79705000	H 0 10.11217800 62.19973700 6.70870200	H 0 14.21405000 58.42910000 4.30256800
C 0 20.63101100 58.32292800 7.39096100	H 0 11.39070500 59.62432800 5.39038200	C -1 9.36875500 64.78772200 13.86321000
C 0 19.89880600 57.26000400 6.57300400	H 0 9.74603200 59.69534100 6.01263600	C 0 10.49096400 64.01670800 13.14602800
N 0 18.69856200 57.64390900 6.06488900	H 0 10.03277400 59.22169300 4.33326100	C 0 11.83267900 64.22124900 13.86135900
O 0 20.37516600 56.13801600 6.41172000	C 0 14.95711600 68.89442100 14.29933500	C 0 10.16095700 62.52814700 13.00581400
H 0 18.99706600 59.22327400 9.98517500	C 0 14.79566700 67.37469500 14.40346300	H 0 9.32287400 64.52114100 14.92583200
H 0 19.19620200 56.52477900 8.86123300	C 0 16.02675500 66.54797800 14.04723000	H 0 10.59407600 64.43403500 12.13517600
H 0 21.42121000 58.56245800 9.39659600	O 0 17.15201000 67.20683100 14.14802500	H 0 12.65267300 63.74788100 13.31479100
H 0 21.63694400 56.94626000 8.71148100	O 0 15.92372100 65.35667100 13.74333300	H 0 12.07653700 65.28430200 13.95118700

H 0 11.80876500 63.79537500 14.87143700  
H 0 11.01797300 61.97255000 12.61959700  
H 0 9.90682300 62.08782800 13.97449400  
H 0 9.30891300 62.36792100 12.33471300  
H -1 15.41796200 51.40131000 3.31782100  
H -1 8.46290600 61.01900900 3.48740900  
H -1 18.76065400 57.25107000 1.87913100  
H -1 19.49893500 52.57382500 8.71137000  
H -1 22.21779100 63.14291600 14.80896800  
H -1 19.93332200 56.70830000 10.41281600  
H -1 6.00262300 59.81689000 7.41863300  
H -1 11.67859700 57.43263400 15.10840500  
H 0 11.10279300 53.57155000 13.01021600  
H -1 9.58972300 65.85842100 13.78326200  
H -1 8.38406900 64.58826600 13.42540800  
H 0 14.93669500 52.33810900 4.74686800  
H -1 13.20184200 54.61266700 8.59409400  
C -1 13.92155800 69.63660200 15.14271400  
H -1 14.06767100 70.72210800 15.13455900  
H -1 12.89126100 69.40617700 14.84979100  
H 0 14.01592400 69.32377900 16.19097900  
H 0 13.34826800 58.93715100 13.96035600  
C -1 9.09336300 66.03184800 8.85513000  
C 0 10.45392900 65.50269700 8.35009700  
C 0 11.57425200 65.61061300 9.36678800  
C 0 11.81757800 66.81076600 10.05306800  
C 0 12.42662200 64.52988700 9.61140600  
C 0 12.85257700 66.91282100 10.98194800  
C 0 13.46485000 64.62941100 10.53738500  
C 0 13.67505700 65.81476700 11.23766400  
H -1 9.29287400 66.79644300 9.61309300  
H -1 8.44505000 65.25547500 9.27475700  
H 0 8.52908500 66.50189800 8.04260100  
H 0 10.37122600 64.46668100 8.00799000  
H 0 10.75135300 66.07578700 7.46530500  
H 0 11.19307400 67.67885400 9.85927700  
H 0 12.27418100 63.60687400 9.06304300  
H 0 13.01615200 67.84861000 11.50948400  
H 0 14.11323800 63.78400200 10.73531800  
H 0 14.45981900 65.85798500 11.98297200  
C -1 12.60587600 56.71568600 17.61678700  
C 0 13.45371800 55.56469700 17.09457400  
O 0 13.78148300 55.72837900 15.70990000  
H -1 12.18861800 56.58082800 18.62026500  
H -1 11.78063800 56.90577200 16.92283800

H 0 13.20483300 57.63393100 17.64292800  
H 0 14.37394300 55.46430400 17.68711500  
H 0 12.91609900 54.61354000 17.15832000  
H 0 14.00239000 56.65606000 15.51544400  
H 0 10.30220700 66.95390900 3.98453500  
C -1 10.41965600 67.50457900 4.92203600  
C 0 11.89589100 67.63144400 5.32601500  
C 0 12.70953600 66.36340600 5.24365700  
C 0 13.46194700 65.92642700 6.33832400  
C 0 12.79072200 65.64794200 4.04080400  
C 0 14.28812600 64.80747200 6.24105400  
C 0 13.61421100 64.53016300 3.93776900  
C 0 14.36287400 64.11012900 5.03616300  
H 0 9.81967700 67.00480800 5.68678200  
H 0 12.36235500 68.38187100 4.67266100  
H 0 11.96125200 68.03839000 6.34144600  
H 0 13.41221300 66.47213800 7.27617500  
H 0 12.22598700 65.98240600 3.17393000  
H 0 14.88236400 64.51165500 7.09680000  
H 0 13.69898000 63.99532100 2.99825200  
H 0 15.00493500 63.24761300 4.93224200  
H -1 10.04574700 68.52176000 4.76338700  
S 0 13.00420800 61.23849600 10.37160400  
C 0 11.57322400 60.12572300 10.37126900  
H 0 11.89643300 59.08590400 10.34904100  
H 0 11.02365200 60.32542700 11.28513000  
H 0 10.96314800 60.35846300 9.49775900  
H 0 14.91614200 62.72076200 8.86710900  
H 0 15.05752600 60.98505500 11.75950500  
**E:MPSO<sub>s</sub>**  
H -1 17.45623800 55.72340200 15.73984700  
H -1 14.36500600 66.87378000 19.12441500  
H -1 8.60683600 62.77683100 18.32963200  
H -1 10.42842100 62.61807800 -1.01087500  
H -1 10.37412700 60.99333000 -0.26687400  
C 0 14.02609899 60.14366815 6.98708048  
C 0 15.03331360 60.95143640 7.50921491  
C 0 14.80362985 61.74272523 8.63259814  
C 0 13.54738288 61.71425592 9.24731583  
C 0 12.52615551 60.90648912 8.72541400  
C 0 12.76702112 60.13195206 7.59268870  
H 0 14.23037037 59.52514775 6.11957415  
H 0 16.01611334 60.95235781 7.05658651

H 0 11.55437151 60.87985065 9.20176796  
H 0 11.96840792 59.52135236 7.18574419  
O 0 16.00822700 59.34333100 12.67518300  
H 0 17.92201100 66.50539300 14.03883000  
C -1 10.91677500 57.40612400 14.32221500  
C 0 11.12686200 56.32184300 13.26527900  
O 0 10.30785400 56.17841800 12.35682500  
C 0 10.63169600 58.77450400 13.69712700  
O 0 11.74744400 59.39411900 13.06404300  
H 0 9.98681600 57.10781100 14.82742400  
H 0 9.80792700 58.65589500 12.98403700  
H 0 10.31168200 59.47272300 14.47379100  
H 0 12.11638600 58.82035600 12.36214700  
N 0 12.22099800 55.53062000 13.40735000  
C 0 12.30252200 54.22467500 12.76587100  
C 0 12.21494600 54.11816100 11.23868500  
O 0 11.92728600 53.02781800 10.75386500  
H 0 12.80272600 55.66264200 14.23467300  
H 0 13.25971300 53.78352200 13.05884000  
N 0 12.53371100 55.20022800 10.49000400  
C -1 12.35105900 55.13829900 9.03891500  
C 0 12.26849900 56.55496400 8.47060700  
S 0 11.65621400 56.60370300 6.73437200  
H 0 12.59814600 56.11066800 10.93052100  
H 0 11.44968400 54.56246800 8.81572700  
H 0 11.60644900 57.17965700 9.07321600  
H 0 13.25026600 57.03584800 8.46364600  
H 0 10.35851600 56.77404300 7.06024700  
C -1 14.81301100 65.87511000 19.15144600  
C 0 16.29018300 65.91832100 18.73188800  
C 0 16.97390900 64.56730000 18.97349700  
C 0 16.44376000 66.35136300 17.27018200  
H 0 14.69580000 65.48787100 20.17053800  
H 0 14.23746000 65.22656000 18.47919800  
H 0 16.79746100 66.66274000 19.36259100  
H 0 18.02160300 64.59667500 18.65790900  
H 0 16.93838700 64.27878100 20.03054600  
H 0 16.47748500 63.77865600 18.39637400  
H 0 17.49176800 66.42343000 16.96399600  
H 0 15.95304500 65.62807700 16.60606000  
H 0 15.97672900 67.32671700 17.09533100  
C -1 8.77987700 61.70537700 18.47134800  
C 0 10.22174900 61.34476900 18.08858300  
C 0 10.53806900 59.87386200 18.38195200  
C 0 10.41594800 61.65409400 16.60348500

H 0 8.54391100 61.44635200 19.50845500	H 0 13.11023700 62.01634400 17.42978200	H 0 20.26204900 65.36190900 10.95278300
H -1 8.12185500 61.13695500 17.80628500	H 0 15.51389000 60.17504900 19.95135100	H 0 19.80157000 65.88609500 9.31918600
H 0 10.91295900 61.96797500 18.67214800	H 0 17.11921100 59.62425000 19.45049400	H 0 17.24958100 69.37960000 9.66905600
H 0 11.56046400 59.62105700 18.08357100	H 0 16.60867000 61.28662800 19.13716500	H 0 17.84847900 68.95437800 11.28067700
H 0 10.42671400 59.64234100 19.44682300	H 0 13.20926000 60.46493800 15.60888300	H 0 18.92120800 68.85336500 9.87646600
H 0 9.85979800 59.21507600 17.82527900	H 0 17.28915900 58.42539700 17.48925700	N 0 18.51413500 63.21328200 9.29443200
H 0 11.42417400 61.42717600 16.25168400	H 0 18.17352100 57.23124300 16.35729000	C -1 18.55260200 62.47051200 8.05098100
H 0 9.71978500 61.05753400 16.00297900	H 0 18.49398700 56.68707100 14.69926700	C 0 17.84436100 61.10790300 8.09033600
H 0 10.21283600 62.70609800 16.38646100	C -1 21.24029700 63.62142200 14.93447100	O 0 17.83193000 60.41172900 7.06673300
C -1 6.93658200 59.40319300 7.02401300	C 0 20.24369500 62.88932500 14.03384600	C 0 20.00890300 62.21386400 7.63970400
C 0 7.99333900 59.47341100 8.10505400	O 0 20.59007500 62.43197800 12.94142700	C 0 20.79646900 63.48844400 7.37201200
C 0 8.41634000 58.33208700 8.79772100	C 0 21.31876700 65.11277300 14.53622100	O 0 20.55843400 61.47260100 8.73981300
C 0 8.52397600 60.71450800 8.48636400	C 0 19.97963900 65.80127800 14.83073600	H 0 19.16091200 62.95534400 10.03057200
C 0 9.32408900 58.42406000 9.85894100	O 0 19.15938500 65.84201200 13.82580100	H -1 18.05377200 63.07793200 7.28928100
C 0 9.44628000 60.81286800 9.52547400	H 0 20.97127400 63.56032400 15.99146400	H 0 19.97597900 61.58896000 6.73915800
C 0 9.84089400 59.66911300 10.22296800	H 0 22.10004900 65.59614100 15.12900100	H 0 21.48983200 61.29547000 8.55917000
H 0 6.74656400 58.37296700 6.71193200	H 0 21.56790500 65.19118900 13.47459400	H 0 21.82601200 63.24741700 7.08460200
H 0 7.21730300 59.98403800 6.14171800	N 0 18.93721200 62.83232100 14.43199900	H 0 20.34586000 64.05436400 6.55064300
H 0 8.00841500 57.36192900 8.52416500	C 0 17.93195600 62.18498400 13.58323300	H 0 20.82443400 64.12210600 8.26127000
H 0 8.20398700 61.61149000 7.96299600	C 0 17.59878100 62.87125000 12.27249200	N 0 17.31240300 60.71777700 9.25770600
H 0 9.60697600 57.53623800 10.41862700	O 0 16.76202100 62.31056100 11.51908100	C 0 16.56621400 59.47571500 9.33379300
H 0 9.85856700 61.77983900 9.79867300	C 0 16.64781100 62.16103700 14.45287500	C 0 17.42352100 58.22079400 9.20687400
H 0 10.53851300 59.75825500 11.04807600	C 0 17.18291500 62.27949600 15.87929600	O 0 16.93992600 57.20177600 8.70715000
C -1 17.74274300 56.74891400 15.48516500	C 0 18.35242000 63.24763500 15.72056800	H 0 17.23250900 61.37915000 10.02997200
N 0 16.89904900 56.37641300 13.02953900	H 0 18.25064100 61.17005100 13.32302100	H 0 16.05332300 59.45933900 10.29613300
C 0 16.56972000 56.12903300 11.71834600	H 0 16.03934000 63.03956800 14.21899500	H 0 15.82695400 59.42370300 8.53446400
O 0 17.20088400 55.36931200 11.00588300	H 0 16.06738800 61.26134600 14.26230900	N 0 18.67838300 58.29946600 9.71904400
N 0 15.39088900 56.73771000 11.20422000	H 0 16.42820800 62.64658300 16.57601800	C -1 19.68152300 57.26470900 9.50387200
C 0 14.58315900 57.60914100 11.86402400	H 0 17.53667400 61.30926700 16.23993000	C 0 20.92630200 57.78904900 8.78728300
C 0 15.25008700 58.26633900 13.08914000	H 0 18.00932600 64.28315100 15.66572700	C 0 20.59848600 58.36097300 7.39988400
O 0 13.46209800 57.91118700 11.44486000	H 0 19.08378300 63.17720200 16.52516200	C 0 19.87317500 57.31922700 6.54759600
C 0 14.75065000 59.02477400 15.30193000	N 0 18.14992800 64.04099700 11.95474900	N 0 18.71157900 57.74197000 5.98335200
N 0 14.25134600 58.53556500 14.09989200	C 0 17.57066700 64.85375500 10.88441100	O 0 20.33049300 56.18830300 6.39526900
C 0 14.08923000 60.00581100 16.04721500	C 0 17.57253700 64.15858700 9.52423600	H 0 18.98797900 59.21792700 10.01125600
C 0 14.56171500 60.42611700 17.29101500	O 0 16.75146100 64.48417500 8.65830400	H 0 19.19498700 56.52687200 8.86087800
C 0 13.88179900 61.54465700 18.03821300	C 0 18.26892600 66.23497200 10.83430100	H 0 21.42739300 58.55456200 9.39372900
C 0 15.71750100 59.81834200 17.82148700	C 0 17.44777000 67.23820000 10.00989800	H 0 21.62101900 56.95149900 8.67155600
C 0 16.26761900 60.24425700 19.15878900	C 0 19.72990200 66.13070800 10.38478600	H 0 20.00532600 59.27078100 7.49082800
C 0 16.39013900 58.85586300 17.06821500	C 0 17.89512200 68.68669500 10.21937300	H 0 21.53037900 58.61870800 6.88256200
C 0 15.94562200 58.47051100 15.79897500	H 0 18.67602700 64.55247200 12.68134500	H 0 18.25020100 58.57052000 6.34530700
C 0 16.27368800 57.30797500 13.68852700	H 0 16.51952000 65.02825500 11.12586500	H 0 18.12650900 57.03192800 5.56294700
N 0 16.61624500 57.52424800 14.98752600	H 0 18.26801500 66.58999700 11.86653400	C -1 19.48696600 53.29107000 7.88404300
H 0 15.14572600 56.46058100 10.26003900	H 0 17.48614800 66.97433200 8.94681100	C 0 18.07057000 53.43591500 7.35292800
H 0 13.41197300 61.19118000 18.96395500	H 0 16.39649400 67.14973600 10.30627800	N 0 17.22369500 54.17806000 8.11047700
H 0 14.59783200 62.32182300 18.32557900	H 0 20.25287100 67.07604000 10.54897100	O 0 17.70690500 52.88392200 6.31222700

H 0 19.88671100 54.24601500 8.23197500	C 0 17.30365200 60.76583800 3.86580100	H -1 22.21791000 63.14352200 14.80760900
H 0 20.11596500 52.91854500 7.07662800	C 0 16.45882300 62.35919400 1.74491200	H -1 19.93348000 56.70799000 10.41258400
H 0 16.29420300 54.32638900 7.74843700	C 0 17.13686100 62.13891400 4.04581300	H -1 6.00257000 59.81702700 7.41836400
H 0 17.49427200 54.73551700 8.91071300	C 0 16.71323600 62.94314300 2.98692600	H -1 11.67867100 57.43282400 15.10834000
C -1 10.76462700 62.01066200 -0.16252400	H 0 18.60714100 58.58224700 0.69036700	H 0 11.51076800 53.56061600 13.12932200
C 0 12.30687700 61.92663500 -0.32834200	H 0 19.43288000 58.84726300 2.23969500	H -1 9.59077400 65.85825900 13.78404900
C 0 12.96790900 60.71359000 0.35881900	H 0 16.43691500 58.25959000 1.85311800	H -1 8.38387600 64.58709200 13.42638600
C 0 12.99045700 63.25658200 0.00751000	H 0 17.22473000 58.19602900 3.41043200	H 0 15.01772100 52.34117400 4.75557100
C 0 12.98525500 60.70320200 1.88692400	H 0 16.42235300 60.53735600 0.59832200	H -1 13.20198800 54.61274800 8.59427300
H 0 10.44033900 62.44409700 0.78682800	H 0 17.63775600 60.16254300 4.70141700	C -1 13.92190500 69.63618900 15.14363300
H 0 12.46723300 61.75507900 -1.40357700	H 0 16.12142300 62.97433100 0.91620300	H -1 14.06735500 70.72214600 15.13397000
H 0 12.46569900 59.80530400 -0.00111700	H 0 17.33709400 62.57275300 5.02109900	H -1 12.89126200 69.40652000 14.84952700
H 0 14.00394200 60.64738300 0.00214900	H 0 16.56046400 64.00725800 3.13303600	H 0 14.02534300 69.31038600 16.18646100
H 0 14.06212300 63.21475700 -0.21394300	C -1 15.09098700 52.38701500 3.66491700	H 0 13.43687800 59.04453600 13.75000600
H 0 12.55956900 64.07485800 -0.58067000	C 0 16.06155900 53.51458600 3.26710700	C -1 9.09367100 66.03150800 8.85578700
H 0 12.88537000 63.52130100 1.06209100	C 0 15.58711500 54.86530600 3.76613000	C 0 10.40499500 65.36807700 8.39140400
H 0 13.44298600 59.78176000 2.26074300	C 0 14.66260800 55.62594500 3.03980500	C 0 11.64652100 66.23534900 8.43765900
H 0 13.57583800 61.53135800 2.28460500	C 0 16.01936600 55.35350500 5.00812700	C 0 11.59877300 67.63364900 8.40559900
H 0 11.97454600 60.76180600 2.30120700	C 0 14.17156600 56.83176900 3.54396700	C 0 12.90157700 65.61927300 8.52143700
C -1 8.85004100 61.71557800 4.23796600	C 0 15.52640200 56.55587800 5.52416100	C 0 12.77107800 68.39089100 8.47435300
C 0 10.27097900 61.36072800 4.69362800	C 0 14.59860000 57.29750800 4.78799100	C 0 14.07493900 66.36524900 8.61310400
C 0 10.71677000 62.25504300 5.85747900	H 0 14.08784500 52.57473300 3.26652000	C 0 14.00968000 67.76066700 8.59190000
C 0 10.40174500 59.87750100 5.05535000	H 0 17.04496500 53.29774600 3.69405200	H -1 9.29270500 66.79679500 9.61278200
H 0 8.15969600 61.67697200 5.09081100	H 0 16.16918700 53.54272400 2.17527700	H -1 8.44477800 65.25556000 9.27449100
H -1 8.80496100 62.73712600 3.84519200	H 0 14.31797300 55.26536300 2.07306200	H 0 8.56510000 66.52014800 8.03142600
H 0 10.94246200 61.55507000 3.84981800	H 0 16.73826700 54.76244100 5.56378200	H 0 10.60012500 64.48652200 9.01369100
H 0 11.76164000 62.07424700 6.12085600	H 0 13.44621500 57.40376900 2.97193200	H 0 10.27982800 64.97393800 7.37416800
H 0 10.62201400 63.31488500 5.60267400	H 0 15.86273400 56.90464700 6.49810200	H 0 10.64196800 68.14139000 8.33327600
H 0 10.11240300 62.05336800 6.74704000	H 0 14.20302200 58.22470300 5.18465200	H 0 12.95857300 64.53493400 8.49683300
H 0 11.43674500 59.62006900 5.29293800	C -1 9.36752900 64.78935000 13.86134600	H 0 12.71092600 69.47551200 8.45039100
H 0 9.79946600 59.62982900 5.93571900	C 0 10.45833000 63.92352600 13.20990700	H 0 15.03082200 65.85698800 8.68574500
H 0 10.07933600 59.23335200 4.22927400	C 0 11.76548600 64.01210100 14.01099300	H 0 14.91978800 68.34852200 8.66248100
C 0 14.94280500 68.90286400 14.26926000	C 0 9.98527300 62.47209100 13.05518800	C -1 12.60583400 56.71580000 17.61658500
C 0 14.70015600 67.38729500 14.22789900	H 0 9.28949800 64.54861100 14.92939300	C 0 13.45264300 55.55216000 17.12554800
C 0 15.91101200 66.52369600 13.88585600	H 0 10.65490400 64.31580500 12.20117900	O 0 13.90229600 55.75600700 15.78177200
O 0 17.05411000 67.11908900 14.12241800	H 0 12.50030000 63.28648100 13.65443000	H -1 12.18869400 56.58078200 18.62029100
O 0 15.77827700 65.36701400 13.48157900	H 0 12.21780500 65.00731700 13.94826700	H -1 11.78061000 56.90561000 16.92284900
H 0 14.92905400 69.30194800 13.24745900	H 0 11.58973200 63.79558700 15.06939300	H 0 13.21202000 57.62968500 17.64473900
H 0 15.94881000 69.08020500 14.65625700	H 0 10.78084900 61.82420000 12.67884100	H 0 14.31444400 55.39516400 17.78973900
H 0 14.38019400 67.04152200 15.22041000	H 0 9.65570200 62.06508300 14.01594300	H 0 12.87867800 54.62100600 17.10481800
H 0 13.89167600 67.11933600 13.54014100	H 0 9.13806800 62.40537000 12.36382000	H 0 14.25495700 56.65482500 15.70435300
C -1 18.60159200 58.32714900 1.75426800	H -1 15.41795000 51.40119200 3.31814700	H 0 9.83417400 66.82323300 4.29769600
C 0 17.26350900 58.68551700 2.43340600	H -1 8.46282100 61.01904100 3.48742300	C -1 10.41975800 67.50474700 4.92139600
C 0 17.05080600 60.16834900 2.62368500	H -1 18.76053900 57.25102400 1.87887600	C 0 11.90508400 67.50939100 4.53013300
C 0 16.62723700 60.98548700 1.56773600	H -1 19.49901600 52.57373300 8.71128800	C 0 12.56040700 66.15163300 4.51719500

C 0 13.69444000 65.89684400 5.29262800	C 0 10.63968200 58.78917500 13.72862500	H 0 9.71767200 61.12181100 16.00607000
C 0 12.05616800 65.12249300 3.71338400	O 0 11.77059600 59.44319600 13.16297100	H 0 10.26456500 62.74777100 16.41994400
C 0 14.30969200 64.64524700 5.27851600	H 0 9.99268500 57.13770200 14.85731700	C -1 6.93689200 59.40353400 7.02388800
C 0 12.66688300 63.87252500 3.69678800	H 0 9.83866400 58.68830800 12.98816500	C 0 7.61232800 58.38191200 7.90415900
C 0 13.79529800 63.62579700 4.47894700	H 0 10.28928200 59.45466000 14.52109500	C 0 7.62485900 57.02853500 7.54743600
H 0 10.28606100 67.22267700 5.96761300	H 0 12.09369800 58.97390700 12.36974100	C 0 8.28094700 58.76295900 9.07710800
H 0 11.99823500 67.96119800 3.53249700	N 0 11.94511300 55.34065300 13.41614400	C 0 8.26981000 56.07773300 8.34345300
H 0 12.44881900 68.16397200 5.21937300	C 0 11.82345600 54.07671900 12.70057700	C 0 8.92105100 57.81711500 9.87703200
H 0 14.08696300 66.68181200 5.92921300	C 0 11.80847500 54.06102900 11.16111500	C 0 8.91624400 56.46656200 9.51673800
H 0 11.17909000 65.29862200 3.09571100	O 0 11.30739900 53.08795800 10.60430900	H 0 6.70695200 58.97770900 6.04277400
H 0 15.17781000 64.47387400 5.90760100	H 0 12.56647200 55.38371200 14.22389000	H 0 7.59865600 60.25879200 6.85197100
H 0 12.25318500 63.08258400 3.08474500	H 0 12.66129900 53.44678400 13.01343300	H 0 7.12678800 56.71726800 6.63279000
H 0 14.26422900 62.65010300 4.46029200	N 0 12.42208300 55.07228700 10.49992200	H 0 8.29550000 59.81213300 9.36368800
H -1 10.04555000 68.52174700 4.76376300	C -1 12.35119000 55.13835700 9.03935500	H 0 8.26418400 55.03241000 8.04854100
S 0 13.16873608 62.59022212 10.75228995	C 0 12.32303600 56.58421400 8.55695400	H 0 9.42567700 58.10759700 10.79156600
C 0 14.55382517 63.75484077 10.93358700	S 0 11.80771100 56.70966100 6.79567900	H 0 9.40728700 55.74441600 10.15807700
H 0 14.45461328 64.56573624 10.21195916	H 0 12.61371800 55.93346200 11.00428800	C -1 17.74208200 56.74968600 15.48424900
H 0 14.52536034 64.15062730 11.94720950	H 0 11.45026200 54.60689400 8.72388300	N 0 16.95703000 56.41845400 13.02887600
H 0 15.49550739 63.23138727 10.81013153	H 0 11.63483900 57.17367700 9.16560400	C 0 16.59418900 56.09658400 11.74482700
H 0 15.61728937 62.34320541 9.01238781	H 0 13.30937600 57.05289800 8.61646900	O 0 17.26199600 55.37739800 11.02572500
H 0 15.52861276 60.15706773 12.84665521	H 0 10.48642200 56.58853800 7.04147000	N 0 15.33129300 56.56300100 11.28579400
O 0 13.06438189 61.55270994 12.05673568	C -1 14.81279800 65.87499300 19.15158400	C 0 14.47377300 57.34063600 12.00118200
O 0 19.73766617 66.19395125 16.00155940	C 0 16.31576100 65.91756100 18.83378700	C 0 15.14375600 58.13130200 13.13664000

## E:MPSOR

H -1 17.45637900 55.72341200 15.74004700	H 0 16.96570300 64.55116700 19.08208600	C 0 14.72149100 58.96111500 15.34320500
H -1 14.36515100 66.87384500 19.12434500	C 0 16.56895600 66.38350400 17.39646200	N 0 14.18647100 58.37038600 14.19035200
H -1 8.60694600 62.77678100 18.32912500	H 0 14.62615800 65.45900600 20.14899200	C 0 14.05716000 59.95459300 16.06392000
H -1 10.42811600 62.61772500 -1.01100700	H 0 14.28240000 65.24788800 18.42410700	C 0 14.57387400 60.45151600 17.26306400
H -1 10.37418200 60.99324000 -0.26621600	H 0 16.78586400 66.63845600 19.51846900	C 0 13.88960500 61.57812200 17.99362100
C 0 14.72694600 60.57693700 6.14927500	H 0 18.03558300 64.57624800 18.85208700	C 0 15.77432800 59.91009100 17.76472500
C 0 15.12042700 61.66830700 6.91821500	H 0 16.84250500 64.22555300 20.12172300	C 0 16.36654000 60.41138500 19.05697400
C 0 14.55677800 61.89633400 8.17190800	H 0 16.51019000 63.79147300 18.43705600	C 0 16.45115100 58.94095500 17.02409700
C 0 13.58588000 61.01520600 8.64633500	H 0 17.63258800 66.42734200 17.14319500	C 0 15.95494700 58.47624000 15.80388800
C 0 13.17437000 59.92198900 7.88224000	H 0 16.09480200 65.69347800 16.68792000	C 0 16.27885900 57.29996100 13.70298300
C 0 13.74370300 59.71005200 6.63196100	H 0 16.14462800 67.37824700 17.22313000	N 0 16.62060800 57.52616400 14.99429800
H 0 15.19776000 60.39948600 5.18796100	C -1 8.77922700 61.70518600 18.47281200	H 0 15.02938100 56.18681700 10.39492800
H 0 15.89399700 62.33337900 6.56303900	C 0 10.22398500 61.34933100 18.09555800	H 0 13.44599500 61.24118400 18.93851500
H 0 12.42552300 59.22922400 8.23969500	C 0 10.53542000 59.87285800 18.36540900	H 0 14.59797600 62.37425200 18.24322500
H 0 13.41779200 58.85273200 6.05964700	C 0 10.43128400 61.68519500 16.61787600	H 0 13.09784500 62.02037500 17.38986500
O 0 15.73981300 59.29241900 12.60086700	H 0 8.54025000 61.44631900 19.50917800	H 0 15.64558400 60.36202600 19.88052900
H 0 18.05170900 66.60623600 14.02804200	H -1 8.12223700 61.13712200 17.80576500	H 0 17.24338700 59.82452300 19.34192800
C -1 10.91707200 57.40613200 14.32178900	H 0 10.91086100 61.96061900 18.69655300	H 0 16.68143000 61.45790900 18.97276800
C 0 11.01606300 56.31185000 13.25981300	H 0 11.56339500 59.62591300 18.08143600	H 0 13.14148900 60.36008800 15.64702300
O 0 10.19819000 56.30259700 12.33837600	H 0 10.40470900 59.62020800 19.42322100	H 0 17.39206600 58.57358200 17.41223800
	H 0 9.86756100 59.22489100 17.78377500	H 0 18.16786100 57.22247500 16.36432600

H 0 18.50035400 56.69243600 14.70533600	C -1 18.55413300 62.47067400 8.05095000	C 0 12.99528700 60.85189000 0.51526500
C -1 21.24006700 63.62185200 14.93270300	C 0 17.89285900 61.08497200 8.08217200	C 0 12.80912100 63.39598600 0.32146600
C 0 20.24457300 62.87029400 14.04087200	O 0 17.95327400 60.36609400 7.07403800	C 0 12.75018200 60.71567300 2.01735900
O 0 20.61705400 62.32557400 12.99825500	C 0 20.02908800 62.26942100 7.68183200	H 0 10.36248200 62.43213000 0.76377700
C 0 21.33549900 65.09960400 14.48791300	C 0 20.78093000 63.57600200 7.47010600	H 0 12.60738300 61.95880900 -1.24470200
C 0 20.01824300 65.83236100 14.76982800	O 0 20.56673000 61.51796900 8.78046300	H 0 12.67597800 59.92627700 0.01747300
O 0 19.21425900 65.92285400 13.75480900	H 0 19.09127200 62.99448300 10.04613900	H 0 14.07490100 60.93436500 0.34176000
O 0 19.78618100 66.21463200 15.92136600	H -1 18.05230800 63.07738100 7.28964500	H 0 13.90150900 63.46086300 0.29866400
H 0 20.96977800 63.58678900 15.99078100	H 0 20.04848200 61.66529000 6.76647700	H 0 12.40971100 64.21563700 -0.28607400
H 0 22.13154400 65.58776600 15.05744400	H 0 21.51676200 61.41163900 8.64782500	H 0 12.48461000 63.56782000 1.35213700
H 0 21.57853700 65.13827500 13.42264200	H 0 21.82864200 63.37751400 7.21748100	H 0 13.32576200 59.87898100 2.42562900
N 0 18.92116600 62.88106100 14.38623500	H 0 20.34173600 64.14313000 6.64324100	H 0 13.05335600 61.61113100 2.56833800
C 0 17.94104400 62.14363700 13.57884200	H 0 20.75065400 64.19283800 8.37107000	H 0 11.69503600 60.52623600 2.23152800
C 0 17.52151200 62.78096400 12.26211000	N 0 17.29973400 60.70505700 9.22385400	C -1 8.84957600 61.71553400 4.23804700
O 0 16.69890600 62.17440200 11.54660400	C 0 16.56316500 59.45748900 9.27185300	C 0 10.26818100 61.36099100 4.69958500
C 0 16.68360400 62.04443900 14.48501300	C 0 17.41879400 58.19917500 9.19078400	C 0 10.74912400 62.29643600 5.81817100
C 0 17.20806000 62.36486700 15.88669700	O 0 16.93054600 57.17341800 8.71253300	C 0 10.36161200 59.89241300 5.12584200
C 0 18.28927500 63.40540700 15.60882400	H 0 17.18278800 61.35945600 10.00259700	H 0 8.15479600 61.67355200 5.08742700
H 0 18.34094100 61.15671200 13.32825400	H 0 16.00104100 59.43569100 10.20438400	H -1 8.80520100 62.73712200 3.84515400
H 0 15.96091500 62.80793500 14.18607600	H 0 15.86166300 59.39114600 8.44101400	H 0 10.94107200 61.50838100 3.84857100
H 0 16.21443300 61.06815100 14.38898200	N 0 18.67090700 58.29204500 9.70832600	H 0 11.77814800 62.06648800 6.10998100
H 0 16.42227700 62.74261600 16.54323700	C -1 19.68171200 57.26437700 9.50351200	H 0 10.72266400 63.34590000 5.50607400
H 0 17.64749600 61.47679000 16.35154800	C 0 20.93180400 57.79363100 8.79945600	H 0 10.11480900 62.19109700 6.70909200
H 0 17.84679200 64.38227100 15.40513500	C 0 20.62491700 58.33515200 7.39400800	H 0 11.38579800 59.61668000 5.38056700
H 0 19.01281600 63.52345800 16.41305700	C 0 19.89605600 57.27331600 6.57153800	H 0 9.74533700 59.69315600 6.01020900
N 0 18.01533100 63.98460500 11.92681700	N 0 18.70605400 57.66411000 6.04395600	H 0 10.02197900 59.22194300 4.32830700
C 0 17.33840200 64.73868000 10.87465500	O 0 20.36603600 56.14706600 6.42156600	C 0 14.95746900 68.89399600 14.30083800
C 0 17.40453800 64.04602800 9.51735100	H 0 18.97591600 59.21779800 9.98264000	C 0 14.80470700 67.37466500 14.41838400
O 0 16.55543500 64.27463900 8.65136200	H 0 19.20580700 56.52067300 8.85911000	C 0 16.03973900 66.55302700 14.06363400
C 0 17.87056200 66.18906400 10.81540100	H 0 21.41095000 58.57700300 9.40038800	O 0 17.16050900 67.21811500 14.15970300
C 0 16.96214100 67.08117600 9.95115000	H 0 21.63935900 56.96312900 8.71366400	O 0 15.94188600 65.35900800 13.76731200
C 0 19.34330700 66.25500600 10.39744200	H 0 20.04076700 59.25336900 7.45437600	H 0 14.89097300 69.19419300 13.24701900
C 0 17.16761800 68.57170700 10.23401900	H 0 21.56516400 58.56578700 6.88002400	H 0 15.96230700 69.16392600 14.63415700
H 0 18.52849400 64.52409400 12.63424600	H 0 18.25221000 58.50456500 6.38831700	H 0 14.58180000 67.11307000 15.46091900
H 0 16.27377900 64.78003200 11.11179700	H 0 18.12098300 56.93760700 5.65342100	H 0 13.95935500 66.99977900 13.83489800
H 0 17.80213500 66.55609500 11.84168500	C -1 19.48707100 53.29098600 7.88391700	C -1 18.60133700 58.32721800 1.75415900
H 0 17.12341400 66.86476100 8.88906000	C 0 18.07853400 53.54232400 7.36849500	C 0 17.50736200 58.77361100 2.73632900
H 0 15.91670000 66.82371900 10.14975900	N 0 17.25186600 54.22321000 8.20228400	C 0 17.27196000 60.26463300 2.76381000
H 0 19.72445200 67.27472800 10.49497200	O 0 17.70375400 53.13350800 6.26782700	C 0 16.69552200 60.92209500 1.66843400
H 0 19.96203400 65.61818500 11.03469600	H 0 19.94827800 54.22398800 8.21702300	C 0 17.63534600 61.02825200 3.88174400
H 0 19.47290000 65.94426700 9.35462100	H 0 20.07723100 52.89202800 7.05952400	C 0 16.49154200 62.30141000 1.68292800
H 0 16.46869600 69.18135800 9.65175400	H 0 16.36734300 54.52051400 7.81918100	C 0 17.42931200 62.40890200 3.89911300
H 0 17.00471700 68.78828400 11.29596100	H 0 17.55676300 54.71983400 9.02959300	C 0 16.85879300 63.05330200 2.80049300
H 0 18.18075200 68.90243700 9.98255600	C -1 10.76510100 62.01132400 -0.16323500	H 0 18.32350800 58.52537800 0.71385700
N 0 18.44835000 63.20714600 9.29264700	C 0 12.30956600 62.03884600 -0.18896500	H 0 19.54739600 58.83917000 1.95688600

H 0 16.57570500 58.25740100 2.48551100	H -1 8.38407300 64.58831300 13.42537800	H 0 12.35865700 68.40535900 4.73650700
H 0 17.78289800 58.43902200 3.73925000	H 0 14.94298400 52.34071400 4.74780000	H 0 11.92794400 68.01426100 6.38622600
H 0 16.40357200 60.34296100 0.79580800	H -1 13.20183800 54.61265800 8.59409700	H 0 13.43136000 66.47653600 7.28921700
H 0 18.06552200 60.54549300 4.75273900	C -1 13.92156000 69.63659100 15.14270800	H 0 12.23225400 66.01175900 3.18741900
H 0 16.04777300 62.79057300 0.82083400	H -1 14.06767200 70.72210800 15.13456000	H 0 14.95258100 64.55656700 7.07286100
H 0 17.71370800 62.98267100 4.77718500	H -1 12.89125900 69.40618300 14.84979200	H 0 13.75251000 64.06433800 2.97620500
H 0 16.68574600 64.12436700 2.82265400	H 0 14.01555700 69.32478900 16.19134100	H 0 15.09319000 63.32816300 4.89030200
C -1 15.09096000 52.38696300 3.66533700	H 0 13.32708700 58.82319900 13.85745800	H -1 10.04576600 68.52177200 4.76342200
C 0 16.13208200 53.46724900 3.31820600	C -1 9.09339000 66.03185300 8.85515400	S 0 13.06964600 61.21980500 10.35848900
C 0 15.61633500 54.86341700 3.58731700	C 0 10.45826300 65.49907000 8.36507600	C 0 11.29693800 60.85760700 10.14830500
C 0 14.82998100 55.52316500 2.63472400	C 0 11.56538000 65.58119200 9.40074300	H 0 11.15744200 59.88456000 9.67824600
C 0 15.87025600 55.50787000 4.80702000	C 0 11.76863100 66.74668600 10.15585900	H 0 10.85818800 60.85443800 11.14287500
C 0 14.30945500 56.79131200 2.88795300	C 0 12.45543900 64.51782400 9.58830400	H 0 10.85893800 61.64778000 9.53558500
C 0 15.35292800 56.77976100 5.06704500	C 0 12.79491500 66.82833700 11.09621800	H 0 14.89897500 62.73621700 8.76384800
C 0 14.57396600 57.42365200 4.10225200	C 0 13.48778100 64.59796200 10.52360200	H 0 15.04197700 59.81314800 12.12382700
H 0 14.12509300 52.60648600 3.19734400	C 0 13.65249800 65.74608200 11.29467700	O 0 13.63797800 60.01969300 11.13566500
H 0 17.03609500 53.28857800 3.90590600	H -1 9.29286600 66.79644500 9.61309300	
H 0 16.39794200 53.38463300 2.25662800	H -1 8.44503900 65.25547500 9.27474000	
H 0 14.62546300 55.03400300 1.68499600	H 0 8.53638000 66.49970600 8.03692000	
H 0 16.47909500 54.98752800 5.54047800	H 0 10.37290800 64.46962100 8.00298000	
H 0 13.70476700 57.29247000 2.13684900	H 0 10.77553300 66.08325900 7.49421500	
H 0 15.56088700 57.26027500 6.02018200	H 0 11.12182900 67.60678000 10.00760200	
H 0 14.18238300 58.41800600 4.27814100	H 0 12.34641500 63.63070100 8.97186200	
C -1 9.36877900 64.78771200 13.86329800	H 0 12.92447400 67.73805600 11.67612000	
C 0 10.48891900 63.97665300 13.19542600	H 0 14.16192200 63.76417800 10.67266700	
C 0 11.82350400 64.19753800 13.91926800	H 0 14.43017400 65.77405400 12.04875200	
C 0 10.12155000 62.48926400 13.14321100	C -1 12.60592000 56.71569800 17.61679900	
H 0 9.30338100 64.54040000 14.93048700	C 0 13.43897600 55.55295400 17.09332200	
H 0 10.61280800 64.33918600 12.16602800	O 0 13.73733800 55.68995900 15.69894100	
H 0 12.64429700 63.68855000 13.40653800	H -1 12.18858700 56.58080400 18.62024900	
H 0 12.08000300 65.26029300 13.96218000	H -1 11.78063300 56.90579400 16.92285500	
H 0 11.78072800 63.82019800 14.94794500	H 0 13.21118500 57.62966600 17.63956200	
H 0 10.98923600 61.86282600 12.92320900	H 0 14.37073000 55.45573300 17.66836000	
H 0 9.72746400 62.15444000 14.10626600	H 0 12.89711200 54.60648400 17.18351000	
H 0 9.34665600 62.29543900 12.39244700	H 0 13.97718000 56.60830100 15.48783700	
H -1 15.41797100 51.40131200 3.31782300	H 0 10.32400100 66.96263100 3.97703100	
H -1 8.46291500 61.01899900 3.48741400	C -1 10.41964400 67.50454400 4.92199300	
H -1 18.76064700 57.25106800 1.87912500	C 0 11.88636300 67.63307200 5.35957200	
H -1 19.49892100 52.57384900 8.71139100	C 0 12.71926900 66.37818400 5.25905300	
H -1 22.21779000 63.14292000 14.80894600	C 0 13.48853900 65.94452800 6.34379300	
H -1 19.93331400 56.70830400 10.41282100	C 0 12.80989400 65.68011900 4.04667100	
H -1 6.00255300 59.81681200 7.41854900	C 0 14.34353200 64.84915400 6.22592400	
H -1 11.67856800 57.43269700 15.10842500	C 0 13.66077900 64.58502900 3.92315900	
H 0 10.89988100 53.56022000 12.98152500	C 0 14.42844000 64.17118500 5.01056200	
H -1 9.58969500 65.85842300 13.78321400	H 0 9.80472200 66.99544600 5.66869900	

## E:MPSR<sub>S(OO)</sub>

H -1 17.45623100 55.72337300 15.73971200
H -1 14.36518900 66.87385500 19.12415300
H -1 8.60702700 62.77679300 18.32911000
H -1 10.42807800 62.61771100 -1.01100100
H -1 10.37421200 60.99319600 -0.26589600
C 0 9.60605400 60.60079300 9.46791800
C 0 10.22989000 61.78866300 9.84169800
C 0 11.56302800 62.02438000 9.51005600
C 0 12.27611800 61.08690200 8.75801000
C 0 11.64713600 59.89647400 8.37833400
C 0 10.32940200 59.65103300 8.74212000
H 0 8.57702800 60.40680500 9.74537300
H 0 9.68393600 62.54137200 10.40036800
H 0 12.04048200 62.93879700 9.82307900
H 0 12.18546400 59.16840200 7.78347500
H 0 9.86391500 58.71826400 8.45130900
S 0 13.92473000 61.34440300 8.17592400
O 0 15.65049500 59.38486900 12.53784200
O 0 14.65293000 59.20840400 11.43842300
H 0 17.95387700 66.53735600 14.07967800
C 0 14.44462600 62.83214700 9.07085000
H 0 14.52943900 62.63930700 10.14164600
H 0 15.42585400 63.08697200 8.68087800
H 0 13.78235200 63.67334300 8.86397200
C -1 10.91628800 57.40527300 14.32281900
C 0 10.72890800 56.14608300 13.48163100



O 0 9.68004200 55.99727300 12.84684100	H 0 11.49757500 61.56314100 16.33125800	H 0 18.20841000 57.21197300 16.35179700
C 0 11.06835900 58.60036100 13.36117500	H 0 9.77817300 61.28442900 16.01049100	H 0 18.47045000 56.68264800 14.67716900
O 0 11.54218000 59.77229000 14.04002000	H 0 10.33150300 62.87081900 16.53322100	C -1 21.24077700 63.62219000 14.93277000
H 0 9.96302400 57.52269300 14.85971600	C -1 6.93652200 59.40393000 7.02355500	C 0 20.25235600 62.89150700 14.01310300
H 0 11.81497400 58.37055100 12.59853600	C 0 7.41390500 58.19189100 7.79410100	O 0 20.63262000 62.41774500 12.93937300
H 0 10.11446100 58.79824200 12.86028600	C 0 8.06513600 57.13890400 7.13846300	C 0 21.32120300 65.11614000 14.54717800
H 0 10.89281000 60.02485400 14.70721000	C 0 7.32117800 58.13357600 9.19278900	C 0 19.98831300 65.81442800 14.85703400
N 0 11.74065300 55.25315000 13.42282800	C 0 8.63775100 56.08590500 7.85887100	O 0 19.17531200 65.89715500 13.85355000
C 0 11.58683100 54.03927200 12.64331300	C 0 7.92540700 57.10511900 9.91921500	O 0 19.76075100 66.17233500 16.01932900
C 0 11.52136000 54.14252700 11.10287900	C 0 8.59556900 56.07512500 9.25461300	H 0 20.96189600 63.55295200 15.98734800
O 0 10.79694300 53.34236300 10.50201800	H 0 6.78806700 59.17246100 5.96498800	H 0 22.10943300 65.59244500 15.13798600
H 0 12.57472000 55.41031600 13.97712000	H 0 7.68944800 60.19899600 7.08237700	H 0 21.56320300 65.20215000 13.48439800
H 0 12.42642700 53.38156000 12.88933100	H 0 8.14361800 57.15650500 6.05410300	N 0 18.93472900 62.85028200 14.37280600
N 0 12.33984000 55.02839700 10.49646200	H 0 6.80198800 58.92946600 9.72161700	C 0 17.94636700 62.17764300 13.51330700
C -1 12.35113500 55.13809200 9.03916200	H 0 9.13180700 55.27606800 7.32988300	C 0 17.59203600 62.84410200 12.19030000
C 0 12.36405800 56.59496300 8.59596700	H 0 7.90597400 57.10467100 11.00475600	O 0 16.79123700 62.25878300 11.44663800
S 0 12.20819300 56.74419200 6.76397200	H 0 9.07270300 55.27802700 9.81700100	C 0 16.65795900 62.13297300 14.37294100
H 0 12.80455900 55.77003900 11.04644400	C -1 17.74271700 56.74915600 15.48521200	C 0 17.17337700 62.26916300 15.80526600
H 0 11.45312800 54.63612800 8.67262300	N 0 16.91875600 56.48398000 13.01474700	C 0 18.32390800 63.26246000 15.64942800
H 0 11.56128300 57.15245400 9.07867400	C 0 16.60871400 56.28942800 11.65509200	H 0 18.29849400 61.17184600 13.26401200
H 0 13.29801500 57.09368600 8.86337700	O 0 17.30610300 55.52713400 10.98542800	H 0 16.03420600 62.99694600 14.12423400
H 0 10.86088700 56.72034000 6.74803400	N 0 15.52869400 56.94526000 11.13322000	H 0 16.08626400 61.22950400 14.17030900
C -1 14.81280200 65.87487600 19.15182600	C 0 14.50597400 57.70688700 11.86234400	H 0 16.40375200 62.62344700 16.49368500
C 0 16.29465500 65.91406700 18.74731800	C 0 15.15925200 58.20692400 13.19248800	H 0 17.54459800 61.30957800 16.17800200
C 0 16.96288100 64.55031700 18.96084700	O 0 13.31819400 57.27530700 11.76881300	H 0 17.95485100 64.28842700 15.57268000
C 0 16.46682500 66.37533800 17.29668300	C 0 14.75377600 59.00086900 15.41841600	H 0 19.04696200 63.22375600 16.46399600
H 0 14.68348200 65.48136700 20.16749100	N 0 14.21469000 58.47477100 14.23799500	N 0 18.12405400 64.04617200 11.89319200
H 0 14.24364900 65.23090500 18.47017700	C 0 14.10885900 59.97650000 16.18061200	C 0 17.52195000 64.85839000 10.83842500
H 0 16.80283600 66.63912300 19.40052900	C 0 14.62242400 60.40766900 17.40649500	C 0 17.62859800 64.23622100 9.45057200
H 0 18.01662000 64.58229200 18.66659300	C 0 13.94476600 61.50889400 18.18276000	O 0 16.96502200 64.68673800 8.51177600
H 0 16.90332500 64.22746700 20.00733400	C 0 15.80461700 59.81985900 17.89186500	C 0 18.12031900 66.28344000 10.86520600
H 0 16.47496500 63.78522600 18.34660400	C 0 16.40227900 60.25854900 19.20504400	C 0 17.29677300 67.26727100 10.01610600
H 0 17.51770900 66.43406000 16.99736000	C 0 16.46046600 58.86055900 17.11741100	C 0 19.60757600 66.28666200 10.49444700
H 0 15.97082900 65.67234400 16.61591100	C 0 15.97241200 58.46074400 15.86910200	C 0 17.46625100 68.71653200 10.48001000
H 0 16.01640800 67.36099400 17.13613400	C 0 16.27163000 57.35470100 13.71389600	H 0 18.61391800 64.55580700 12.63521600
C -1 8.77918900 61.70511700 18.47248900	N 0 16.62076400 57.53369900 15.03211500	H 0 16.44726500 64.93422900 11.03247500
C 0 10.23270700 61.36551600 18.11630400	H 0 15.33540600 56.72976700 10.16336600	H 0 18.04002200 66.60580300 11.90441900
C 0 10.53597600 59.87428600 18.29930700	H 0 13.49684500 61.14014600 19.11469500	H 0 17.56361000 67.16604200 8.95910600
C 0 10.48722100 61.79673000 16.67206400	H 0 14.65397200 62.29472800 18.46408000	H 0 16.23993600 66.99411300 10.07504000
H 0 8.53218000 61.44428100 19.50707100	H 0 13.15460000 61.97750900 17.59569500	H 0 20.04030600 67.28084200 10.64020100
H -1 8.12206900 61.13704500 17.80599800	H 0 15.68286300 60.18175600 20.02905700	H 0 20.17120000 65.58864100 11.11887300
H 0 10.90164600 61.93578500 18.77530900	H 0 17.27367300 59.65066600 19.46334000	H 0 19.74983900 66.00850100 9.44373400
H 0 11.57396400 59.64517600 18.04010500	H 0 16.72862100 61.30547100 19.16735100	H 0 16.84494900 69.39709600 9.88668400
H 0 10.36405700 59.55242900 19.33233900	H 0 13.20083400 60.40542800 15.77554700	H 0 17.17904900 68.82201700 11.53263900
H 0 9.89285700 59.26594600 17.65085500	H 0 17.38157200 58.44351100 17.50353200	H 0 18.50422400 69.05625000 10.39087700

N 0 18.47202300 63.18789600 9.29635100	C 0 12.31192300 62.01338800 -0.16808900	H 0 19.17898100 58.82279000 2.53959400
C -1 18.55299200 62.47002100 8.05107700	C 0 12.95269500 60.76850400 0.47898000	H 0 16.56229800 58.40019000 0.99916100
C 0 17.86193200 61.10365700 8.01155900	C 0 12.85152400 63.32252200 0.42259300	H 0 16.69387800 57.94518800 2.68435900
O 0 17.92948500 60.44755800 6.95900300	C 0 12.76650000 60.61641400 1.98810300	H 0 16.59918400 60.84146500 0.37649500
C 0 20.02188800 62.25128800 7.66134700	H 0 10.35699900 62.43052500 0.76177800	H 0 16.96804000 59.58257900 4.46284500
C 0 20.78907700 63.55154300 7.46571500	H 0 12.62016300 61.98230400 -1.22405600	H 0 16.18423900 63.16445700 1.13516400
O 0 20.56296200 61.48221200 8.74731600	H 0 12.55530500 59.87749800 -0.02677100	H 0 16.58390400 61.87374700 5.22412300
H 0 19.02324200 62.87200200 10.08376700	H 0 14.02814600 60.78889600 0.26663300	H 0 16.13825800 63.69371900 3.56700300
H -1 18.05419800 63.07816700 7.28919000	H 0 13.94397400 63.35926400 0.37942400	C -1 15.09105900 52.38697200 3.66512200
H 0 20.02250800 61.65861800 6.73912000	H 0 12.45826100 64.19065800 -0.11912700	C 0 16.09546300 53.48983100 3.27928900
H 0 21.48814000 61.28638000 8.55601400	H 0 12.56512900 63.43407700 1.47326700	C 0 15.65828300 54.87089700 3.72843200
H 0 21.83330800 63.34502400 7.20314800	H 0 13.25500100 59.70558100 2.34596100	C 0 14.72527300 55.61181700 2.99204300
H 0 20.34869700 64.14110800 6.65532800	H 0 13.22210800 61.44771300 2.53257200	C 0 16.15344700 55.42418700 4.91839700
H 0 20.77229100 64.14733100 8.38128500	H 0 11.70977600 60.56068600 2.26417300	C 0 14.29713700 56.86650600 3.43037100
N 0 17.23659700 60.66724700 9.11133600	C -1 8.84994300 61.71559800 4.23793700	C 0 15.72362400 56.67647800 5.36775600
C 0 16.54976600 59.39044900 9.05910300	C 0 10.26707900 61.39232600 4.72518300	C 0 14.79586000 57.40426800 4.61779000
C 0 17.45857000 58.17558700 9.01654700	C 0 10.60236700 62.24284900 5.95584000	H 0 14.09927800 52.59000700 3.24618700
O 0 17.07259900 57.15482200 8.44091300	C 0 10.44543300 59.89698300 5.00811100	H 0 17.06001100 53.25493400 3.73826100
H 0 17.10955300 61.27401900 9.92626200	H 0 8.14976800 61.66900900 5.08272300	H 0 16.23550400 53.48916800 2.18975900
H 0 15.89001700 59.32188800 9.92632500	H -1 8.80486300 62.73709300 3.84511600	H 0 14.33014700 55.20085800 2.06488700
H 0 15.93583100 59.33480000 8.16093500	H 0 10.96751500 61.66843200 3.92675900	H 0 16.87164100 54.84936800 5.49227500
N 0 18.64769800 58.26973800 9.66915000	H 0 11.64067800 62.11054800 6.26419100	H 0 13.57070000 57.42465600 2.84598300
C -1 19.68167600 57.26476100 9.50386100	H 0 10.45630200 63.30866600 5.75085500	H 0 16.09803300 57.06177000 6.31312600
C 0 20.94799300 57.81547800 8.84000200	H 0 9.96778600 61.96541400 6.80437000	H 0 14.45662700 58.37574200 4.96169100
C 0 20.67969700 58.41153200 7.45210500	H 0 11.46218900 59.67030500 5.34035900	C -1 9.36793400 64.78910200 13.86163500
C 0 20.01856400 57.39021600 6.52608900	H 0 9.76865200 59.56281800 5.80151900	C 0 10.42948900 63.96555300 13.11648500
N 0 18.94718000 57.85976500 5.83399700	H 0 10.24182300 59.29653400 4.11331100	C 0 11.83387400 64.19552200 13.68596800
O 0 20.45710100 56.24641900 6.41190700	C 0 14.94155600 68.91430000 14.26606800	C 0 10.05684600 62.48163400 13.12324500
H 0 18.90340400 59.18496100 10.01627200	C 0 14.71657400 67.39985100 14.25535400	H 0 9.33245400 64.52012600 14.92430400
H 0 19.24099100 56.51628700 8.84154700	C 0 15.93265100 66.55960400 13.88271000	H 0 10.43491300 64.31257000 12.07346200
H 0 21.41513500 58.57761000 9.47795200	O 0 17.06807000 67.13912700 14.19227600	H 0 12.59043200 63.63953000 13.12381200
H 0 21.65760800 56.98735800 8.74163700	O 0 15.80560600 65.43859600 13.39312500	H 0 12.10996800 65.25446600 13.65621900
H 0 20.06781500 59.30930200 7.53540400	H 0 14.90349400 69.29858400 13.23852400	H 0 11.89235000 63.86356600 14.72978300
H 0 21.63223400 58.70257300 6.99032400	H 0 15.95034500 69.11217300 14.63561100	H 0 10.81318600 61.85960800 12.64239100
H 0 18.47778400 58.69848900 6.16500100	H 0 14.43898600 67.06828700 15.26506400	H 0 9.94946300 62.13049800 14.15111300
H 0 18.37753400 57.16910900 5.36302800	H 0 13.88636800 67.11885900 13.60225000	H 0 9.10012400 62.30856700 12.61836400
C -1 19.48696300 53.29105900 7.88402400	C -1 18.60102000 58.32707000 1.75346600	H -1 15.41790900 51.40123700 3.31797600
C 0 18.06279800 53.44891400 7.37165700	C 0 17.09683600 58.62520300 1.93004700	H -1 8.46288100 61.01872200 3.48768800
N 0 17.22157700 54.16549700 8.15365800	C 0 16.80976200 60.04266900 2.36387700	H -1 18.76090800 57.25115900 1.87957500
O 0 17.69684100 52.91435500 6.31948400	C 0 16.58893700 61.07084200 1.43996600	H -1 19.49899800 52.57372700 8.71128500
H 0 19.89923900 54.24206500 8.22845000	C 0 16.80061400 60.36250600 3.72844200	H -1 22.21785000 63.14300400 14.80909700
H 0 20.10081500 52.91155300 7.06798000	C 0 16.35434100 62.37958800 1.86725000	H -1 19.93338800 56.70794700 10.41258200
H 0 16.30771600 54.36124200 7.77265200	C 0 16.57096800 61.66692000 4.15981500	H -1 6.00246000 59.81657600 7.41857800
H 0 17.50004900 54.73655700 8.94643400	C 0 16.33944200 62.68241400 3.22971800	H -1 11.67899100 57.43245100 15.10802100
C -1 10.76489400 62.01139000 -0.16383800	H 0 18.98526500 58.65504700 0.78290500	H 0 10.65808100 53.53325000 12.91796500

H -1 9.59019300 65.85839200 13.78418800  
H -1 8.38384200 64.58790700 13.42608700  
H 0 14.99861900 52.34380900 4.75410000  
H -1 13.20194400 54.61291200 8.59399700  
C -1 13.92125400 69.63689100 15.14221500  
H -1 14.06789700 70.72208000 15.13487700  
H -1 12.89124500 69.40603100 14.84996800  
H 0 14.02914900 69.30823000 16.18386700  
H 0 13.39238600 58.97897800 13.91548600  
C -1 9.09332900 66.03210800 8.85521100  
C 0 10.49166400 65.46039400 8.45941300  
C 0 11.61712900 66.20650500 9.15050500  
C 0 11.94106600 67.51640000 8.76647400  
C 0 12.32906500 65.64649000 10.21782200  
C 0 12.94121300 68.23239500 9.42237800  
C 0 13.34939900 66.34516400 10.86821300  
C 0 13.65208700 67.64828000 10.47408000  
H -1 9.29273500 66.79649000 9.61308200  
H -1 8.44502100 65.25539800 9.27457100  
H 0 8.57717700 66.50017100 8.01225700  
H 0 10.54996000 64.39951500 8.70884700  
H 0 10.64201400 65.51710600 7.37637400  
H 0 11.40444100 67.97442100 7.93949100  
H 0 12.08622300 64.64707700 10.55575700  
H 0 13.17558300 69.24541800 9.10592700  
H 0 13.91034900 65.86919000 11.66791900  
H 0 14.43918100 68.20107500 10.97667500  
C -1 12.60582900 56.71581800 17.61681100  
C 0 13.44637600 55.56910900 17.06411800  
O 0 13.72518200 55.72650800 15.67361000  
H -1 12.18864900 56.58067400 18.62025800  
H -1 11.78065300 56.90597700 16.92283200  
H 0 13.20549300 57.63383600 17.64112800  
H 0 14.38350600 55.47356700 17.63399900  
H 0 12.91295400 54.61639300 17.14962900  
H 0 13.95705900 56.64767600 15.46681800  
H 0 9.95609800 66.83192000 4.19518200  
C -1 10.41987200 67.50474800 4.92194000  
C 0 11.95121200 67.55839100 4.77168100  
C 0 12.69833300 66.28346400 5.08960600  
C 0 13.65432600 66.26462900 6.11146900  
C 0 12.48576600 65.11063100 4.35126400  
C 0 14.38369100 65.11087500 6.40233200  
C 0 13.20985900 63.95465600 4.63517600  
C 0 14.15582200 63.95093800 5.66256600

H 0 10.12871200 67.17719100 5.92366500  
H 0 12.18301900 67.87039500 3.74343500  
H 0 12.33552700 68.35393500 5.42045600  
H 0 13.82830200 67.16373600 6.69403200  
H 0 11.75357200 65.10396500 3.54663600  
H 0 15.12471900 65.12092100 7.19489500  
H 0 13.03472800 63.04961700 4.06361100  
H 0 14.69639600 63.04102700 5.88931600  
H -1 10.04551200 68.52168000 4.76343000

### E:MPSR<sub>R</sub>(OO)

H -1 17.45612500 55.72344500 15.73988200  
H -1 14.36508700 66.87380700 19.12401200  
H -1 8.60703900 62.77678600 18.32902700  
H -1 10.42804400 62.61790900 -1.01084500  
H -1 10.37408500 60.99325200 -0.26598600  
C 0 13.46957300 59.72815100 6.80426300  
C 0 12.73465100 59.86074800 7.98126600  
C 0 13.02626800 60.87440900 8.88721600  
C 0 14.04940000 61.78641400 8.60716100  
C 0 14.76924900 61.66748900 7.41014800  
C 0 14.48614800 60.64010700 6.51538300  
H 0 13.24156200 58.90729200 6.13954300  
H 0 11.91937400 59.18062200 8.18926800  
H 0 12.46598800 60.94441600 9.80957900  
H 0 15.57385200 62.36436400 7.21083400  
H 0 15.07946500 60.54353400 5.61096700  
S 0 14.48446900 63.11804600 9.68360400  
O 0 15.68049600 59.42748700 12.66404300  
O 0 14.74039900 59.33988500 11.51247600  
H 0 17.91359100 66.46985100 14.12035300  
C 0 13.90098800 62.53087100 11.30121000  
H 0 14.23343700 61.50875900 11.48116800  
H 0 14.36689400 63.19223600 12.03346100  
H 0 12.81386200 62.59966100 11.38895100  
C -1 10.91597800 57.40507300 14.32301800  
C 0 10.88125100 56.18994000 13.39793300  
O 0 9.92061700 56.03367200 12.64028000  
C 0 10.98059700 58.69042600 13.48411400  
O 0 11.42576700 59.81137500 14.26410900  
H 0 9.95487900 57.38494800 14.85757700  
H 0 11.71902600 58.56626100 12.68882000  
H 0 10.00488200 58.89388200 13.03122000  
H 0 10.82111500 59.92389700 15.00791500

N 0 11.92394900 55.33297600 13.44732800  
C 0 11.90044000 54.08527900 12.70818000  
C 0 11.88271200 54.09066900 11.16692100  
O 0 11.43993600 53.08026300 10.61535300  
H 0 12.66518500 55.49314000 14.12209300  
H 0 12.78174000 53.51236000 13.01206900  
N 0 12.40886200 55.14033800 10.50067300  
C -1 12.35106400 55.13796000 9.03907200  
C 0 12.23849300 56.54299800 8.47100500  
S 0 11.88182800 56.51553300 6.66504900  
H 0 12.73935500 55.97825700 11.00378100  
H 0 11.47213700 54.55496400 8.75324100  
H 0 11.39209900 57.06337400 8.92266000  
H 0 13.12568900 57.15231900 8.65543200  
H 0 13.10952200 56.14110500 6.25180800  
C -1 14.81300300 65.87499500 19.15198900  
C 0 16.30187400 65.91701100 18.77557200  
C 0 16.97315300 64.56085700 19.02548600  
C 0 16.49583300 66.35670000 17.32128900  
H 0 14.66514900 65.47570800 20.16301300  
H 0 14.25666800 65.23463800 18.45660600  
H 0 16.79345400 66.65537200 19.42657600  
H 0 18.03008000 64.58999100 18.74240200  
H 0 16.90331700 64.26129800 20.07825200  
H 0 16.49499500 63.77998500 18.42369700  
H 0 17.55058400 66.42003200 17.03714900  
H 0 16.01612400 65.64014700 16.64318000  
H 0 16.04095900 67.33591100 17.13704200  
C -1 8.77899400 61.70500200 18.47300700  
C 0 10.23243000 61.38685000 18.09010400  
C 0 10.51778600 59.88112200 18.11931900  
C 0 10.50776300 61.97296500 16.70306900  
H 0 8.54531500 61.43427100 19.50751300  
H -1 8.12211700 61.13713200 17.80587600  
H 0 10.90270200 61.87536800 18.81057400  
H 0 11.55798800 59.66588600 17.85758000  
H 0 10.32241500 59.45250900 19.10846500  
H 0 9.87758900 59.35123800 17.40155500  
H 0 11.51000500 61.74416300 16.33446900  
H 0 9.78759000 61.58026300 15.97526800  
H 0 10.39626500 63.06137100 16.69921200  
C -1 6.93602500 59.40307100 7.02304500  
C 0 8.00321700 59.48735900 8.09443300  
C 0 8.39417600 58.36327300 8.83253500  
C 0 8.58309000 60.72360200 8.41221200

C 0 9.33214100 58.46517300 9.86530600	O 0 19.13107400 65.85198500 13.87890000	H 0 18.96727100 62.81677200 10.09895500
C 0 9.53348900 60.83106400 9.42532900	O 0 19.79053800 66.19225800 16.01341300	H -1 18.05426900 63.07820900 7.28917700
C 0 9.91005400 59.70221700 10.15553900	H 0 20.97751400 63.57751000 15.99309700	H 0 20.04452300 61.71605200 6.72462600
H 0 6.74905400 58.36817500 6.72425200	H 0 22.11085700 65.59841200 15.07159800	H 0 21.51759600 61.34960500 8.54466100
H 0 7.20956300 59.97427700 6.13227600	H 0 21.51516300 65.17374500 13.44315700	H 0 21.81882600 63.43046500 7.24336200
H 0 7.95639400 57.39541900 8.60215500	N 0 18.94144100 62.82574500 14.44300600	H 0 20.32026600 64.20513600 6.70204800
H 0 8.29172700 61.60830400 7.85218000	C 0 17.94875300 62.15271100 13.59839000	H 0 20.72796100 64.18036400 8.43064900
H 0 9.60398600 57.58951200 10.44958400	C 0 17.64514600 62.75333100 12.23287500	N 0 17.26395900 60.66397200 9.10342600
H 0 9.99150500 61.79247400 9.63716600	O 0 16.92428900 62.07699400 11.48972000	C 0 16.55438200 59.40148800 9.07556300
H 0 10.66002800 59.77915300 10.93405500	C 0 16.64726500 62.20088300 14.43362500	C 0 17.44681100 58.17457000 9.01974800
C -1 17.74298800 56.74900600 15.48500100	C 0 17.15341400 62.31243300 15.87123500	O 0 17.05239900 57.16059900 8.43817700
N 0 16.82780700 56.47568500 13.03417700	C 0 18.35573300 63.24626000 15.72910000	H 0 17.11748500 61.29561000 9.89690300
C 0 16.49355800 56.30991000 11.67657900	H 0 18.25873800 61.12118500 13.40528200	H 0 15.93015100 59.35249800 9.96934500
O 0 17.15763500 55.53462900 10.99084900	H 0 16.08880200 63.10526600 14.17256000	H 0 15.90901500 59.34850100 8.19901200
N 0 15.42543700 57.00275700 11.16935200	H 0 16.02338000 61.33260400 14.23029900	N 0 18.63986900 58.26227800 9.67078800
C 0 14.45742100 57.82880400 11.89186400	H 0 16.39663500 62.70671300 16.55232600	C -1 19.68203100 57.26507300 9.50400600
C 0 15.12029100 58.24705500 13.25205600	H 0 17.46995100 61.33445300 16.24629200	C 0 20.94436700 57.82311700 8.83912200
O 0 13.23731700 57.52271600 11.74741000	H 0 18.04328600 64.29182300 15.68212100	C 0 20.67577900 58.39122000 7.43738700
C 0 14.74371400 59.00914300 15.48639200	H 0 19.07686300 63.14726100 16.54167400	C 0 20.01160100 57.34381600 6.54467300
N 0 14.18326700 58.50302400 14.30547300	N 0 18.10049600 63.98433200 11.91811600	N 0 18.87473500 57.75626200 5.92263100
C 0 14.11177000 59.97632700 16.26886400	C 0 17.46704400 64.78545700 10.86291500	O 0 20.49345800 56.22003300 6.40466000
C 0 14.64275500 60.39168300 17.49231900	C 0 17.61383200 64.21876800 9.45355100	H 0 18.89113800 59.17706100 10.02315100
C 0 13.96936100 61.47701600 18.29357900	O 0 17.01168000 64.72003700 8.50235600	H 0 19.24449300 56.51341600 8.84173700
C 0 15.83364500 59.79953700 17.95040900	C 0 17.99790500 66.23669100 10.92759200	H 0 21.39497200 58.60352800 9.46622500
C 0 16.45248800 60.22515400 19.25798400	C 0 17.10337200 67.21070200 10.14223400	H 0 21.66721000 57.00426400 8.75938600
C 0 16.47600200 58.84734700 17.15573500	C 0 19.47231200 66.32090600 10.51610900	H 0 20.06588700 59.29195200 7.49985800
C 0 15.96841200 58.45835900 15.91134700	C 0 17.25981100 68.65804900 10.61693100	H 0 21.62947300 58.66546800 6.96907300
C 0 16.21334100 57.35356600 13.75165700	H 0 18.57070700 64.51724600 12.65583100	H 0 18.38552000 58.56992400 6.28710500
N 0 16.60261900 57.53336300 15.05942400	H 0 16.39001200 64.80919200 11.05019000	H 0 18.30725800 57.02907000 5.50760100
H 0 15.21953700 56.80315400 10.19866300	H 0 17.93490400 66.52022400 11.97804600	C -1 19.48699800 53.29099300 7.88398800
H 0 13.55553900 61.09471300 19.23581700	H 0 17.30853700 67.12898000 9.07086700	C 0 18.05430200 53.49222900 7.41141800
H 0 14.67207300 62.27437500 18.55879900	H 0 16.05965400 66.90791500 10.26141100	N 0 17.23481500 54.16676700 8.25051200
H 0 13.15368600 61.93303300 17.73185500	H 0 19.86837600 67.32485800 10.69487400	O 0 17.65874900 53.02113900 6.33958400
H 0 15.74865300 60.13271400 20.09377700	H 0 20.08184600 65.62062300 11.09379000	H 0 19.93445900 54.23081300 8.21576100
H 0 17.33282900 59.62065500 19.49253800	H 0 19.59426900 66.09420700 9.45063800	H 0 20.06772500 52.89684100 7.05105300
H 0 16.77006700 61.27491900 19.22716800	H 0 16.57069500 69.32290400 10.08369800	H 0 16.31242200 54.38430700 7.90445700
H 0 13.19661100 60.40985400 15.88422800	H 0 17.05153900 68.74047400 11.68988500	H 0 17.52739200 54.70748300 9.05855000
H 0 17.40230600 58.42504000 17.52326100	H 0 18.27501600 69.03661700 10.45265900	C -1 10.76502200 62.01098600 -0.16399700
H 0 18.22682500 57.21186700 16.34120600	N 0 18.44933600 63.16264000 9.30292600	C 0 12.31032800 62.03495100 -0.17044400
H 0 18.44854400 56.68736100 14.65718600	C -1 18.55293800 62.47004400 8.05108700	C 0 12.97885800 60.80490100 0.47495800
C -1 21.24101700 63.62205400 14.93297800	C 0 17.89293400 61.08845000 8.00545300	C 0 12.81078700 63.35833200 0.42163800
C 0 20.24737500 62.86738400 14.05120600	O 0 17.99121400 60.41684000 6.96336500	C 0 12.71875900 60.58608500 1.96455800
O 0 20.60654800 62.37478200 12.97871000	C 0 20.02778600 62.28573000 7.66153400	H 0 10.35543400 62.42805400 0.76164300
C 0 21.30687100 65.10830600 14.51446200	C 0 20.76782900 63.60648300 7.50185600	H 0 12.62240700 62.01150600 -1.22538800
C 0 19.98092300 65.80557900 14.85375100	O 0 20.58231400 61.49956900 8.72794400	H 0 12.65691200 59.91179900 -0.07847500

H 0 14.06063800 60.88871200 0.31855300	H 0 16.57822300 64.04014700 3.03790800	H 0 14.02091000 69.31492900 16.18702100
H 0 13.90339500 63.41108700 0.43266200	C -1 15.09103000 52.38698800 3.66506400	H 0 13.35689100 59.00924900 13.99980800
H 0 12.43368800 64.21300300 -0.15176100	C 0 16.15438400 53.46533400 3.39066100	C -1 9.09291900 66.03209800 8.85498000
H 0 12.46308900 63.48025000 1.45140200	C 0 15.66624800 54.85938900 3.72608300	C 0 10.49476400 65.47611200 8.46033900
H 0 13.28416600 59.72352800 2.33011600	C 0 14.83299000 55.55399400 2.84021000	C 0 11.58293500 66.21645400 9.20847500
H 0 13.02966100 61.44386000 2.56721100	C 0 16.00879400 55.47415000 4.93981300	C 0 11.82615300 67.57477300 8.95161600
H 0 11.66105700 60.39746900 2.16603900	C 0 14.36608100 56.83185600 3.14703800	C 0 12.31474400 65.59529200 10.22143700
C -1 8.84994100 61.71601900 4.23801900	C 0 15.54469800 56.75559200 5.25527800	C 0 12.77714800 68.28260100 9.68386700
C 0 10.29050900 61.36245600 4.62824300	C 0 14.73040200 57.44038000 4.34804000	C 0 13.27413900 66.29354500 10.95887400
C 0 10.82592700 62.27597000 5.73854100	H 0 14.14686500 52.62657300 3.16303700	C 0 13.50309800 67.64274700 10.69271100
C 0 10.40701300 59.88241300 5.00388700	H 0 17.04498400 53.24102400 3.98301200	H -1 9.29292400 66.79663500 9.61288500
H 0 8.18580300 61.66882300 5.10975300	H 0 16.43685300 53.43242100 2.32981100	H -1 8.44518700 65.25542800 9.27488100
H -1 8.80503000 62.73704300 3.84496700	H 0 14.55293300 55.08800300 1.89758800	H 0 8.57204100 66.49833200 8.01347700
H 0 10.91166400 61.53581100 3.74183500	H 0 16.64712400 54.93039200 5.62783600	H 0 10.56719200 64.40789400 8.68465800
H 0 11.87506400 62.06140600 5.95562300	H 0 13.72603200 57.35963800 2.44514600	H 0 10.66499100 65.56584800 7.38251200
H 0 10.75673200 63.33193800 5.45490300	H 0 15.82143200 57.20496000 6.20638100	H 0 11.26186100 68.07759200 8.16975200
H 0 10.26541300 62.12903700 6.66733100	H 0 14.39122000 58.44531100 4.56551500	H 0 12.14872000 64.54416600 10.41784700
H 0 11.44459200 59.59860000 5.17812200	C -1 9.36805400 64.78884000 13.86240300	H 0 12.95805900 69.33176200 9.46569500
H 0 9.85761800 59.66360900 5.92546700	C 0 10.48412300 64.01909400 13.13893800	H 0 13.85448500 65.78401100 11.72256000
H 0 10.00830800 59.23732400 4.21163400	C 0 11.81237000 64.20383200 13.88359600	H 0 14.25091100 68.18968400 11.25272500
C 0 14.93704400 68.89192400 14.28095400	C 0 10.12881600 62.54375900 12.93432400	C -1 12.60598200 56.71597900 17.61698100
C 0 14.68105500 67.38091800 14.28367500	H 0 9.32383600 64.51706600 14.92386000	C 0 13.45715600 55.56861400 17.08889900
C 0 15.88017300 66.51595200 13.91279900	H 0 10.59943300 64.47334000 12.14587000	O 0 13.80071600 55.74183500 15.71458300
O 0 17.02122700 67.06715000 14.24500400	H 0 12.63930400 63.71025600 13.37213600	H -1 12.18849200 56.58058500 18.62018300
O 0 15.73466700 65.40357600 13.40540700	H 0 12.06912400 65.26461900 13.97377300	H -1 11.78075200 56.90571300 16.92272900
H 0 14.91576300 69.26723400 13.25003900	H 0 11.75418000 63.78771200 14.89525500	H 0 13.20434300 57.63460600 17.64428200
H 0 15.94629500 69.07335900 14.65734800	H 0 10.95684800 61.98447800 12.49106700	H 0 14.36854500 55.46081800 17.69645200
H 0 14.40332700 67.06487200 15.29869200	H 0 9.90164400 62.05307700 13.88428300	H 0 12.91427500 54.61887700 17.14076200
H 0 13.84194300 67.11134600 13.63751900	H 0 9.25571500 62.43277900 12.28181600	H 0 14.00176000 56.67366700 15.52572700
C -1 18.60100400 58.32699800 1.75300600	H -1 15.41791300 51.40122300 3.31802000	H 0 10.13777100 66.88837500 4.06336300
C 0 17.28016300 58.70827100 2.43867800	H -1 8.46287300 61.01871700 3.48769700	C -1 10.42003500 67.50491400 4.92173600
C 0 17.08081500 60.19550200 2.59666400	H -1 18.76096700 57.25121400 1.87996100	C 0 11.94762100 67.62763700 5.06550500
C 0 16.64242900 60.98833100 1.52874900	H -1 19.49900000 52.57374900 8.71130400	C 0 12.73401200 66.33945500 5.14331800
C 0 17.35857100 60.81979400 3.81982400	H -1 22.21785200 63.14302200 14.80903500	C 0 13.56797400 66.08173500 6.23809100
C 0 16.47319000 62.36538700 1.67941400	H -1 19.93309900 56.70764100 10.41247400	C 0 12.71522100 65.42366500 4.08183000
C 0 17.18586700 62.19489200 3.97463700	H -1 6.00283400 59.81699400 7.41902400	C 0 14.37607300 64.94492200 6.27859300
C 0 16.73791800 62.97485900 2.90713600	H -1 11.67902300 57.43291100 15.10797700	C 0 13.52315000 64.28953800 4.11454100
H 0 18.60020700 58.57422700 0.68628100	H 0 11.01474600 53.50024500 12.97444500	C 0 14.35473300 64.05167100 5.20863000
H 0 19.44307200 58.84387700 2.22395200	H -1 9.58995900 65.85841500 13.78383200	H 0 9.95768000 67.08021600 5.81684100
H 0 16.44330200 58.27449400 1.88128200	H -1 8.38395800 64.58811600 13.42572900	H 0 12.31723400 68.20929300 4.20874700
H 0 17.25332000 58.24213700 3.42582700	H 0 14.89626900 52.32207100 4.73935400	H 0 12.16981100 68.22961900 5.95315700
H 0 16.42760700 60.51821600 0.57166600	H -1 13.20196600 54.61300400 8.59393100	H 0 13.59438800 66.78231500 7.06622700
H 0 17.70838700 60.23881900 4.66528300	C -1 13.92101700 69.63696900 15.14204800	H 0 12.08364600 65.61289300 3.21613200
H 0 16.13178300 62.96284100 0.83859000	H -1 14.06799200 70.72206600 15.13497400	H 0 15.03063600 64.78138900 7.12898300
H 0 17.39489000 62.64832800 4.93858700	H -1 12.89121500 69.40607300 14.85004200	H 0 13.52826500 63.59463800 3.28211300

H 0 14.97882800 63.16997200 5.21444100  
H -1 10.04529200 68.52161800 4.76354700

## MPS-TS<sub>s(00)</sub>

H -1 17.45624400 55.72342900 15.73993800  
H -1 14.36523000 66.87387800 19.12421200  
H -1 8.60702000 62.77676700 18.32892500  
H -1 10.42829800 62.61758200 -1.01118000  
H -1 10.37415100 60.99324300 -0.26613400  
C 0 9.57801700 60.28359800 9.49976900  
C 0 10.46678200 59.42385800 10.14204900  
C 0 11.76445000 59.84798800 10.43872200  
C 0 12.17224900 61.13673800 10.08749200  
C 0 11.30970000 61.95835800 9.35366300  
C 0 10.01068600 61.54256100 9.08521400  
H 0 8.56349400 59.96571600 9.31303000  
H 0 10.14370500 58.42551800 10.41997100  
H 0 12.48272700 59.19711300 10.92049100  
H 0 11.65207700 62.92198100 9.00782500  
H 0 9.32828400 62.20781500 8.56412700  
S 0 13.72249200 61.73411700 10.75174000  
O 0 16.17539400 59.14535700 12.34181800  
O 0 14.94262900 60.18304600 11.61404100  
H 0 17.99120100 66.60896100 14.02559000  
C 0 14.46391800 62.40681000 9.22939400  
H 0 13.81900000 63.16575900 8.78479800  
H 0 15.39643600 62.87193700 9.53039700  
H 0 14.65080100 61.60556900 8.51253800  
C -1 10.91600800 57.40531800 14.32287200  
C 0 10.81339300 56.13431600 13.48964300  
O 0 9.78536000 55.88162500 12.85870400  
C 0 11.12468300 58.55055900 13.33942600  
O 0 11.32463300 59.76992800 14.05260900  
H 0 9.94850900 57.53338700 14.82120900  
H 0 11.99010000 58.31491800 12.71771200  
H 0 10.24258600 58.61918300 12.69528500  
H 0 11.39415600 60.47284300 13.39244300  
N 0 11.92352200 55.35220500 13.39745000  
C 0 11.82525200 54.08087900 12.69871000  
C 0 11.66728800 54.11492900 11.16494300  
O 0 10.99740700 53.23979700 10.61581300  
H 0 12.68207800 55.50842800 14.05707100  
H 0 12.73343700 53.51121400 12.91957500  
N 0 12.37190600 55.05597000 10.49680800  
C -1 12.35173900 55.13842100 9.03948700

C 0 12.35237100 56.59966600 8.58576900  
S 0 12.21978100 56.79046400 6.75903300  
H 0 12.81915200 55.81703300 11.00185900  
H 0 11.45193700 54.62339800 8.69569500  
H 0 11.53128500 57.14680600 9.04814500  
H 0 13.27291900 57.10287300 8.88244700  
H 0 10.88122700 56.92872800 6.73587200  
C -1 14.81273800 65.87485700 19.15171200  
C 0 16.28114900 65.89870600 18.69958200  
C 0 16.93150900 64.51766100 18.85091000  
C 0 16.41839400 66.39303300 17.25639800  
H 0 14.71308800 65.49212500 20.17479100  
H 0 14.21958900 65.22595500 18.49540700  
H 0 16.82419500 66.59677300 19.35437100  
H 0 17.97804100 64.54588300 18.53197000  
H 0 16.89096500 64.15825500 19.88642700  
H 0 16.41765200 63.78219200 18.22075100  
H 0 17.46195100 66.44071300 16.93064800  
H 0 15.89362700 65.71243900 16.57451300  
H 0 15.97840800 67.38901900 17.13305700  
C -1 8.77929000 61.70482600 18.47294400  
C 0 10.21215100 61.34850100 18.04633400  
C 0 10.52551300 59.86965600 18.30164600  
C 0 10.37865000 61.68360400 16.56075600  
H 0 8.56180100 61.43972600 19.51270400  
H -1 8.12210500 61.13733300 17.80571800  
H 0 10.92060300 61.95566800 18.62698700  
H 0 11.54078200 59.62063100 17.97870100  
H 0 10.42870700 59.61299200 19.36319700  
H 0 9.83884800 59.22785600 17.73629800  
H 0 11.35373500 61.38628700 16.17655800  
H 0 9.64072900 61.13951100 15.96181700  
H 0 10.24236000 62.75428000 16.37645200  
C -1 6.93705400 59.40465000 7.02405500  
C 0 7.39838700 58.18083600 7.78784800  
C 0 8.18250300 57.20157200 7.16516300  
C 0 7.14075700 58.03705800 9.15908200  
C 0 8.71912500 56.13668700 7.89419000  
C 0 7.70561500 56.99534900 9.89909100  
C 0 8.50774400 56.04065500 9.27069700  
H 0 6.79624700 59.18592900 5.96162000  
H 0 7.69241700 60.19659600 7.09035100  
H 0 8.38734700 57.28338600 6.10047000  
H 0 6.52208600 58.77653700 9.66275600  
H 0 9.32092200 55.38768900 7.38886200

H 0 7.54563500 56.93265000 10.97108300  
H 0 8.96226100 55.23990400 9.84647900  
C -1 17.74256100 56.74924200 15.48468800  
N 0 17.12867600 56.30768700 12.99151600  
C 0 16.90015500 56.02080600 11.66497700  
O 0 17.65450600 55.32384500 10.99624900  
N 0 15.69368400 56.47432700 11.09876500  
C 0 14.80962300 57.32384700 11.71290700  
C 0 15.42763800 58.12561800 12.86592800  
O 0 13.66407100 57.47008700 11.29828000  
C 0 14.77577200 59.01972400 15.01212400  
N 0 14.36413600 58.57163900 13.76065300  
C 0 14.10289900 60.04274700 15.69487400  
C 0 14.47062900 60.44371400 16.97814000  
C 0 13.81652300 61.63289700 17.63449000  
C 0 15.50475900 59.75461200 17.64193600  
C 0 15.92327800 60.14173000 19.03756000  
C 0 16.18718200 58.74673000 16.96338100  
C 0 15.87902800 58.40658400 15.63994100  
C 0 16.40191700 57.21825300 13.58415600  
N 0 16.63318500 57.46832600 14.89754600  
H 0 15.55703700 56.25091500 10.11855100  
H 0 13.22672100 61.34809600 18.51386100  
H 0 14.56723500 62.35249300 17.97967300  
H 0 13.15710200 62.15388500 16.94061000  
H 0 15.07942900 60.13120800 19.73785000  
H 0 16.68701900 59.46003100 19.42264200  
H 0 16.34150900 61.15612600 19.06430700  
H 0 13.28057900 60.52519700 15.18144800  
H 0 16.99433500 58.24717700 17.48287600  
H 0 18.10754600 57.26405800 16.36864500  
H 0 18.54092000 56.68313200 14.74707900  
C -1 21.24080500 63.62221600 14.93280300  
C 0 20.27903400 62.93103100 13.95696500  
O 0 20.69064700 62.52427500 12.86628900  
C 0 21.32990600 65.12714100 14.59693500  
C 0 19.98033200 65.81162000 14.86851600  
O 0 19.23445600 65.97632800 13.82476300  
O 0 19.68460500 66.09094100 16.03780700  
H 0 20.93488600 63.51689600 15.97636500  
H 0 22.08930400 65.58972700 15.23514900  
H 0 21.61658500 65.24627100 13.54872900  
N 0 18.95670500 62.85778200 14.28463300  
C 0 17.99364700 62.22558700 13.36821600  
C 0 17.63924500 62.98995800 12.10648600

O 0 16.81096100 62.48490300 11.33599300	C 0 16.53133700 59.42440100 9.19657400	C 0 10.27836400 61.39951700 4.69838600
C 0 16.69969700 62.06197900 14.20250100	C 0 17.41331700 58.18562400 9.12901000	C 0 10.74385900 62.45560200 5.70650400
C 0 17.19313700 62.13358100 15.64891700	O 0 16.97812300 57.15369700 8.59883200	C 0 10.39999500 59.98530400 5.27769000
C 0 18.31190800 63.17375200 15.57112900	H 0 17.15253900 61.29104400 10.02822200	H 0 8.16245600 61.67343000 5.09334800
H 0 18.37518100 61.25274600 13.04259900	H 0 15.89803300 59.42516500 10.09827900	H -1 8.80497500 62.73707400 3.84505100
H 0 16.03308300 62.90487000 13.99916900	H 0 15.89379500 59.37310300 8.31006900	H 0 10.93416700 61.46372500 3.82250900
H 0 16.18688000 61.14584500 13.91730800	N 0 18.64548300 58.27341600 9.69327800	H 0 11.74949600 62.24514800 6.07906200
H 0 16.40607600 62.42370100 16.34722100	C -1 19.68139100 57.26468500 9.50390600	H 0 10.76210000 63.45513100 5.26225700
H 0 17.59276700 61.16704200 15.97417400	C 0 20.93792700 57.82635500 8.83495900	H 0 10.07294500 62.47829500 6.56919200
H 0 17.90811600 64.18984600 15.54979400	C 0 20.65149700 58.43039600 7.45436400	H 0 11.43664800 59.74176700 5.52806500
H 0 19.02317800 63.11481800 16.39481700	C 0 19.96947500 57.41650700 6.53718800	H 0 9.81905200 59.88294800 6.20067300
N 0 18.20621600 64.18153300 11.84244600	N 0 18.86158400 57.88174200 5.90365900	H 0 10.04197000 59.22980100 4.56781900
C 0 17.61143200 64.97845200 10.77571300	O 0 20.41689200 56.28031400 6.38437000	C 0 14.94145900 68.92571500 14.25281400
C 0 17.63487500 64.26290300 9.42313700	H 0 18.90831800 59.18178700 10.05367300	C 0 14.74485800 67.40660700 14.23224700
O 0 16.86821600 64.60857400 8.52015900	H 0 19.23396000 56.52091700 8.84099800	C 0 15.97755300 66.59124300 13.85050200
C 0 18.27045300 66.37391700 10.72351200	H 0 21.40614600 58.58612500 9.47418600	O 0 17.10563500 67.20496300 14.12447400
C 0 17.50002100 67.32598400 9.79171400	H 0 21.65003500 57.00184700 8.72487700	O 0 15.87220400 65.45870800 13.38536600
C 0 19.76309300 66.29610800 10.38337100	H 0 20.04413600 59.32893200 7.55507500	H 0 14.88861000 69.31673300 13.22808700
C 0 17.75434600 68.79961300 10.11904400	H 0 21.59730600 58.71992100 6.97865100	H 0 15.95096700 69.13677200 14.61304100
H 0 18.69337400 64.68407200 12.59200100	H 0 18.39724500 58.71315400 6.26140500	H 0 14.47647100 67.06271000 15.23960500
H 0 16.54774600 65.11411800 10.99440500	H 0 18.28845500 57.19597200 5.43047800	H 0 13.92089900 67.10882500 13.57833000
H 0 18.18258500 66.76584500 11.74120000	C -1 19.48639900 53.29116500 7.88411500	C -1 18.60122000 58.32714100 1.75286400
H 0 17.75611200 67.11391600 8.74778900	C 0 18.06904700 53.44206400 7.35642600	C 0 17.12222400 58.64019500 2.06038500
H 0 16.42843900 67.12085100 9.87416700	N 0 17.23584200 54.19029800 8.11823700	C 0 16.87509100 60.08240900 2.43273400
H 0 20.23388900 67.27997500 10.46994200	O 0 17.70243100 52.88875000 6.31536600	C 0 16.63495000 61.06534900 1.46464100
H 0 20.28608600 65.61907300 11.06343000	H 0 19.88895000 54.24423700 8.23380800	C 0 16.92804800 60.47353800 3.77731200
H 0 19.91192900 65.94032800 9.35746800	H 0 20.11199800 52.91587700 7.07479200	C 0 16.44930000 62.40033300 1.82978800
H 0 17.17959100 69.45730600 9.45733900	H 0 16.32825400 54.40120100 7.73096300	C 0 16.74724800 61.80480700 4.14722400
H 0 17.46364800 69.02091900 11.15263400	H 0 17.53815700 54.75410500 8.90676700	C 0 16.50300000 62.77553000 3.17375900
H 0 18.81159300 69.06662700 10.01238400	C -1 10.76487700 62.01133800 -0.16325100	H 0 18.89613700 58.63527900 0.74513500
N 0 18.53748000 63.25980700 9.25707400	C 0 12.31096500 62.03514200 -0.11994300	H 0 19.25214400 58.83197700 2.47328500
C -1 18.55245800 62.46967200 8.05109400	C 0 12.94848800 60.76100400 0.46998800	H 0 16.49892600 58.35871500 1.20304600
C 0 17.82646900 61.11580900 8.07590100	C 0 12.80557500 63.30675600 0.58269300	H 0 16.79846600 58.00738700 2.88972500
O 0 17.82391600 60.45424100 7.02137800	C 0 12.65021900 60.47586500 1.94144400	H 0 16.59532100 60.78013000 0.41545500
C 0 20.00250000 62.20014200 7.62327100	H 0 10.33226200 62.42587100 0.75380300	H 0 17.11213900 59.73248600 4.54663800
C 0 20.78989200 63.47170300 7.33853400	H 0 12.66000700 62.08068800 -1.16211200	H 0 16.26638000 63.14943000 1.06380000
O 0 20.56843400 61.46930100 8.72249700	H 0 12.62536300 59.90272200 -0.13516200	H 0 16.80763400 62.06593700 5.19813200
H 0 19.12324200 62.98448000 10.03493500	H 0 14.03532000 60.83471300 0.34645800	H 0 16.34514400 63.80928000 3.46304800
H -1 18.05448100 63.07839600 7.28919000	H 0 13.89823200 63.35548600 0.60405500	C -1 15.09113700 52.38689200 3.66638500
H 0 19.95977300 61.56794500 6.72837800	H 0 12.43095100 64.20662600 0.08139800	C 0 16.09681200 53.48729700 3.27708600
H 0 21.49457300 61.28446500 8.52451100	H 0 12.45651100 63.34064400 1.61964800	C 0 15.66434100 54.86729800 3.73160100
H 0 21.81833500 63.22801500 7.04631000	H 0 13.18024100 59.57878200 2.27363000	C 0 14.74090700 55.61797800 2.99403300
H 0 20.33221100 64.03257400 6.51739000	H 0 12.98251000 61.29303200 2.58760800	C 0 16.15125200 55.40762500 4.93084500
H 0 20.82107100 64.10999100 8.22439600	H 0 11.58158800 60.31825300 2.11645100	C 0 14.31506500 56.87052800 3.43975000
N 0 17.26291000 60.68121800 9.20977100	C -1 8.84980100 61.71529700 4.23807800	C 0 15.72097500 56.65634100 5.38917300

C 0 14.80504300 57.39571000 4.63597000	C 0 13.44153200 65.90569100 10.89444600	H -1 10.37408300 60.99322400 -0.26570500
H 0 14.09857000 52.59116900 3.25014900	C 0 13.75005100 67.25110800 10.69763400	C 0 13.79237200 60.40171000 6.24322000
H 0 17.06308400 53.24869100 3.73054700	H -1 9.29268100 66.79641600 9.61317100	C 0 13.09104900 59.76448000 7.26747100
H 0 16.23120000 53.48823800 2.18699500	H -1 8.44512400 65.25525100 9.27445900	C 0 13.21705000 60.20258400 8.58311000
H 0 14.35138600 55.21646100 2.06046200	H 0 8.57975400 66.49468600 8.00756400	C 0 14.01498200 61.31723700 8.87503700
H 0 16.86562200 54.82544300 5.50134600	H 0 10.48215100 64.37262800 8.61651300	C 0 14.68436300 61.98517900 7.83829500
H 0 13.59499700 57.43551600 2.85446800	H 0 10.69132100 65.60564000 7.40608700	C 0 14.59184900 61.50503900 6.53526500
H 0 16.08462800 57.03338900 6.34233100	H 0 11.36858500 68.01422800 8.39040800	H 0 13.70575200 60.05781900 5.21738800
H 0 14.46699400 58.36496000 4.98611500	H 0 12.15940500 64.28144800 10.36635900	H 0 12.45667600 58.91621100 7.04191200
C -1 9.36796700 64.78841300 13.86198700	H 0 13.22877900 69.05816700 9.64128400	H 0 12.72124300 59.65499500 9.37186000
C 0 10.41657700 64.00268500 13.04899400	H 0 14.02086800 65.31430300 11.59765600	H 0 15.28826500 62.85770100 8.06025700
C 0 11.81322200 64.06743400 13.67685700	H 0 14.57399700 67.70381900 11.23898100	H 0 15.13382300 61.99403800 5.73832300
C 0 9.97652800 62.55430100 12.81311900	C -1 12.60592800 56.71592200 17.61691400	S 0 14.38071300 61.83311600 10.53594100
H 0 9.35378900 64.49210400 14.91628800	C 0 13.44626000 55.56363600 17.08401200	O 0 16.42567800 59.20867500 12.51805000
H 0 10.47838300 64.48623700 12.06475000	O 0 13.82943500 55.78090100 15.72337800	O 0 15.53174500 60.39548900 11.59023900
H 0 12.55193300 63.55617000 13.05137300	H -1 12.18857400 56.58067900 18.62022700	H 0 18.53512700 66.86258500 14.20039800
H 0 12.15000300 65.10158600 13.80369000	H -1 11.78074300 56.90562900 16.92269400	C 0 12.91450500 61.27305500 11.42027800
H 0 11.81984400 63.58913200 14.66380000	H 0 13.21058500 57.63125500 17.64225100	H 0 12.87679500 60.18576000 11.38933400
H 0 10.68898800 62.03634000 12.16365900	H 0 14.33835200 55.41038100 17.70982700	H 0 13.04785400 61.58385800 12.45433500
H 0 9.89157000 62.00329600 13.75498400	H 0 12.88014200 54.62668100 17.08237000	H 0 12.00546700 61.72220500 11.01653100
H 0 9.00370400 62.50698900 12.31151500	H 0 14.19826700 56.67449200 15.64745700	C -1 10.91700800 57.40452100 14.32249000
H -1 15.41793800 51.40158500 3.31701600	H 0 9.86693700 66.80349900 4.28998100	C 0 10.97781600 56.11970400 13.50347600
H -1 8.46291700 61.01885100 3.48754900	C -1 10.41974800 67.50433200 4.92193600	O 0 9.99927200 55.68181200 12.90193900
H -1 18.76070500 57.25118800 1.88007700	C 0 11.93068900 67.50983000 4.60255300	C 0 11.14884300 58.57611600 13.35631700
H -1 19.49930100 52.57362100 8.71118900	C 0 12.71369000 66.28096800 5.01411200	O 0 11.44010800 59.80389900 14.01861700
H -1 22.21784500 63.14300300 14.80907100	C 0 13.41183500 66.26574000 6.22883800	H 0 9.92848300 57.46912800 14.78773200
H -1 19.93371900 56.70800500 10.41252600	C 0 12.80470900 65.15831400 4.18051200	H 0 12.01826200 58.35694700 12.73510800
H -1 6.00214600 59.81615700 7.41827300	C 0 14.17814900 65.16451800 6.61389900	H 0 10.27716200 58.68030600 12.70089300
H -1 11.67902200 57.43284700 15.10800100	C 0 13.57091000 64.05378200 4.55490900	H 0 10.61909200 60.17705500 14.35851300
H 0 10.96124000 53.51078000 13.05113000	C 0 14.25669400 64.05415300 5.77180200	N 0 12.21962600 55.56222000 13.40285200
H -1 9.59016800 65.85837000 13.78382200	H 0 10.24053800 67.23618700 5.96711000	C 0 12.38172500 54.26331400 12.77454200
H -1 8.38381400 64.58827100 13.42598700	H 0 12.05648900 67.67653200 3.52502200	C 0 12.18558900 54.16225100 11.25575400
H 0 15.00237000 52.34273400 4.75560300	H 0 12.37731200 68.37942100 5.09911300	O 0 11.83587400 53.08182400 10.78453700
H -1 13.20148400 54.61251300 8.59359100	H 0 13.36730000 67.13198300 6.88056100	H 0 12.91530900 55.83211500 14.09403100
C -1 13.92122300 69.63678900 15.14202300	H 0 12.28623400 65.15694300 3.22411400	H 0 13.39798600 53.92122900 12.99324000
H -1 14.06792500 70.72207700 15.13503900	H 0 14.73992000 65.18190200 7.54240300	N 0 12.48259500 55.24020200 10.49033500
H -1 12.89123000 69.40612100 14.84995000	H 0 13.65024900 63.19777700 3.89254500	C -1 12.34994600 55.13789100 9.03938500
H 0 14.03500400 69.30295200 16.18107500	H 0 14.86186000 63.20055800 6.05791700	C 0 12.18374300 56.50601700 8.39227800
H 0 13.88627400 59.30182300 13.22324700	H -1 10.04570300 68.52177200 4.76357300	S 0 11.81169100 56.36732100 6.59568100
C -1 9.09325500 66.03253700 8.85522700		H 0 12.79806200 56.11346000 10.90301300
C 0 10.48758500 65.45122800 8.47106800	<b>MPS-TS<sub>R</sub>(OO)</b>	H 0 11.47722500 54.51454100 8.83187000
C 0 11.62646700 66.06324400 9.26874600	H -1 17.45614800 55.72344100 15.73989600	H 0 11.33006200 57.03413600 8.82202800
C 0 11.94441200 67.41975200 9.09663600	H -1 14.36507900 66.87378800 19.12346500	H 0 13.06178200 57.13993600 8.53457900
C 0 12.38346600 65.32544200 10.18766600	H -1 8.60700700 62.77681200 18.32925400	H 0 13.07064100 56.13378400 6.17364800
C 0 12.99368500 68.00896100 9.79942100	H -1 10.42793700 62.61777300 -1.01090000	C -1 14.81307200 65.87498200 19.15262100



C 0 16.32061700 65.90131900 18.86216000  
C 0 16.93613100 64.51010000 19.06083800  
C 0 16.60939800 66.41679900 17.44990800  
H 0 14.60312000 65.44896800 20.14189300  
H 0 14.29339500 65.25711000 18.40976000  
H 0 16.79341600 66.58302100 19.58562000  
H 0 18.00818900 64.52091200 18.84044800  
H 0 16.79421400 64.14356100 20.08506700  
H 0 16.47204600 63.78794900 18.37929300  
H 0 17.67875900 66.45159200 17.22658400  
H 0 16.15359500 65.75714200 16.70291100  
H 0 16.19931500 67.42098400 17.29898900  
C -1 8.77915000 61.70506400 18.47245800  
C 0 10.21564300 61.32614200 18.08784700  
C 0 10.49843800 59.84455100 18.36248700  
C 0 10.42501500 61.64649200 16.60641200  
H 0 8.54058300 61.44710700 19.50961000  
H -1 8.12193300 61.13706800 17.80611000  
H 0 10.91942600 61.92734300 18.67865300  
H 0 11.51691800 59.57515800 18.06750800  
H 0 10.37147200 59.59982900 19.42304900  
H 0 9.81287400 59.20787600 17.78923000  
H 0 11.39369700 61.30439300 16.24067300  
H 0 9.64869500 61.14477800 16.01391200  
H 0 10.33910900 62.71848200 16.40771200  
C -1 6.93568000 59.40204800 7.02271700  
C 0 8.01624100 59.45888200 8.07660600  
C 0 8.35503500 58.33206400 8.83475300  
C 0 8.67861500 60.66511700 8.34181000  
C 0 9.32638200 58.40477700 9.83668900  
C 0 9.66517500 60.73996300 9.32169200  
C 0 9.98910400 59.60949100 10.07272900  
H 0 6.73580800 58.37272200 6.71213200  
H 0 7.20863000 59.97815000 6.13496100  
H 0 7.85351200 57.38759900 8.64067200  
H 0 8.42610900 61.54896000 7.76277000  
H 0 9.56481600 57.52627700 10.43132900  
H 0 10.18993500 61.67512700 9.49143600  
H 0 10.76022900 59.66674200 10.82855900  
C -1 17.74272300 56.74938100 15.48460200  
N 0 16.99777400 56.27876900 12.99799100  
C 0 16.77995500 56.06587200 11.65216400  
O 0 17.46706400 55.30882500 10.98184100  
N 0 15.65572800 56.68424700 11.05872600  
C 0 14.85078200 57.61814600 11.65423600  
C 0 15.50203800 58.27665100 12.88731700  
O 0 13.75079600 57.91711600 11.18894100  
C 0 14.79979100 59.07981600 15.06197200  
N 0 14.43538200 58.75033100 13.76599100  
C 0 14.13304400 60.07345300 15.79261900  
C 0 14.45973200 60.37107500 17.11427200  
C 0 13.82678800 61.54236300 17.82164500  
C 0 15.44009500 59.59841600 17.76725500  
C 0 15.81092700 59.86961300 19.20290700  
C 0 16.11750100 58.61789800 17.04349000  
C 0 15.86080300 58.38573600 15.68446400  
C 0 16.35252400 57.23911500 13.59915100  
N 0 16.61281700 57.46729500 14.91719700  
H 0 15.51489300 56.47020200 10.07595800  
H 0 13.22216500 61.23099600 18.68169000  
H 0 14.59151800 62.22644600 18.20659800  
H 0 13.18862800 62.11395000 17.14700900  
H 0 14.93901300 59.83404900 19.86715800  
H 0 16.53892300 59.13885000 19.56626400  
H 0 16.25550200 60.86627400 19.31985000  
H 0 13.36354100 60.63601700 15.27761300  
H 0 16.88012600 58.04639000 17.55646600  
H 0 18.12484300 57.27243700 16.35686700  
H 0 18.51996400 56.68540000 14.72430000  
C -1 21.24034900 63.62209300 14.93436500  
C 0 20.25633100 62.87126900 14.06057000  
O 0 20.60224900 62.52009100 12.92970200  
C 0 21.35621200 65.10159200 14.52883300  
C 0 20.11203700 65.87073600 14.96245100  
O 0 19.52149800 66.48856000 13.97465000  
O 0 19.74148600 65.85226600 16.13483800  
H 0 20.97902200 63.58632000 15.99474200  
H 0 22.21989000 65.54102700 15.04148600  
H 0 21.50521900 65.19009300 13.45160900  
N 0 19.00510800 62.62860900 14.53724900  
C 0 18.04669600 61.87578300 13.70630900  
C 0 17.99883300 62.37351300 12.26931200  
O 0 18.30686700 61.58214600 11.36729200  
C 0 16.72315900 62.00615800 14.46483300  
C 0 17.18117900 62.08607500 15.92386700  
C 0 18.42211900 62.98284200 15.84753100  
H 0 18.34706000 60.82785300 13.62623100  
H 0 16.21155700 62.93443600 14.19432200  
H 0 16.07651500 61.16940600 14.21905000  
H 0 16.41913000 62.50157800 16.58559400  
H 0 17.44601200 61.09106500 16.29589200  
H 0 18.15297900 64.04142600 15.87307300  
H 0 19.13203200 62.79752600 16.65770700  
N 0 17.62132900 63.65800700 12.13415000  
C 0 17.31643400 64.52534700 10.99031000  
C 0 17.44899000 63.98294900 9.57845300  
O 0 16.69481300 64.41936100 8.70006400  
C 0 18.13152900 65.84372400 11.13788600  
C 0 17.55600700 66.97702200 10.27464800  
C 0 19.63298400 65.63295800 10.92619900  
C 0 18.02094000 68.35689100 10.75089300  
H 0 17.37870000 64.16287100 12.99097500  
H 0 16.26221600 64.79212800 11.08053800  
H 0 17.98304800 66.12713300 12.17987200  
H 0 17.82141100 66.82187300 9.22193300  
H 0 16.46190300 66.93632100 10.31131800  
H 0 20.19163000 66.47777400 11.33477300  
H 0 19.97967200 64.73245500 11.44113500  
H 0 19.87195100 65.53480000 9.86197800  
H 0 17.55103000 69.15635800 10.16638000  
H 0 17.76438300 68.50196200 11.80576900  
H 0 19.10608000 68.47230800 10.65696500  
N 0 18.46421500 63.13669700 9.31350400  
C -1 18.55277200 62.46953200 8.05054700  
C 0 17.86083300 61.09273100 7.95940700  
O 0 17.89664700 60.49719900 6.86583300  
C 0 20.02046300 62.27894500 7.64352100  
C 0 20.77294000 63.59475900 7.50001600  
O 0 20.58656900 61.46459500 8.67702900  
H 0 18.85494700 62.62141900 10.10745600  
H -1 18.05423800 63.07861700 7.28952300  
H 0 20.01580600 61.73390400 6.69063900  
H 0 21.53268600 61.37270200 8.51227100  
H 0 21.81150800 63.41196500 7.19798500  
H 0 20.30879700 64.22674800 6.73586800  
H 0 20.77334600 64.13429100 8.44916400  
N 0 17.25035100 60.61213800 9.04325700  
C 0 16.54268400 59.35099600 9.01785100  
C 0 17.43652100 58.12817300 9.03635000  
O 0 17.04443400 57.07384800 8.51115400  
H 0 17.32095600 61.07465600 9.95465800  
H 0 15.91177500 59.37002900 9.91747300  
H 0 15.92663600 59.27764300 8.12202800  
N 0 18.62647700 58.24826200 9.66930500  
C -1 19.68124700 57.26508800 9.50425800

C 0 20.94130000 57.84931900 8.85811500	H 0 10.31604200 62.19176700 6.61678800	H 0 14.81902400 58.19120400 5.52233900
C 0 20.67361400 58.44929400 7.47129300	H 0 11.47229400 59.59937100 5.09014200	C -1 9.36882900 64.78810200 13.86227800
C 0 20.01245300 57.43641900 6.53955600	H 0 9.94537900 59.70125800 5.95396100	C 0 10.41914600 63.94440900 13.12858200
N 0 18.92093800 57.90306200 5.87616100	H 0 9.96641900 59.25001100 4.24140200	C 0 11.78856300 64.03865500 13.81011200
O 0 20.45894400 56.29829200 6.39620200	C 0 14.95664300 68.90155100 14.29220800	C 0 9.90436400 62.50335400 13.00884800
H 0 18.83583200 59.14306200 10.09768700	C 0 14.90087400 67.37758200 14.45003600	H 0 9.32439200 64.52136000 14.92537300
H 0 19.26456100 56.51311100 8.83110700	C 0 16.23566200 66.66772100 14.15709900	H 0 10.53370800 64.34844200 12.11353200
H 0 21.38115400 58.61930300 9.50423900	O 0 17.27285600 67.40348700 14.28542200	H 0 12.56361700 63.53643800 13.22773100
H 0 21.66946400 57.03663500 8.76408900	O 0 16.20908700 65.45041400 13.86596900	H 0 12.10066100 65.08187100 13.92220700
H 0 20.06751900 59.34959300 7.55980200	H 0 14.84414300 69.17153300 13.23342500	H 0 11.76870500 63.58486000 14.80765800
H 0 21.62731600 58.74114300 7.01295200	H 0 15.96115000 69.21792600 14.58311100	H 0 10.66978600 61.81258100 12.65997500
H 0 18.44230600 58.73224900 6.22477400	H 0 14.65986100 67.12942400 15.49189600	H 0 9.55410800 62.14600000 13.98454000
H 0 18.36124700 57.21094100 5.39669800	H 0 14.11370400 66.92053300 13.84362900	H 0 9.05472300 62.44584400 12.31940400
C -1 19.48684900 53.29127700 7.88424700	C -1 18.60083100 58.32699800 1.75280900	H -1 15.41789200 51.40134400 3.31765700
C 0 18.07630400 53.36473300 7.32254100	C 0 17.19575100 58.69541500 2.26595600	H -1 8.46262500 61.01884700 3.48770500
N 0 17.20731200 54.13957300 8.01285500	C 0 17.01830500 60.18129000 2.46711900	H -1 18.76106000 57.25125100 1.88014400
O 0 17.74388300 52.71827800 6.32355100	C 0 16.64805500 61.02547200 1.41260600	H -1 19.49913600 52.57352800 8.71111200
H 0 19.83620900 54.26023000 8.24593500	C 0 17.28112100 60.75431400 3.71764300	H -1 22.21780100 63.14325000 14.80776900
H 0 20.15210800 52.94121000 7.09557400	C 0 16.53848100 62.40437700 1.60173600	H -1 19.93368700 56.70766500 10.41232600
H 0 16.28960600 54.26402600 7.61273900	C 0 17.18050200 62.13120600 3.90847300	H -1 6.00336700 59.81804300 7.41918000
H 0 17.47682900 54.78740000 8.74590000	C 0 16.80394900 62.96438400 2.85335800	H -1 11.67871000 57.43256300 15.10823200
C -1 10.76536000 62.01122000 -0.16407900	H 0 18.73949800 58.59921100 0.70160600	H 0 11.67972900 53.53293600 13.18846900
C 0 12.31119900 62.04628400 -0.11247000	H 0 19.36527500 58.84021800 2.34421300	H -1 9.58982200 65.85843100 13.78366500
C 0 12.95919800 60.76230300 0.44340800	H 0 16.43715400 58.31187000 1.57364300	H -1 8.38384200 64.58847100 13.42583200
C 0 12.79298200 63.30360200 0.62537500	H 0 17.02104800 58.18543300 3.21693700	H 0 15.33243300 52.42941500 4.73217600
C 0 12.68052500 60.44004800 1.91149800	H 0 16.44683900 60.59613200 0.43362800	H -1 13.20261800 54.61377100 8.59427300
H 0 10.32738700 62.42439600 0.75124000	H 0 17.56995900 60.13378300 4.55707400	C -1 13.92183700 69.63633800 15.14281800
H 0 12.66452700 62.12284900 -1.15136300	H 0 16.25176100 63.04252400 0.77016300	H -1 14.06746700 70.72213300 15.13459100
H 0 12.63457300 59.91654200 -0.17833000	H 0 17.40104400 62.53562100 4.89104700	H -1 12.89127300 69.40639200 14.84958800
H 0 14.04386000 60.84542000 0.30876800	H 0 16.71146100 64.03510500 3.00692000	H 0 14.02052600 69.32241100 16.19063200
H 0 13.88537600 63.36353300 0.64275300	C -1 15.09107500 52.38696300 3.66558400	H 0 13.93290700 59.49012100 13.28591800
H 0 12.40796600 64.21251600 0.14916500	C 0 15.80514200 53.54093000 2.94008400	C -1 9.09329700 66.03245900 8.85500300
H 0 12.44722100 63.30735700 1.66461700	C 0 15.54476200 54.87174700 3.61505600	C 0 10.45998400 65.45404300 8.39852200
H 0 13.21627300 59.53353100 2.20836500	C 0 14.62001800 55.79302000 3.11188400	C 0 11.59788700 65.81859900 9.33101200
H 0 13.01866600 61.24039000 2.57582300	C 0 16.20184300 55.16892400 4.81885000	C 0 11.83541200 67.16251300 9.66310000
H 0 11.61553500 60.27285600 2.09673400	C 0 14.35861800 56.98683200 3.79058700	C 0 12.45521500 64.84895900 9.85867200
C -1 8.84995600 61.71530800 4.23734500	C 0 15.93364700 56.35173900 5.50995300	C 0 12.88993900 67.52439700 10.49977300
C 0 10.29987900 61.37490600 4.59725700	C 0 15.01625600 57.26978000 4.98844400	C 0 13.50533900 65.20596100 10.70646400
C 0 10.84645000 62.32795600 5.66852900	H 0 14.00419800 52.46202700 3.55671400	C 0 13.72794500 66.54200200 11.03088700
C 0 10.42984100 59.90036500 4.99280900	H 0 16.88332700 53.34454900 2.94626400	H -1 9.29271300 66.79651000 9.61306600
H 0 8.19886600 61.66459900 5.11801400	H 0 15.49137200 53.58348300 1.88960400	H -1 8.44520300 65.25532200 9.27471100
H -1 8.80495200 62.73722600 3.84544900	H 0 14.09713200 55.57350100 2.18345000	H 0 8.54807500 66.49773700 8.02751800
H 0 10.89555900 61.53181200 3.68963900	H 0 16.90883200 54.44775200 5.21787900	H 0 10.40851500 64.36554800 8.29728000
H 0 11.90581700 62.15225500 5.86197100	H 0 13.62987300 57.68776900 3.39362800	H 0 10.70779600 65.82608200 7.39846300
H 0 10.73502300 63.37430200 5.36190500	H 0 16.42091000 56.56072300 6.45849200	H 0 11.19178500 67.93660500 9.25115100

H 0 12.32351600 63.80519400 9.58883600	H 0 14.94314500 60.34228300 5.67027800	C 0 10.22192000 61.34997600 18.08540400
H 0 13.05983000 68.57106500 10.73732900	H 0 15.56827800 62.32601800 7.02656200	C 0 10.53276200 59.87179400 18.34702300
H 0 14.14919800 64.43099400 11.10075600	H 0 12.04445000 59.19273800 8.64398800	C 0 10.42310600 61.69213400 16.60760400
H 0 14.55028500 66.80511100 11.68524300	H 0 13.16215800 58.79358000 6.48172000	H 0 8.54545100 61.44455900 19.50962100
C -1 12.60577800 56.71564600 17.61659600	O 0 16.04901500 59.30838700 12.65824500	H -1 8.12212600 61.13717900 17.80582600
C 0 13.45239200 55.55744400 17.10965200	O 0 15.10313600 60.28455000 12.09740000	H 0 10.91283700 61.95786500 18.68537600
O 0 13.97312800 55.82438100 15.80696100	H 0 17.91733700 66.49937100 14.05071100	H 0 11.55802100 59.62373600 18.05379300
H -1 12.18866400 56.58056500 18.62025100	C -1 10.91650800 57.40592400 14.32231500	H 0 10.40968700 59.61497800 19.40476300
H -1 11.78056900 56.90636900 16.92306500	C 0 11.15145300 56.32578100 13.26757500	H 0 9.85922900 59.22760900 17.76789200
H 0 13.21434700 57.62797000 17.64710100	O 0 10.33747000 56.15822300 12.36022500	H 0 11.42205200 61.43774900 16.24748300
H 0 14.27383600 55.34301700 17.80989200	C 0 10.63817300 58.77722300 13.70750700	H 0 9.70533100 61.13563200 15.99422000
H 0 12.85831300 54.64368500 17.01024600	O 0 11.76481100 59.38181100 13.07545400	H 0 10.25887600 62.75600700 16.41498200
H 0 14.46002700 56.66232600 15.85105500	H 0 9.98683700 57.09974600 14.82222900	C -1 6.93625900 59.40309200 7.02341000
H 0 10.47815200 67.01410100 3.94667400	H 0 9.81388600 58.67461200 12.99365100	C 0 7.97406100 59.36147900 8.11647700
C -1 10.42062300 67.50500200 4.92207200	H 0 10.33008200 59.47713000 14.48719700	C 0 8.32012800 58.16261300 8.75088400
C 0 11.80214300 67.69321500 5.56694000	H 0 12.10331600 58.81808300 12.35172000	C 0 8.57328300 60.54946600 8.55638000
C 0 12.78349300 66.54347900 5.54720800	N 0 12.27198000 55.56983200 13.41049500	C 0 9.22797900 58.14769000 9.81361400
C 0 13.66950500 66.40299500 6.62220400	C 0 12.39628300 54.26253400 12.77636300	C 0 9.49609400 60.54211900 9.59786600
C 0 12.93774600 65.70332900 4.43690900	C 0 12.31623300 54.13721300 11.24967000	C 0 9.81855800 59.34074800 10.23079900
C 0 14.71387700 65.48488000 6.58182800	O 0 12.10165400 53.02403500 10.78035100	H 0 6.72080700 58.40420400 6.63419300
C 0 13.98121300 64.77676500 4.38894100	H 0 12.84287400 55.71631900 14.24243000	H 0 7.25289500 60.03266200 6.18804400
C 0 14.88008900 64.68514600 5.45151700	H 0 13.36557600 53.85330400 13.07537600	H 0 7.85616700 57.23482900 8.42493700
H 0 9.73173800 66.93883600 5.55422400	N 0 12.55706300 55.22964100 10.48623200	H 0 8.31193300 61.48655100 8.07292400
H 0 12.28785900 68.54035800 5.05978400	C -1 12.35125200 55.13834400 9.03918000	H 0 9.46564200 57.22231800 10.32991500
H 0 11.66733100 68.02035100 6.60445800	C 0 12.22655300 56.53032900 8.43579200	H 0 9.97370000 61.46460700 9.91158800
H 0 13.54635000 67.03004700 7.49966900	S 0 11.62305900 56.50115100 6.69735400	H 0 10.53089500 59.34091200 11.04371000
H 0 12.25911500 65.78500400 3.59190900	H 0 12.54247200 56.14649800 10.91495100	C -1 17.74268200 56.74912200 15.48505700
H 0 15.38582100 65.38481800 7.42469400	H 0 11.45869200 54.53836800 8.84222000	N 0 16.86795300 56.32613600 13.04877400
H 0 14.10105000 64.13442600 3.52096300	H 0 11.53514200 57.14068200 9.01802700	C 0 16.54446700 56.07530500 11.73124800
H 0 15.70621400 63.98701900 5.40798000	H 0 13.18744400 57.04956600 8.42178100	O 0 17.17033300 55.30094900 11.03624200
H -1 10.04492500 68.52145600 4.76338200	H 0 10.32009700 56.65683000 7.00752800	N 0 15.38101500 56.70198300 11.20491900
	C -1 14.81292200 65.87502100 19.15209200	C 0 14.57743400 57.58174700 11.85410600
	C 0 16.30065500 65.92487100 18.77217600	C 0 15.23472300 58.21233000 13.09592300
	C 0 16.98753600 64.58297800 19.05308500	O 0 13.46688300 57.90990500 11.44181000
	C 0 16.48697800 66.34205400 17.30974200	C 0 14.75428400 59.03009900 15.28323600
	H 0 14.66958000 65.47894600 20.16450500	N 0 14.26138200 58.54293800 14.07559600
	H 0 14.25580100 65.23233100 18.45911100	C 0 14.08784900 60.01507500 16.01795500
	H 0 16.78494400 66.68123000 19.40661400	C 0 14.56161400 60.44820700 17.25641800
	H 0 18.04097400 64.61091000 18.75688400	C 0 13.88058700 61.57141000 17.99457400
	H 0 16.93377800 64.31647600 20.11508400	C 0 15.72031700 59.84762500 17.79189100
	H 0 16.50623500 63.77909900 18.48437300	C 0 16.26875600 60.28655600 19.12539500
	H 0 17.54021400 66.41463200 17.02252000	C 0 16.39433400 58.87907200 17.04959200
	H 0 16.01094500 65.61172700 16.64274100	C 0 15.94702700 58.47926400 15.78523800
	H 0 16.02213400 67.31395600 17.11343500	C 0 16.26603700 57.27572200 13.69519000
	C -1 8.77933400 61.70507600 18.47267400	N 0 16.61544900 57.52050300 14.98541600

## E:indene<sub>1R,2S</sub>

H -1 17.45621700 55.72340300 15.73982800		
H -1 14.36507800 66.87379900 19.12395100		
H -1 8.60699900 62.77679200 18.32914400		
H -1 10.42811400 62.61773400 -1.01099900		
H -1 10.37422600 60.99320000 -0.26599400		
C 0 14.44033000 60.52871900 6.61412700		
C 0 14.79887700 61.64792900 7.37523000		
C 0 14.17959700 61.86013100 8.59647900		
C 0 13.20677800 60.95518800 9.07665400		
C 0 12.82185100 59.86234700 8.30353800		
C 0 13.45138900 59.65301500 7.07356700		

H 0 15.14160100 56.43032400 10.25680400	H 0 17.98253100 66.60130600 11.88261900	C -1 19.48694900 53.29109000 7.88410600
H 0 13.40249100 61.22078500 18.91696400	H 0 17.50683900 67.07778100 8.92234300	C 0 18.07448900 53.44923700 7.34305200
H 0 14.59813700 62.34533300 18.28541500	H 0 16.17834400 66.91763000 10.03452800	N 0 17.22440000 54.18228300 8.10727900
H 0 13.11603400 62.04474000 17.37918400	H 0 19.96992600 67.26374500 10.59007700	O 0 17.71354100 52.91433900 6.29355400
H 0 15.51295600 60.22512300 19.91620800	H 0 20.13061100 65.59481500 11.12756800	H 0 19.89092000 54.24454700 8.23146100
H 0 17.11981900 59.66970300 19.42455400	H 0 19.69848700 65.94827700 9.43877000	H 0 20.11747900 52.91809600 7.07793900
H 0 16.60909500 61.32848200 19.09273700	H 0 16.75739000 69.31898600 9.78401200	H 0 16.30447600 54.35410200 7.73121700
H 0 13.20787400 60.46933900 15.57503000	H 0 17.08297600 68.79632600 11.44758300	H 0 17.50373900 54.75742200 8.89079100
H 0 17.29483000 58.45473100 17.47323300	H 0 18.41584500 69.01434200 10.31145300	C -1 10.76494000 62.01136400 -0.16354900
H 0 18.16927600 57.23326900 16.35784600	N 0 18.47045700 63.18529700 9.30176900	C 0 12.30998100 61.96601800 -0.27450200
H 0 18.49646000 56.68853100 14.70126300	C -1 18.55224700 62.47032200 8.05123800	C 0 12.97089100 60.74867200 0.40415600
C -1 21.24047000 63.62192900 14.93288400	C 0 17.86865600 61.09546500 8.05214700	C 0 12.93137000 63.30139700 0.14931400
C 0 20.22833300 62.87837300 14.06346300	O 0 17.90369600 60.40628300 7.02470900	C 0 12.92404700 60.69980300 1.93064800
O 0 20.55628100 62.36923400 12.98907800	C 0 20.01999600 62.24479500 7.66293500	H 0 10.41136900 62.44005500 0.77828100
C 0 21.31750400 65.10301300 14.49071300	C 0 20.79428700 63.53908500 7.46109700	H 0 12.52548000 61.84145800 -1.34637500
C 0 19.98793700 65.80871500 14.79062100	O 0 20.55506100 61.47175500 8.75065800	H 0 12.50259000 59.84082300 -0.00004800
O 0 19.15236800 65.84614200 13.79899400	H 0 19.08300900 62.91345500 10.06033400	H 0 14.02141700 60.71382200 0.08951600
O 0 19.77198400 66.20870100 15.93908700	H -1 18.05402600 63.07805200 7.28920800	H 0 14.01542300 63.30223100 -0.00081200
H 0 20.98186300 63.59205900 15.99402000	H 0 20.01848900 61.64982500 6.74184100	H 0 12.51047600 64.12967000 -0.43187600
H 0 22.11140000 65.59856300 15.05603100	H 0 21.49720400 61.33171600 8.59492100	H 0 12.74813300 63.51757700 1.20531600
H 0 21.55018600 65.14916800 13.42348000	H 0 21.83575600 63.32511500 7.19548500	H 0 13.37930200 59.77611100 2.30121900
N 0 18.92050000 62.87307900 14.46409000	H 0 20.35653100 64.12616600 6.64783600	H 0 13.48729900 61.52355800 2.37559600
C 0 17.90929600 62.22052000 13.63273000	H 0 20.78488600 64.14211600 8.37203100	H 0 11.89749900 60.73678100 2.30463500
C 0 17.58891100 62.85416200 12.29077400	N 0 17.29777600 60.68839200 9.19722500	C -1 8.84986300 61.71587000 4.23798500
O 0 16.78512000 62.22647100 11.55302200	C 0 16.55152600 59.44576800 9.22940100	C 0 10.27519400 61.36580500 4.68750900
C 0 16.61884000 62.26099300 14.49352500	C 0 17.41220800 58.18761400 9.20075900	C 0 10.71534200 62.22845600 5.87755400
C 0 17.14866600 62.40241000 15.91966400	O 0 16.92843500 57.13986300 8.76303100	C 0 10.41259700 59.87388200 5.00742000
C 0 18.34631000 63.33230200 15.74225100	H 0 17.20905300 61.33995800 9.97541700	H 0 8.16240800 61.67571100 5.09294500
H 0 18.21272500 61.19127700 13.41272400	H 0 15.93129500 59.45101700 10.12572600	H -1 8.80512900 62.73708400 3.84506300
H 0 16.03681700 63.14808000 14.22645100	H 0 15.89108400 59.38054000 8.36448800	H 0 10.94840300 61.59445500 3.85210500
H 0 16.00483500 61.37732800 14.33392100	N 0 18.66901900 58.29552800 9.70587000	H 0 11.75444000 62.02763600 6.14989900
H 0 16.40081800 62.81192800 16.60002700	C -1 19.68173000 57.26468300 9.50386500	H 0 10.63366800 63.29606600 5.65063200
H 0 17.47244900 61.43243100 16.30853000	C 0 20.92713100 57.79222400 8.79148700	H 0 10.09847300 62.01207300 6.75586500
H 0 18.03320800 64.37505700 15.66653000	C 0 20.60666300 58.34762500 7.39523000	H 0 11.44354900 59.61961400 5.25983300
H 0 19.07441900 63.25794400 16.54959700	C 0 19.87368100 57.29983600 6.55650500	H 0 9.79556900 59.59785400 5.86965200
N 0 18.09062400 64.03422900 11.94012100	N 0 18.71406200 57.72224400 5.99132400	H 0 10.10768500 59.25163300 4.15795200
C 0 17.47553400 64.82193200 10.86083300	O 0 20.32313700 56.16313800 6.42021500	C 0 14.93927100 68.90102300 14.27263700
C 0 17.56318400 64.18079600 9.47730300	H 0 18.98005700 59.23316500 9.92965800	C 0 14.69763000 67.38701700 14.26666600
O 0 16.83475900 64.57118800 8.56495300	H 0 19.20588800 56.52062800 8.85960300	C 0 15.89927500 66.52902700 13.89296500
C 0 18.06665400 66.25140600 10.85266300	H 0 21.41873900 58.56702900 9.39366800	O 0 17.04443700 67.09960100 14.17884700
C 0 17.23220200 67.20174800 9.97502000	H 0 21.62745800 56.95749400 8.69030200	O 0 15.75952300 65.39908700 13.42148800
C 0 19.55286600 66.25910400 10.47945100	H 0 20.02374700 59.26544200 7.47003600	H 0 14.90891700 69.28081700 13.24333800
C 0 17.38178300 68.66424800 10.40129000	H 0 21.54253100 58.58810300 6.87714400	H 0 15.94861800 69.09134500 14.64437200
H 0 18.61853600 64.56701600 12.64990000	H 0 18.27016700 58.57321600 6.32211000	H 0 14.41983100 67.06102100 15.27845000
H 0 16.40694700 64.90049700 11.07790800	H 0 18.12844100 57.01949700 5.56024300	H 0 13.86180400 67.11228900 13.61760600

C -1 18.60108700 58.32705400 1.75355300	H -1 15.41789000 51.40124700 3.31793200	H 0 10.04235000 66.87173500 4.11389800
C 0 17.23028800 58.67262900 2.36471600	H -1 8.46285400 61.01887000 3.48756600	C -1 10.41975100 67.50456700 4.92172300
C 0 17.00640200 60.14881600 2.58486700	H -1 18.76091000 57.25115200 1.87950700	C 0 11.95351400 67.56538400 4.93205800
C 0 16.59441600 60.99003200 1.54420300	H -1 19.49902000 52.57367800 8.71124000	C 0 12.64151100 66.22394300 4.99898700
C 0 17.23175400 60.71480900 3.84671100	H -1 22.21783100 63.14300900 14.80892700	C 0 13.58523500 65.94586000 5.99377700
C 0 16.39930700 62.35507500 1.75937700	H -1 19.93338100 56.70798600 10.41260700	C 0 12.37445100 65.24532500 4.03248100
C 0 17.03360200 62.07723400 4.06649900	H -1 6.00277500 59.81702600 7.41885000	C 0 14.26283700 64.72584000 6.01925500
C 0 16.61116700 62.90451200 3.02474200	H -1 11.67891800 57.43284600 15.10808800	C 0 13.04081400 64.02497900 4.05948500
H 0 18.66240900 58.59026200 0.69330600	H 0 11.62556400 53.57663700 13.14442000	C 0 13.98994600 63.76429400 5.04688700
H 0 19.40381100 58.84691300 2.28551400	H -1 9.59010600 65.85838600 13.78385700	H 0 10.02327800 67.12102200 5.86580700
H 0 16.43601200 58.26415000 1.73011000	H -1 8.38392600 64.58804700 13.42583300	H 0 12.28251700 68.08948600 4.02375900
H 0 17.13675900 58.15745600 3.32415600	H 0 14.94394200 52.33013300 4.74759600	H 0 12.28587800 68.18317600 5.77332700
H 0 16.41814700 60.56782100 0.55770400	H -1 13.20183400 54.61269700 8.59404100	H 0 13.79245800 66.68967600 6.75726100
H 0 17.56530200 60.09271700 4.66868700	C -1 13.92146700 69.63679200 15.14255100	H 0 11.64709700 65.44336800 3.24911900
H 0 16.07481100 62.99013300 0.94059500	H -1 14.06772700 70.72210100 15.13466900	H 0 14.99994500 64.54251300 6.79473900
H 0 17.20171700 62.48292700 5.05918200	H -1 12.89126300 69.40609000 14.84985800	H 0 12.81471700 63.26690000 3.31957900
H 0 16.43096800 63.95949400 3.20270200	H 0 14.02554500 69.31233700 16.18598100	H 0 14.50097100 62.81274300 5.05223700
C -1 15.09108800 52.38695600 3.66518900	H 0 13.42622300 59.01912100 13.72242200	H -1 10.04563300 68.52175000 4.76358900
C 0 16.12023000 53.48446500 3.33743400	C -1 9.09315100 66.03208600 8.85508800	C 0 12.81227900 61.38472000 10.42119600
C 0 15.62034400 54.86353000 3.71514700	C 0 10.47482300 65.45414700 8.41960100	C 0 13.48242100 62.50912100 10.74637800
C 0 14.75973200 55.57058400 2.86616200	C 0 11.60863900 66.14295300 9.14752900	C 0 14.39913900 62.92897500 9.63045300
C 0 15.96479200 55.44370600 4.94488700	C 0 11.96496800 67.46418000 8.83924700	H 0 15.42784900 62.94486400 9.98753200
C 0 14.25574200 56.81864100 3.23148900	C 0 12.27764600 65.50627500 10.19577400	H 0 14.19432200 63.93433400 9.24856200
C 0 15.45764100 56.69177800 5.32127600	C 0 12.95859100 68.12342400 9.56147700	H 0 12.14176100 60.84067400 11.07002400
C 0 14.60436700 57.38432800 4.45796100	C 0 13.28025500 66.15492300 10.92173500	H 0 13.43418400 63.02749900 11.69440900
H 0 14.12243200 52.60578400 3.20240600	C 0 13.61675700 67.47193700 10.60842900	H 0 15.73737600 61.05015000 11.97058400
H 0 17.04608700 53.27122900 3.87820700	H -1 9.29287900 66.79639600 9.61313900	
H 0 16.34509300 53.46429700 2.26326800	H -1 8.44509000 65.25543500 9.27474400	
H 0 14.48236500 55.13532400 1.90859600	H 0 8.56191700 66.50407500 8.02336900	
H 0 16.63554000 54.89565300 5.59734800	H 0 10.52144600 64.37987100 8.62145300	
H 0 13.59028200 57.35330800 2.55939600	H 0 10.61836700 65.56130600 7.33983200	
H 0 15.72844100 57.11432800 6.28613600	H 0 11.45477200 67.97796100 8.02856500	
H 0 14.21728500 58.35871800 4.72879100	H 0 12.02413200 64.47857100 10.42996000	
C -1 9.36832400 64.78823200 13.86201700	H 0 13.22398700 69.14573300 9.30681800	
C 0 10.48295100 63.98219500 13.17869100	H 0 13.80770400 65.63634400 11.71794900	
C 0 11.80791200 64.17687900 13.92805000	H 0 14.39112900 67.98501300 11.16929600	
C 0 10.11220600 62.50165700 13.04167200	C -1 12.60588600 56.71571300 17.61687600	
H 0 9.30602800 64.53477500 14.92802100	C 0 13.44527200 55.54267800 17.13618000	
H 0 10.61366600 64.38826700 12.16779300	O 0 13.94645400 55.76321200 15.81248800	
H 0 12.62740000 63.62363600 13.46213600	H -1 12.18859300 56.58082400 18.62025500	
H 0 12.09883600 65.23184900 13.95472600	H -1 11.78068900 56.90575100 16.92277700	
H 0 11.72623500 63.82786100 14.96406300	H 0 13.21764400 57.62585400 17.64605100	
H 0 10.94133000 61.91157700 12.64509000	H 0 14.27993100 55.35487400 17.82638400	
H 0 9.84201800 62.07362200 14.01151100	H 0 12.85326200 54.62489200 17.07751500	
H 0 9.25401800 62.36828500 12.37378900	H 0 14.34735500 56.64367000 15.78871200	

## E:indene<sub>1S,2R</sub>

H -1 17.45623000 55.72339200 15.73980100
H -1 14.36508300 66.87380100 19.12396100
H -1 8.60700100 62.77679100 18.32913500
H -1 10.42809800 62.61778200 -1.01095900
H -1 10.37422100 60.99319800 -0.26594500
C 0 13.41748500 59.72038900 6.88551000
C 0 12.65307200 59.85623000 8.05076600
C 0 12.98923000 60.84967900 8.95422200
C 0 14.05288300 61.73809700 8.68331600
C 0 14.78031600 61.63067700 7.49978300
C 0 14.46778900 60.60045500 6.60826800
H 0 13.17786800 58.91483100 6.20420100
H 0 11.81329300 59.19548900 8.22850700
H 0 15.58623700 62.32406300 7.29506000
H 0 15.05248900 60.48216300 5.70127200
O 0 16.06992700 59.30430600 12.61088000

O 0 15.11889800 60.27326000 12.04728600	H 0 10.91655100 61.96765200 18.64822900	H 0 17.05105300 59.68711800 19.39243700
H 0 17.92006500 66.50996200 14.02601900	H 0 11.55687200 59.62645500 18.02655600	H 0 16.53525000 61.34081700 19.04426700
C -1 10.91660300 57.40590000 14.32222900	H 0 10.43736000 59.63133400 19.40135600	H 0 13.18203600 60.44068100 15.49048100
C 0 11.13253500 56.24092700 13.35658200	H 0 9.85344100 59.22439100 17.78101100	H 0 17.25780000 58.46257500 17.45076600
O 0 10.23795600 55.89384900 12.58728400	H 0 11.38601500 61.43753200 16.20572800	H 0 18.15162100 57.23885200 16.36308600
C 0 10.65610400 58.74214300 13.62864900	H 0 9.67052500 61.10324300 15.98710400	H 0 18.51153700 56.68711400 14.71639900
O 0 11.78384100 59.30189400 12.96668500	H 0 10.20571200 62.73746200 16.38066900	C -1 21.24045500 63.62192300 14.93286900
H 0 9.97867900 57.15193800 14.83484200	C -1 6.93631100 59.40333500 7.02342700	C 0 20.23233800 62.86730500 14.06746600
H 0 9.82656600 58.60776600 12.92462700	C 0 7.81036200 58.80953700 8.09776900	O 0 20.56695900 62.34633700 13.00081800
H 0 10.35224300 59.48498600 14.36985300	C 0 7.87388300 57.42217800 8.28048100	C 0 21.31356200 65.09954100 14.47971800
H 0 12.09538900 58.71441000 12.25249600	C 0 8.57144500 59.62886100 8.94245900	C 0 19.98205800 65.80471500 14.77310200
N 0 12.34170800 55.61730700 13.39881400	C 0 8.65392900 56.86752200 9.29497800	O 0 19.15345300 65.84846200 13.77614500
C 0 12.49894700 54.30008400 12.78960400	C 0 9.34969300 59.07870100 9.96153300	O 0 19.75994600 66.20042600 15.92202900
C 0 12.30937500 54.15389100 11.27235200	C 0 9.38873800 57.69542500 10.14503100	H 0 20.98219700 63.59789900 15.99420800
O 0 12.03484000 53.04356700 10.82819400	H 0 6.66764100 58.65273000 6.27459500	H 0 22.10579400 65.60119600 15.04207100
H 0 12.95636000 55.82494200 14.18470000	H 0 7.44924400 60.21670300 6.50335200	H 0 21.54725200 65.13840100 13.41243200
H 0 13.51136400 53.95744000 13.02292400	H 0 7.29848200 56.77424100 7.62400100	N 0 18.92260800 62.86157100 14.46176400
N 0 12.53933300 55.23145600 10.48732000	H 0 8.55181600 60.70632000 8.79941500	C 0 17.91945800 62.18856600 13.63580600
C -1 12.35119400 55.13826900 9.03916700	H 0 8.68853700 55.79131900 9.43552700	C 0 17.58715300 62.82359100 12.29838800
C 0 12.25158100 56.53149300 8.42944400	H 0 9.92672100 59.72770200 10.61265300	O 0 16.78502400 62.20637700 11.55219500
S 0 11.65070800 56.50554000 6.69280600	H 0 9.95911800 57.24449600 10.94698900	C 0 16.63129100 62.20777000 14.50118200
H 0 12.67162000 56.14486700 10.90250600	C -1 17.74263600 56.74914400 15.48510300	C 0 17.16040500 62.38479000 15.92405800
H 0 11.45435200 54.54721100 8.83755300	N 0 16.92407300 56.32657600 13.02932200	C 0 18.33672800 63.33714900 15.72834200
H 0 11.57712300 57.15833000 9.01207600	C 0 16.63195300 56.07494100 11.70610600	H 0 18.24156800 61.16548100 13.41495600
H 0 13.22275900 57.03173000 8.40603800	O 0 17.28762500 55.31825000 11.01847000	H 0 16.02480500 63.07491300 14.22443500
H 0 10.34022800 56.50389300 7.01403100	N 0 15.46284300 56.67603800 11.16282800	H 0 16.04145500 61.30577300 14.35596700
C -1 14.81292100 65.87501300 19.15207200	C 0 14.64455800 57.55566400 11.79373000	H 0 16.40350900 62.78817700 16.59792400
C 0 16.29934700 65.92450900 18.76599400	C 0 15.26837200 58.19718700 13.04514300	H 0 17.50730000 61.42896100 16.32828000
C 0 16.98876100 64.58494000 19.05067700	O 0 13.54173900 57.87590000 11.35438900	H 0 17.99922300 64.36997600 15.62608900
C 0 16.47993600 66.33642200 17.30117700	C 0 14.74165000 59.00961300 15.22225400	H 0 19.06491500 63.30039600 16.53779100
H 0 14.67380200 65.48065400 20.16567000	N 0 14.27555000 58.51971600 14.00613400	N 0 18.07718300 64.01152800 11.95565800
H 0 14.25302400 65.23114700 18.46229600	C 0 14.05924100 59.99306600 15.94546300	C 0 17.42807800 64.77270000 10.88258700
H 0 16.78502000 66.68410100 19.39551200	C 0 14.51788500 60.43871000 17.18563100	C 0 17.47705600 64.08387200 9.52270900
H 0 18.04064400 64.61224000 18.74905400	C 0 13.83369600 61.57173000 17.90462400	O 0 16.65027400 64.36474900 8.65342700
H 0 16.94062100 64.32450000 20.11444500	C 0 15.67145600 59.84700400 17.74150700	C 0 18.00404800 66.20650700 10.81580700
H 0 16.50542100 63.77693500 18.48963200	C 0 16.20038100 60.29728600 19.07885100	C 0 17.15553300 67.10295700 9.89563800
H 0 17.53216200 66.40697700 17.00951800	C 0 16.35968500 58.87833300 17.01399800	C 0 19.49062900 66.22457700 10.44537500
H 0 16.00044800 65.60481100 16.63811400	C 0 15.93202400 58.47096600 15.74524500	C 0 17.29210500 68.58744700 10.24156300
H 0 16.01525600 67.30838800 17.10461000	C 0 16.30175100 57.27243000 13.66292500	H 0 18.59918300 64.55522800 12.66136100
C -1 8.77938300 61.70505000 18.47266500	N 0 16.62400900 57.51712000 14.95927700	H 0 16.36644000 64.85169000 11.13018300
C 0 10.21782700 61.35068400 18.06715000	H 0 15.27634300 56.44272200 10.19162900	H 0 17.91149900 66.59722600 11.83114400
C 0 10.53764900 59.87635400 18.33845900	H 0 13.37616100 61.24060800 18.84414000	H 0 17.42696000 66.92782900 8.84872800
C 0 10.38973800 61.67833100 16.58200900	H 0 14.54727400 62.36133400 18.16223300	H 0 16.10436400 66.81355700 9.97456800
H 0 8.55424900 61.44232500 19.51057600	H 0 13.05405900 62.01905900 17.28996300	H 0 19.88762600 67.24109400 10.51330000
H -1 8.12211900 61.13718900 17.80582500	H 0 15.43494000 60.23619200 19.86034100	H 0 20.07824600 65.60131900 11.12425100

H 0 19.64553000 65.87163800 9.41994200	H 0 20.11817400 52.91773600 7.07855700	C 0 16.45016300 62.35997100 1.70303500
H 0 16.65137800 69.19977800 9.59848100	H 0 16.30972100 54.36604100 7.72475000	C 0 17.06247500 62.13612000 4.02186800
H 0 17.00279700 68.77099300 11.28284100	H 0 17.50994400 54.75767300 8.88915100	C 0 16.65209400 62.93943500 2.95684900
H 0 18.32043600 68.94498300 10.12114500	C -1 10.76497200 62.01131900 -0.16366000	H 0 18.62992300 58.58128800 0.68952200
N 0 18.47101000 63.18638500 9.30247800	C 0 12.30886000 62.02473400 -0.16969800	H 0 19.42524500 58.84596100 2.25300600
C -1 18.55225200 62.47030500 8.05120700	C 0 12.95942300 60.80827600 0.51801300	H 0 16.43942900 58.26391600 1.81049400
C 0 17.87094900 61.09378600 8.04696000	C 0 12.81860400 63.36285400 0.37961800	H 0 17.19702800 58.20215200 3.37975500
O 0 17.91485700 60.40505800 7.01935900	C 0 12.65410900 60.62305100 2.00362100	H 0 16.47356900 60.54369600 0.54553200
C 0 20.02099300 62.24881800 7.66625300	H 0 10.35695700 62.43067700 0.76170800	H 0 17.58284600 60.16529800 4.67725700
C 0 20.79219400 63.54352900 7.45368300	H 0 12.62328600 61.96427700 -1.22203300	H 0 16.14202600 62.97647500 0.86352300
O 0 20.55922500 61.48495800 8.75829800	H 0 12.64874700 59.90424400 -0.02347100	H 0 17.22311600 62.56724000 5.00520300
H 0 19.12159100 62.95185600 10.04190600	H 0 14.04534400 60.88453800 0.39016400	H 0 16.47561400 63.99927000 3.10747900
H -1 18.05402200 63.07807100 7.28922700	H 0 13.91150700 63.40121300 0.40727100	C -1 15.09108700 52.38696100 3.66518700
H 0 20.02045800 61.64829500 6.74882400	H 0 12.46398900 64.19889300 -0.23370500	C 0 16.12749400 53.47438600 3.32909500
H 0 21.50115400 61.34454700 8.60144600	H 0 12.45297600 63.53093400 1.39665700	C 0 15.64167400 54.86073900 3.69395800
H 0 21.83263100 63.32887500 7.18463500	H 0 13.19682200 59.76128200 2.40436100	C 0 14.80176800 55.57487300 2.83059900
H 0 20.35068200 64.12488100 6.63832600	H 0 12.95708800 61.49029200 2.59642200	C 0 15.98328000 55.44275300 4.92348700
H 0 20.78699600 64.15285500 8.36035600	H 0 11.58792000 60.45216300 2.17574300	C 0 14.32287600 56.83760000 3.17773300
N 0 17.29171900 60.68455000 9.18714900	C -1 8.84985200 61.71579600 4.23806300	C 0 15.50012900 56.70509700 5.28184000
C 0 16.54839100 59.44003000 9.20603200	C 0 10.26279400 61.35443800 4.70522200	C 0 14.67610200 57.40906900 4.39985800
C 0 17.41178200 58.18439200 9.18329700	C 0 10.70562800 62.23437300 5.88188500	H 0 14.12304300 52.60813100 3.20259000
O 0 16.93195200 57.13673900 8.73776800	C 0 10.35740700 59.86433600 5.04777000	H 0 17.05187600 53.25747200 3.87098400
H 0 17.17910600 61.33996400 9.95989300	H 0 8.15152700 61.67856600 5.08484900	H 0 16.35181100 53.44294900 2.25509800
H 0 15.91610100 59.44400800 10.09376000	H -1 8.80513400 62.73707100 3.84502800	H 0 14.52507400 55.13553800 1.87473500
H 0 15.89924300 59.37476700 8.33232900	H 0 10.94897600 61.55452200 3.87523000	H 0 16.63604000 54.88472600 5.58592700
N 0 18.66233800 58.29082200 9.70153400	H 0 11.73308900 62.01316400 6.18005000	H 0 13.67918600 57.38182900 2.49223600
C -1 19.68173500 57.26469500 9.50387700	H 0 10.65743300 63.29788300 5.62456500	H 0 15.76901500 57.13153200 6.24540100
C 0 20.92855700 57.80030400 8.80020900	H 0 10.06207100 62.06431300 6.75514400	H 0 14.32452300 58.40215900 4.64894800
C 0 20.61574900 58.35504300 7.40232000	H 0 11.38218200 59.57526300 5.27790300	C -1 9.36835300 64.78826700 13.86199900
C 0 19.89537800 57.30333300 6.55778100	H 0 9.75005800 59.61901100 5.92657500	C 0 10.50003200 64.00270400 13.17871100
N 0 18.74051900 57.72105500 5.97921200	H 0 10.00979800 59.24125800 4.21551200	C 0 11.81737200 64.23678900 13.93177000
O 0 20.34942400 56.16773500 6.42874400	C 0 14.93993800 68.89834900 14.27504200	C 0 10.16297700 62.51240300 13.05022300
H 0 18.96721600 59.22841100 9.93482400	C 0 14.69954300 67.38389100 14.27077800	H 0 9.30906000 64.53268500 14.92750900
H 0 19.21309100 56.51894000 8.85656600	C 0 15.90362300 66.52266700 13.91017300	H 0 10.62514000 64.40890400 12.16622600
H 0 21.41196200 58.57687300 9.40662800	O 0 17.04968900 67.11360400 14.14774400	H 0 12.67076400 63.76565000 13.43725300
H 0 21.63353300 56.96900500 8.70308900	O 0 15.76604300 65.37272800 13.48914500	H 0 12.04305700 65.30530100 14.00801300
H 0 20.02666200 59.26920700 7.47296300	H 0 14.91152200 69.27707300 13.24532800	H 0 11.76264700 63.83481200 14.95050900
H 0 21.55401000 58.60173700 6.89149100	H 0 15.94887200 69.08988400 14.64714300	H 0 11.00743900 61.92895600 12.67527200
H 0 18.29024500 58.57042500 6.30469400	H 0 14.41179900 67.05894000 15.28006300	H 0 9.88134700 62.09203400 14.01983600
H 0 18.16100000 57.01508200 5.54513000	H 0 13.87018200 67.10494300 13.61491100	H 0 9.31726200 62.35798000 12.37033500
C -1 19.48695100 53.29110800 7.88411000	C -1 18.60108000 58.32705700 1.75354600	H -1 15.41789200 51.40124600 3.31793600
C 0 18.07602500 53.45153700 7.34060900	C 0 17.25563700 58.68984600 2.40391200	H -1 8.46287900 61.01889200 3.48753100
N 0 17.22668800 54.18561500 8.10448500	C 0 17.03899900 60.17179000 2.58842200	H -1 18.76091400 57.25115300 1.87951300
O 0 17.71666600 52.92024800 6.28885600	C 0 16.64014800 60.98906200 1.52357100	H -1 19.49901100 52.57367400 8.71123700
H 0 19.89183900 54.24405500 8.23196800	C 0 17.25761700 60.76779200 3.83734600	H -1 22.21783600 63.14301600 14.80893900

H -1 19.93337500 56.70797700 10.41260400	C 0 12.68903600 65.39467900 4.01348900	O 0 11.72363000 59.37096900 13.03338600
H -1 6.00269400 59.81684600 7.41884900	C 0 14.17253700 64.78267500 6.29940900	H 0 9.99101800 57.10304000 14.83387400
H -1 11.67882200 57.43295100 15.10818100	C 0 13.42602300 64.21469400 4.07410000	H 0 9.76811200 58.67394700 13.04160500
H 0 11.79527200 53.58220000 13.22277100	C 0 14.16515600 63.90628100 5.21591700	H 0 10.35149600 59.47953700 14.50903800
H -1 9.59009800 65.85838500 13.78382400	H 0 9.98787700 67.10017000 5.84128000	H 0 12.15143000 58.72952200 12.42610600
H -1 8.38390500 64.58803700 13.42588400	H 0 12.30356000 68.14823700 4.11537400	N 0 12.19567200 55.51764600 13.40512800
H 0 14.94648300 52.33361300 4.74802500	H 0 12.22248400 68.22316700 5.86501000	C 0 12.25941100 54.21277900 12.76064100
H -1 13.20187400 54.61274500 8.59406000	H 0 13.46691600 66.66082100 7.06427600	C 0 12.17192500 54.11554600 11.23310800
C -1 13.92146700 69.63679100 15.14260600	H 0 12.12503600 65.63561900 3.11480000	O 0 11.85537700 53.03568100 10.74252500
H -1 14.06772900 70.72210000 15.13463300	H 0 14.75548000 64.56408200 7.18719200	H 0 12.78250900 55.64533100 14.22967100
H -1 12.89126600 69.40608600 14.84985300	H 0 13.45131900 63.54010400 3.22629900	H 0 13.20975800 53.75678500 13.05318200
H 0 14.02425600 69.31341200 16.18654500	H 0 14.73095400 62.98654100 5.24653800	N 0 12.52267700 55.19231400 10.49116600
H 0 13.43794400 58.97910300 13.63543700	H -1 10.04562900 68.52174700 4.76357600	C -1 12.35125900 55.13837300 9.03916400
C -1 9.09318400 66.03208900 8.85509700	C 0 14.20661700 62.63117000 9.83266400	C 0 12.27940600 56.54971300 8.47011200
C 0 10.48742600 65.47105900 8.44315000	C 0 13.30365400 62.30433400 10.77822400	S 0 11.68168400 56.59584100 6.73090900
C 0 11.59928600 66.17549000 9.19232800	C 0 12.41982500 61.17774400 10.30901400	H 0 12.61638300 56.09877400 10.93567200
C 0 11.84682000 67.54232200 8.99043300	H 0 11.36732500 61.48799500 10.24993300	H 0 11.44995200 54.56478100 8.80992000
C 0 12.36643700 65.49991300 10.14312800	H 0 12.45614400 60.32741200 10.99090000	H 0 11.61633000 57.16963800 9.07367300
C 0 12.83401900 68.20498400 9.71795300	H 0 14.93478600 63.42496500 9.88085400	H 0 13.26091800 57.03021400 8.46573700
C 0 13.35701000 66.15468200 10.87981600	H 0 13.20182800 62.77399500 11.74674600	H 0 10.37297000 56.68342800 7.04581900
C 0 13.59012400 67.51380600 10.66919900	H 0 15.74737400 61.04859900 11.93369400	C -1 14.81299900 65.87497900 19.15217900
H -1 9.29289800 66.79635700 9.61317400		C 0 16.30083100 65.91580000 18.72483000
H -1 8.44504200 65.25545400 9.27470400		C 0 16.97530500 64.56503400 19.04145400
H 0 8.56674900 66.50028500 8.01850700		C 0 16.49072600 66.33920900 17.31268100
H 0 10.54763400 64.39725800 8.64269400		H 0 14.66816500 65.47933600 20.16461000
H 0 10.65017400 65.58189800 7.36624600		H 0 14.25407100 65.23253800 18.46035400
H 0 11.26119900 68.08783300 8.25422200		H 0 16.79198300 66.66349300 19.41204800
H 0 12.20510300 64.44044300 10.29222800		H 0 18.03017000 64.58803000 18.75000700
H 0 13.01681600 69.26163400 9.54328200		H 0 16.91481900 64.28653400 20.10003800
H 0 13.94441500 65.60981300 11.61417600		H 0 16.49045000 63.77188300 18.46076000
H 0 14.35865600 68.03058800 11.23470600		H 0 17.54429500 66.40438200 17.02522300
C -1 12.60584300 56.71569500 17.61685000		H 0 16.01004700 65.61434700 16.64311000
C 0 13.44456400 55.54237600 17.13317400		H 0 16.03319400 67.31557200 17.12078100
O 0 14.00746600 55.79915600 15.84143900		C -1 8.77936300 61.70508400 18.47258200
H -1 12.18862300 56.58083200 18.62026900		C 0 10.22409300 61.35446000 18.08909900
H -1 11.78071100 56.90570200 16.92275800		C 0 10.53146500 59.87127100 18.32481100
H 0 13.21887900 57.62481800 17.64854100		C 0 10.43993400 61.72505800 16.62002600
H 0 14.24436700 55.31396100 17.85199000		H 0 8.54435100 61.44363300 19.50906200
H 0 12.83833800 54.63946600 17.01763500		H -1 8.12210400 61.13716300 17.80586100
H 0 14.47381900 56.64552500 15.89228800		H 0 10.91095500 61.94972400 18.70604900
H 0 10.09709500 66.87678000 4.08604900		H 0 11.55897900 59.62805900 18.03650200
C -1 10.41975300 67.50455500 4.92175300		H 0 10.39823200 59.59464300 19.37632700
C 0 11.95291900 67.60348400 5.00261400		H 0 9.86260000 59.23903100 17.72735000
C 0 12.69337300 66.29080900 5.09162300		H 0 11.44349500 61.47838800 16.26712300
C 0 13.44428000 65.97029800 6.22798200		H 0 9.72967300 61.17882300 15.98881900

### indene-TS<sub>1R,2S</sub>

H -1 17.45621900 55.72340800 15.73985100		
H -1 14.36506400 66.87379000 19.12384500		
H -1 8.60699200 62.77679700 18.32919600		
H -1 10.42844700 62.61838300 -1.01066700		
H -1 10.37415500 60.99336300 -0.26730600		
C 0 14.41970800 60.70981200 6.66123200		
C 0 14.77509200 61.72031900 7.56029600		
C 0 14.13762200 61.76925100 8.78835300		
C 0 13.13033400 60.82268700 9.11329000		
C 0 12.73329500 59.84948200 8.18453400		
C 0 13.40442200 59.78979400 6.97087400		
H 0 14.94697600 60.63072100 5.71549700		
H 0 15.55742500 62.43031000 7.32866900		
H 0 11.93033500 59.16224400 8.40893000		
H 0 13.13980800 59.00885400 6.27104400		
O 0 15.99498800 59.35776700 12.67708200		
O 0 14.67987600 60.54521400 11.86051600		
H 0 17.90430800 66.46800200 14.05142600		
C -1 10.91651700 57.40589900 14.32220700		
C 0 11.11425400 56.32448600 13.26100100		
O 0 10.29214400 56.19515900 12.35355300		
C 0 10.62465100 58.77734800 13.71750900		



H 0 10.27614300 62.79273700 16.44688200	C -1 21.24016900 63.62251500 14.93331500	C 0 17.84297900 61.10487400 8.07022500
C -1 6.93623400 59.40296600 7.02350600	C 0 20.23892900 62.86903700 14.06449500	O 0 17.81516700 60.42959700 7.03162100
C 0 7.95205600 59.23305000 8.12190200	O 0 20.56962700 62.39492700 12.97421800	C 0 20.01103400 62.22270900 7.64559900
C 0 8.25668400 57.96852900 8.64081700	C 0 21.30550800 65.10266100 14.49067600	C 0 20.79319000 63.50425000 7.39362600
C 0 8.58315300 60.35492600 8.67475300	C 0 19.96988900 65.79367500 14.79701100	O 0 20.55915400 61.47442700 8.74181400
C 0 9.15790300 57.82372000 9.69763300	O 0 19.13386200 65.83272700 13.80443900	H 0 19.15917600 62.96616100 10.02927700
C 0 9.49061600 60.21792700 9.72156700	O 0 19.74992200 66.18409200 15.94743000	H -1 18.05386400 63.07796700 7.28924500
C 0 9.77911200 58.95179200 10.23357200	H 0 20.98104100 63.59199800 15.99421600	H 0 19.98684700 61.60575200 6.73903100
H 0 6.69826800 58.44745400 6.54781100	H 0 22.09612100 65.60610200 15.05368600	H 0 21.49351000 61.30811000 8.56612700
H 0 7.29390900 60.08406600 6.24689500	H 0 21.53375300 65.15114800 13.42269600	H 0 21.82732300 63.27223700 7.11514600
H 0 7.76684800 57.09165500 8.22472200	N 0 18.94082200 62.81466300 14.48354800	H 0 20.34657700 64.07241900 6.57169600
H 0 8.35654500 61.34195800 8.28043900	C 0 17.93857900 62.16255300 13.64263800	H 0 20.80745000 64.13305500 8.28697400
H 0 9.37279000 56.84945600 10.12448500	C 0 17.63961300 62.80234400 12.30468900	N 0 17.31267600 60.70142200 9.23259200
H 0 9.97190600 61.09749900 10.13637900	O 0 16.86759000 62.16635600 11.54682400	C 0 16.56590100 59.46111200 9.32085400
H 0 10.48148100 58.83823400 11.04642600	C 0 16.63863800 62.20599500 14.48492100	C 0 17.42144800 58.20777100 9.18883600
C -1 17.74268100 56.74911700 15.48499500	C 0 17.15745600 62.31230400 15.91882100	O 0 16.94587800 57.19500700 8.66986700
N 0 16.90571100 56.40418800 13.02854400	C 0 18.36813100 63.23430700 15.77649100	H 0 17.30232700 61.32738700 10.03817100
C 0 16.57815300 56.15998300 11.71822700	H 0 18.22924900 61.12974900 13.42539900	H 0 16.06078600 59.45370400 10.28844000
O 0 17.21295200 55.40559200 11.00267600	H 0 16.07229000 63.10737900 14.22968900	H 0 15.81996300 59.40475600 8.52848400
N 0 15.39355600 56.76172800 11.20870700	H 0 16.02476900 61.32941800 14.28789000	N 0 18.66977400 58.28785400 9.71676200
C 0 14.57643400 57.61289400 11.88349600	H 0 16.40865100 62.71241200 16.60395000	C -1 19.68173200 57.26458800 9.50368000
C 0 15.25001200 58.29072200 13.09610500	H 0 17.46642200 61.33007000 16.28780100	C 0 20.92485100 57.79991000 8.79214000
O 0 13.43863600 57.87915300 11.48220700	H 0 18.07037300 64.28446600 15.74060400	C 0 20.59623100 58.37323100 7.40558500
C 0 14.75575000 59.03633300 15.32129800	H 0 19.09308400 63.11757200 16.58279300	C 0 19.87826500 57.33131100 6.54742700
N 0 14.24972400 58.56225300 14.11509100	N 0 18.10769300 64.00416100 11.97247200	N 0 18.72402800 57.75626700 5.96904700
C 0 14.10086000 60.01384900 16.07716400	C 0 17.45664100 64.76534900 10.90012800	O 0 20.33530300 56.19960400 6.40038600
C 0 14.57135100 60.41579500 17.32777700	C 0 17.49760300 64.08199400 9.53660000	H 0 18.96925300 59.20329400 10.02757400
C 0 13.89514600 61.52836500 18.08711300	O 0 16.65048700 64.34979100 8.68093900	H 0 19.20445100 56.52371600 8.85712800
C 0 15.72026000 59.79283300 17.85471500	C 0 18.03479400 66.19889000 10.83414500	H 0 21.41816100 58.56819200 9.40134100
C 0 16.26870300 60.19783200 19.19921500	C 0 17.19734200 67.09259800 9.90056100	H 0 21.62628600 56.96796300 8.67637100
C 0 16.38733200 58.83396700 17.09171100	C 0 19.52528700 66.21472500 10.47977100	H 0 19.99887200 59.28009100 7.49785300
C 0 15.94520600 58.46774200 15.81591000	C 0 17.31141300 68.57613000 10.25842900	H 0 21.52757600 58.63822500 6.89078700
C 0 16.27258600 57.32591800 13.69514700	H 0 18.61490000 64.55289900 12.68499300	H 0 18.25916700 58.58388800 6.32925200
N 0 16.61466700 57.52860300 14.99609800	H 0 16.39580000 64.85003700 11.14802800	H 0 18.14341500 57.04644700 5.54221600
H 0 15.13866900 56.47469400 10.27008200	H 0 17.93102300 66.59271900 11.84739300	C -1 19.48686200 53.29109100 7.88417300
H 0 13.42148500 61.16578900 19.00746700	H 0 17.49523200 66.92745600 8.85896700	C 0 18.06839100 53.46922600 7.36687600
H 0 14.61414500 62.29866800 18.38542800	H 0 16.14774000 66.79134500 9.95352000	N 0 17.23247100 54.18840300 8.15748800
H 0 13.12696800 62.01117000 17.48307400	H 0 19.92091900 67.23237600 10.54037700	O 0 17.69242900 52.96048700 6.30873900
H 0 15.51254600 60.12165300 19.98890300	H 0 20.10495900 65.59869400 11.17157700	H 0 19.90844300 54.23883100 8.22674400
H 0 17.11646800 59.56978000 19.48481200	H 0 19.69193900 65.84980000 9.46029100	H 0 20.09920700 52.90909600 7.06834700
H 0 16.61484100 61.23879500 19.19258900	H 0 16.69051400 69.18937700 9.59671700	H 0 16.31067400 54.37760700 7.79479700
H 0 13.22399600 60.48399300 15.64386100	H 0 16.98506500 68.75229600 11.28997000	H 0 17.51783700 54.73372900 8.96101900
H 0 17.28067500 58.39002800 17.51076300	H 0 18.34122700 68.94002400 10.17657700	C -1 10.76453400 62.01020000 -0.16232300
H 0 18.18067100 57.22921100 16.35498800	N 0 18.50256400 63.20331100 9.29545000	C 0 12.30911800 62.02359900 -0.16815800
H 0 18.48810900 56.68769700 14.69383800	C -1 18.55247200 62.47040900 8.05116500	C 0 12.96158200 60.79545800 0.49655100

C 0 12.82251700 63.35077900 0.40350700	H 0 17.11978100 58.15715900 3.30750000	H 0 14.93461100 52.32713100 4.74643900
C 0 12.67761500 60.59415200 1.98433300	H 0 16.43910400 60.58386900 0.54857100	H -1 13.20182000 54.61267300 8.59404400
H 0 10.35520400 62.42854200 0.76300400	H 0 17.57909700 60.08533700 4.65859700	C -1 13.92237000 69.63583500 15.14420800
H 0 12.62227400 61.98119200 -1.22160600	H 0 16.14691500 63.01333400 0.92989400	H -1 14.06701500 70.72219100 15.13388500
H 0 12.63937600 59.89923800 -0.05082200	H 0 17.27101700 62.48156700 5.04848200	H -1 12.89134000 69.40676900 14.84905200
H 0 14.04599800 60.86793500 0.35484200	H 0 16.52849900 63.97638900 3.19131600	H 0 14.02145900 69.31635000 16.18957500
H 0 13.91566800 63.39137800 0.41728200	C -1 15.09114600 52.38697300 3.66549700	H 0 13.46297100 59.10837200 13.76231100
H 0 12.45773900 64.19929400 -0.18608600	C 0 16.12599500 53.48232800 3.34986300	C -1 9.09328600 66.03226200 8.85518100
H 0 12.47178500 63.49569200 1.42950800	C 0 15.63258800 54.86369300 3.72904500	C 0 10.47659300 65.44139000 8.44276000
H 0 13.22359900 59.72585200 2.36600100	C 0 14.78310900 55.58010700 2.87655800	C 0 11.60171100 66.05710100 9.24582200
H 0 12.99428200 61.45383400 2.58147100	C 0 15.98017500 55.44060400 4.95955100	C 0 11.95948600 67.39907900 9.04562800
H 0 11.61351900 60.42595500 2.17152100	C 0 14.29960800 56.83798100 3.23567100	C 0 12.27293900 65.33761600 10.23821400
C -1 8.85007600 61.71625900 4.23763700	C 0 15.49459800 56.69890400 5.32990300	C 0 12.96484400 67.99457400 9.80438400
C 0 10.27555700 61.36301800 4.67425000	C 0 14.65891900 57.40332700 4.45918900	C 0 13.28293700 65.92570900 11.00717500
C 0 10.74076700 62.24767100 5.83875200	H 0 14.12680500 52.60972300 3.19543800	C 0 13.63028500 67.25818100 10.78769400
C 0 10.38892800 59.87415800 5.01591100	H 0 17.04746300 53.26365400 3.89573900	H -1 9.29282200 66.79636500 9.61318400
H 0 8.16619400 61.67564800 5.09532100	H 0 16.35790500 53.46582100 2.27708200	H -1 8.44509800 65.25537800 9.27465300
H -1 8.80495900 62.73712900 3.84520100	H 0 14.50166400 55.14662500 1.91938000	H 0 8.57045100 66.49718900 8.01490800
H 0 10.93853900 61.56695300 3.82614900	H 0 16.63899700 54.88270800 5.61567000	H 0 10.48706000 64.35565100 8.57851400
H 0 11.78423000 62.05017400 6.09636700	H 0 13.64638300 57.38149300 2.55868400	H 0 10.66852800 65.60940200 7.37825200
H 0 10.66069400 63.31095700 5.58921400	H 0 15.77256500 57.11985400 6.29361800	H 0 11.44523900 67.97646900 8.28134800
H 0 10.13659600 62.05656200 6.73391900	H 0 14.30177700 58.39249900 4.71884600	H 0 12.00198700 64.29953300 10.40462900
H 0 11.42243100 59.58833100 5.21120700	C -1 9.36853800 64.78823800 13.86185200	H 0 13.23531200 69.03153300 9.62667300
H 0 9.81180500 59.62941800 5.91454500	C 0 10.48751900 63.99591400 13.17117000	H 0 13.80820800 65.35982700 11.77110400
H 0 10.01939600 59.24811600 4.19564200	C 0 11.81223200 64.21128000 13.91478300	H 0 14.41789700 67.71674600 11.37498400
C 0 14.93530000 68.88649700 14.28162500	C 0 10.13608100 62.51072800 13.03325900	C -1 12.60587600 56.71568900 17.61686500
C 0 14.68694400 67.37337800 14.30242400	H 0 9.31022700 64.53143400 14.92692400	C 0 13.45371500 55.55572800 17.11900500
C 0 15.87596400 66.51043500 13.89996500	H 0 10.60487200 64.40888600 12.16168900	O 0 13.88622600 55.76040500 15.76950000
O 0 17.02605100 67.06892100 14.18256400	H 0 12.65525600 63.73085300 13.41163200	H -1 12.18860100 56.58082400 18.62025800
O 0 15.72078600 65.39051400 13.40801300	H 0 12.05306900 65.27595400 13.99444100	H -1 11.78068900 56.90578600 16.92278600
H 0 14.90157800 69.25069400 13.24645400	H 0 11.76229100 63.80279200 14.93030100	H 0 13.21077800 57.63042000 17.64536900
H 0 15.94741800 69.07712800 14.64544000	H 0 10.96412200 61.92855200 12.62157100	H 0 14.32422900 55.40503600 17.77308900
H 0 14.44235700 67.06328200 15.32729000	H 0 9.89107200 62.07360200 14.00520700	H 0 12.88508900 54.62113600 17.10611000
H 0 13.82983000 67.09322200 13.68441200	H 0 9.26653500 62.36870200 12.38170900	H 0 14.22741100 56.66307400 15.68324400
C -1 18.60140900 58.32721200 1.75399500	H -1 15.41785400 51.40131600 3.31770300	H 0 10.11410300 66.88431000 4.07329200
C 0 17.22644700 58.67598000 2.35182300	H -1 8.46290900 61.01873200 3.48766600	C -1 10.41949800 67.50429700 4.92097200
C 0 17.01724300 60.15311700 2.57578900	H -1 18.76062900 57.25107400 1.87919400	C 0 11.94916800 67.61125300 5.03338600
C 0 16.62012000 61.00226600 1.53579500	H -1 19.49908700 52.57364200 8.71120800	C 0 12.70713800 66.30853700 5.12841400
C 0 17.25456500 60.71375500 3.83781600	H -1 22.21764000 63.14274100 14.80846200	C 0 13.53401700 66.04615000 6.22646700
C 0 16.45368500 62.37133800 1.75055300	H -1 19.93334000 56.70809500 10.41268600	C 0 12.65866500 65.37319900 4.08509200
C 0 17.08657600 62.08036200 4.05678600	H -1 6.00276900 59.81701300 7.41884700	C 0 14.30426300 64.88483100 6.28955700
C 0 16.68075100 62.91671000 3.01507600	H -1 11.67887700 57.43285300 15.10812300	C 0 13.43339400 64.21729000 4.13707600
H 0 18.67433900 58.59277100 0.69504700	H 0 11.45729400 53.55932200 13.12046300	C 0 14.25696900 63.97369000 5.23592700
H 0 19.39957600 58.84440000 2.29526700	H -1 9.59005700 65.85839700 13.78387700	H 0 9.97043500 67.09053100 5.82808100
H 0 16.43578100 58.27764800 1.70653300	H -1 8.38389900 64.58801500 13.42590700	H 0 12.31367400 68.16513300 4.15718500

H 0 12.19787200 68.22996300 5.90282200	C 0 12.36035400 54.24545300 12.77567400	C 0 9.24303300 59.48612700 10.05440100
H 0 13.58612400 66.76376000 7.03838000	C 0 12.22318800 54.13045000 11.25106200	C 0 9.53106100 58.13260600 10.23173200
H 0 12.03280600 65.56529800 3.21651100	O 0 11.92325200 53.03807200 10.77901000	H 0 6.67691200 58.57164500 6.36272100
H 0 14.95036800 64.71470500 7.14436600	H 0 12.86787900 55.72144700 14.20953300	H 0 7.39754800 60.18151700 6.40890600
H 0 13.42131400 63.51208600 3.31400000	H 0 13.33997900 53.83574500 13.03866700	H 0 7.72348800 56.86592600 7.64461300
H 0 14.86358100 63.07979600 5.25085100	N 0 12.52152000 55.20954100 10.48973300	H 0 8.19846300 60.95066800 8.87140100
H -1 10.04586900 68.52192300 4.76414400	C -1 12.35121000 55.13827400 9.03917300	H 0 9.19646900 56.13669400 9.51814700
C 0 12.76131300 61.01235000 10.48071500	C 0 12.30854400 56.54487600 8.44787500	H 0 9.65267800 60.21766500 10.74233100
C 0 13.56286400 61.99657000 11.06078700	S 0 11.78893500 56.55899100 6.68423200	H 0 10.15061000 57.78837200 11.04761000
C 0 14.39033200 62.64622900 9.97600500	H 0 12.62712000 56.11971200 10.92333400	C -1 17.74260200 56.74928100 15.48502500
H 0 15.43998700 62.71571500 10.24082300	H 0 11.44564200 54.57181700 8.80893600	N 0 16.91234100 56.40351200 13.01977100
H 0 14.06557100 63.67422200 9.78823700	H 0 11.63122500 57.18597500 9.01145400	C 0 16.58336500 56.14707300 11.71144400
H 0 12.04591100 60.42277700 11.03254900	H 0 13.29487800 57.01597700 8.47063000	O 0 17.21999400 55.39139000 11.00077500
H 0 13.34985700 62.46849100 12.00832900	H 0 10.46496200 56.58213400 6.94270100	N 0 15.39152600 56.73644600 11.20201400
H 0 15.47265500 61.13767200 11.85279500	C -1 14.81293000 65.87501400 19.15210700	C 0 14.57564300 57.59214900 11.86965200

## indene-TS<sub>1S,2R</sub>

H -1 17.45621300 55.72339100 15.73977900	C 0 16.30302300 65.91481100 18.78068300	C 0 15.24364800 58.27796500 13.07761500
H -1 14.36507700 66.87379700 19.12393100	C 0 16.97187200 64.56026100 19.04480400	O 0 13.43934900 57.86432800 11.47073600
H -1 8.60699700 62.77679000 18.32913400	C 0 16.50267400 66.34643500 17.32450400	C 0 14.75265300 59.03569900 15.29823100
H -1 10.42809900 62.61778100 -1.01096000	H 0 14.66227000 65.47653200 20.16257600	N 0 14.25318000 58.55863800 14.09193600
H -1 10.37422000 60.99319800 -0.26594500	H 0 14.25734900 65.23497300 18.45532300	C 0 14.09156800 60.01354800 16.04916200
C 0 13.41884900 59.87377700 6.80950300	H 0 16.79265300 66.65692600 19.42784100	C 0 14.56137800 60.42609800 17.29623000
C 0 12.65164600 59.86872400 7.97932100	H 0 18.02899100 64.58234800 18.76156300	C 0 13.88221500 61.54160700 18.04830600
C 0 12.99674400 60.74478500 8.99201500	H 0 16.90248400 64.27376700 20.10071600	C 0 15.71439500 59.81286700 17.82703300
C 0 14.07281300 61.64932500 8.82191700	H 0 16.48925600 63.77312200 18.45406500	C 0 16.26135400 60.22979700 19.16837500
C 0 14.78812900 61.70074600 7.61929900	H 0 17.55783200 66.40656000 17.04164200	C 0 16.38629900 58.85333600 17.07029200
C 0 14.46873500 60.78298600 6.62277700	H 0 16.02054700 65.62892900 16.64818700	C 0 15.94487700 58.47597800 15.79723000
H 0 13.18771400 59.14578600 6.04386800	H 0 16.05227300 67.32688000 17.13692700	C 0 16.28128300 57.32862700 13.68138300
H 0 11.81775000 59.18589500 8.07938800	C -1 8.77935900 61.70506200 18.47268400	N 0 16.61936300 57.53360500 14.98351800
H 0 15.58788900 62.41946300 7.50209600	C 0 10.22273500 61.35124200 18.08708400	H 0 15.14054200 56.44774200 10.26269500
H 0 15.04593600 60.75956700 5.70453500	C 0 10.53053000 59.87024100 18.33585600	H 0 13.40697100 61.18272500 18.96916700
O 0 15.98317700 59.35091900 12.63180500	C 0 10.43160200 61.70686000 16.61332600	H 0 14.60027500 62.31343000 18.34448400
O 0 14.80252000 60.50439600 11.78750700	H 0 8.54487400 61.44409800 19.50937600	H 0 13.11539900 62.02106600 17.44019900
H 0 17.92816200 66.50518800 14.03648000	H -1 8.12211100 61.13718100 17.80584000	H 0 15.50505100 60.15734600 19.95812700
C -1 10.91655900 57.40585400 14.32225100	H 0 10.91227600 61.95240900 18.69520000	H 0 17.11088900 59.60648200 19.45888300
C 0 11.12020400 56.28466100 13.30413500	H 0 11.55628600 59.62340400 18.04415400	H 0 16.60433000 61.27158500 19.15356400
O 0 10.25622200 56.05083700 12.45872300	H 0 10.40300400 59.60403900 19.39074900	H 0 13.21263900 60.47676700 15.61294000
C 0 10.62204500 58.76885800 13.70405100	H 0 9.85804500 59.23250000 17.74841000	H 0 17.28330500 58.41841600 17.49083600
O 0 11.73022300 59.37191000 13.05104100	H 0 11.43234600 61.45421300 16.25698800	H 0 18.17312600 57.23137800 16.35734600
H 0 9.99070000 57.11211900 14.83846200	H 0 9.71670600 61.15572700 15.99164200	H 0 18.49466900 56.68699900 14.70007300
H 0 9.77917000 58.65810800 13.01173300	H 0 10.26943100 62.77300000 16.43001800	C -1 21.24044100 63.62189700 14.93288500
H 0 10.32223000 59.46685000 14.48963800	C -1 6.93633300 59.40333600 7.02345700	C 0 20.23873800 62.87269300 14.05837100
H 0 12.12096500 58.75038800 12.40411600	C 0 7.85892400 58.95813900 8.12781600	O 0 20.57530600 62.38682900 12.97543000
N 0 12.26085200 55.55549000 13.40714200	C 0 8.15704800 57.60270900 8.31623000	C 0 21.31542200 65.10225800 14.49219300
	C 0 8.41913600 59.89463400 9.00695200	C 0 19.98225000 65.80198400 14.78798900
	C 0 8.98317900 57.18973200 9.36228700	O 0 19.16002600 65.86025700 13.78531400

O 0 19.75223300 66.18215500 15.94009600	H -1 18.05401300 63.07807500 7.28923600	H 0 13.90271900 63.41168200 0.43696100
H 0 20.97840300 63.59031400 15.99299300	H 0 19.98942900 61.60826800 6.74278300	H 0 12.43765800 64.20993000 -0.16141600
H 0 22.10488000 65.60040500 15.06164200	H 0 21.49902600 61.32076500 8.56593600	H 0 12.45833900 63.49747300 1.45122800
H 0 21.55292900 65.15037800 13.42620300	H 0 21.82208300 63.28003900 7.09761800	H 0 13.20089400 59.75069300 2.40075200
N 0 18.93453600 62.83379700 14.46401500	H 0 20.33601200 64.07830200 6.56667700	H 0 12.96416000 61.48007900 2.60277000
C 0 17.93297100 62.17858700 13.62225900	H 0 20.81369900 64.14237200 8.27716300	H 0 11.59208100 60.44505600 2.18073100
C 0 17.61870200 62.83811000 12.29675300	N 0 17.30512500 60.69482300 9.22275700	C -1 8.84984900 61.71578900 4.23806100
O 0 16.81870600 62.23995500 11.53616400	C 0 16.56110600 59.45023800 9.27780100	C 0 10.25747900 61.34593300 4.70829000
C 0 16.63864600 62.19218300 14.47585400	C 0 17.42093700 58.19840100 9.17841500	C 0 10.70839500 62.24139800 5.87013500
C 0 17.16102800 62.32613000 15.90638600	O 0 16.94744000 57.17532700 8.67685300	C 0 10.32290900 59.85863000 5.07170100
C 0 18.35120200 63.27054600 15.74591300	H 0 17.24992900 61.33296100 10.01696800	H 0 8.14980200 61.68105300 5.08365200
H 0 18.24139500 61.15454600 13.38795100	H 0 16.01017800 59.44146500 10.21855200	H -1 8.80513400 62.73707200 3.84503000
H 0 16.04477000 63.07435700 14.21762800	H 0 15.85035600 59.39517600 8.45314100	H 0 10.94550800 61.52264800 3.87482000
H 0 16.04651000 61.29793200 14.29269500	N 0 18.66678000 58.28672800 9.71068400	H 0 11.74229300 62.03581800 6.15579100
H 0 16.40630600 62.71965700 16.58887600	C -1 19.68176400 57.26465100 9.50389500	H 0 10.64647100 63.30133300 5.60144400
H 0 17.49281000 61.35575000 16.28706400	C 0 20.92913400 57.80310900 8.80175800	H 0 10.07812700 62.07411000 6.75342500
H 0 18.02947400 64.31230700 15.68353100	C 0 20.61245600 58.37418100 7.41163900	H 0 11.34278500 59.53977700 5.28066100
H 0 19.07698100 63.19137100 16.55530800	C 0 19.90276500 57.32953200 6.54999700	H 0 9.72805200 59.64272400 5.96631900
N 0 18.11509400 64.02924700 11.97020400	N 0 18.74956800 57.74982800 5.96698900	H 0 9.94086200 59.23435900 4.25580400
C 0 17.46920600 64.78412400 10.89468800	O 0 20.36431800 56.19916400 6.40628200	C 0 14.93355600 68.88696800 14.27778400
C 0 17.46952200 64.04857600 9.55806100	H 0 18.96529200 59.20879400 10.00299100	C 0 14.70801500 67.37004000 14.32138700
O 0 16.57060000 64.25029200 8.73726800	H 0 19.21073700 56.52267400 8.85412900	C 0 15.90644900 66.52024000 13.91629100
C 0 18.07709400 66.20169000 10.78257000	H 0 21.41515400 58.57289400 9.41493800	O 0 17.05205000 67.10236900 14.17238800
C 0 17.27554200 67.06581000 9.79069600	H 0 21.63348800 56.97267000 8.69322200	O 0 15.76590000 65.39019800 13.44475000
C 0 19.57503500 66.18250200 10.46207600	H 0 20.01360600 59.28077100 7.49650500	H 0 14.88322000 69.23581400 13.23793100
C 0 17.40768300 68.56243300 10.08044600	H 0 21.54830000 58.63829300 6.90468200	H 0 15.94723400 69.09585000 14.62704200
H 0 18.62706300 64.57435100 12.68244400	H 0 18.28279200 58.57940600 6.31981300	H 0 14.47951400 67.06980400 15.35271000
H 0 16.41481700 64.90210400 11.15572000	H 0 18.17385100 57.03963700 5.53433400	H 0 13.85070200 67.06542400 13.71532900
H 0 17.95658000 66.63839900 11.77760500	C -1 19.48694800 53.29112400 7.88409600	C -1 18.60108000 58.32705400 1.75354600
H 0 17.59620800 66.84756900 8.76519700	C 0 18.06961800 53.45574100 7.35904300	C 0 17.24570800 58.68783800 2.38408200
H 0 16.21958600 66.78492600 9.83103500	N 0 17.22845200 54.18382200 8.13638600	C 0 17.03965500 60.16825000 2.58961800
H 0 19.98285700 67.19680400 10.48891800	O 0 17.69845100 52.92861100 6.30847600	C 0 16.62863400 61.00193300 1.54232100
H 0 20.13063800 65.58935000 11.19212200	H 0 19.89931000 54.24188200 8.22930900	C 0 17.28627700 60.74678600 3.84163200
H 0 19.75820300 65.77356300 9.46277100	H 0 20.10735300 52.91337200 7.07238800	C 0 16.45613300 62.37260800 1.74086700
H 0 16.82182800 69.15421600 9.36942100	H 0 16.30629400 54.36203600 7.76892600	C 0 17.11097100 62.11513300 4.04472800
H 0 17.04908900 68.79408200 11.09005100	H 0 17.51237300 54.74717200 8.92766700	C 0 16.69008600 62.93557200 2.99661300
H 0 18.44689000 68.90246400 10.01733500	C -1 10.76497300 62.01131900 -0.16365900	H 0 18.64727200 58.58521300 0.69110100
N 0 18.50162300 63.20859300 9.29399600	C 0 12.30899200 62.03220400 -0.15477600	H 0 19.41654500 58.84443400 2.26852600
C -1 18.55224900 62.47025900 8.05122100	C 0 12.95930800 60.80904500 0.52114300	H 0 16.43727000 58.27854600 1.76884500
C 0 17.85362100 61.10101200 8.06855500	C 0 12.80987000 63.36164500 0.42384100	H 0 17.16638600 58.18505800 3.35050900
O 0 17.85262400 60.41928800 7.03419100	C 0 12.65813200 60.61555600 2.00670200	H 0 16.43983300 60.56970300 0.56254000
C 0 20.01267800 62.22947100 7.64618600	H 0 10.34861600 62.42964200 0.75883800	H 0 17.61985100 60.13093900 4.66835200
C 0 20.79047300 63.51181400 7.38545300	H 0 12.63435700 61.99080100 -1.20453300	H 0 16.13793100 63.00189500 0.91473500
O 0 20.56557900 61.48860500 8.74505100	H 0 12.64653200 59.90905100 -0.02549000	H 0 17.29893600 62.53130800 5.02965800
H 0 19.18302000 62.99870300 10.01354000	H 0 14.04497600 60.88509300 0.39163000	H 0 16.53156700 63.99621400 3.16133200

C -1 15.09107500 52.38696600 3.66519800	H 0 13.44003000 59.07085300 13.74547900	H -1 10.04563100 68.52174500 4.76355600
C 0 16.13484600 53.47152400 3.34416200	C -1 9.09318500 66.03206800 8.85511700	C 0 14.28661500 62.33594000 10.06807800
C 0 15.65663500 54.85872800 3.71671200	C 0 10.46601200 65.43146100 8.42564600	C 0 13.44292400 61.81993500 11.04149500
C 0 14.82181400 55.58369700 2.85732300	C 0 11.61141700 65.94840300 9.27030900	C 0 12.44771900 60.89488000 10.38087000
C 0 16.00583100 55.43328900 4.94751900	C 0 11.93853400 67.31333100 9.24710300	H 0 11.45981300 61.37248200 10.36638000
C 0 14.35979700 56.85189600 3.20756000	C 0 12.35778900 65.10503100 10.09855600	H 0 12.33509000 59.94562900 10.89185400
C 0 15.54013300 56.70098400 5.30953500	C 0 12.98247700 67.81549900 10.02081900	H 0 15.02711600 63.10564600 10.21323300
C 0 14.72540000 57.41696500 4.42896800	C 0 13.39778100 65.60281500 10.88946700	H 0 13.26758100 62.27735700 12.00363100
H 0 14.12846200 52.61313700 3.19352700	C 0 13.71378700 66.95994800 10.84827100	H 0 15.55512200 61.14666900 11.83337900
H 0 17.05463200 53.24580900 3.89016000	H -1 9.29290300 66.79636900 9.61316100	
H 0 16.36584300 53.44720200 2.27133500	H -1 8.44503600 65.25545600 9.27469900	
H 0 14.53818300 55.15012400 1.90083600	H 0 8.56331800 66.49651000 8.01870900	
H 0 16.65269400 54.86767800 5.60858800	H 0 10.44188200 64.33891300 8.47893700	
H 0 13.72237100 57.40537500 2.52351100	H 0 10.67591800 65.66914100 7.37762200	
H 0 15.81794000 57.12130300 6.27344400	H 0 11.37180000 67.98398500 8.60538700	
H 0 14.39695400 58.41810000 4.67748600	H 0 12.12724600 64.04510700 10.11897500	
C -1 9.36838200 64.78822100 13.86198900	H 0 13.22878300 68.87270000 9.97889800	
C 0 10.47828000 63.98541100 13.16494200	H 0 13.96088100 64.95111900 11.54880500	
C 0 11.81312000 64.18551200 13.89396100	H 0 14.52717100 67.34353400 11.45281800	
C 0 10.10240900 62.50353400 13.04386500	C -1 12.60584300 56.71569900 17.61684300	
H 0 9.31258100 64.52999800 14.92677100	C 0 13.45157800 55.55029200 17.12763100	
H 0 10.59637900 64.38867000 12.15046300	O 0 13.93991100 55.77499200 15.80059200	
H 0 12.64128900 63.69163900 13.37928900	H -1 12.18862500 56.58082900 18.62027000	
H 0 12.07089200 65.24687100 13.96425800	H -1 11.78070900 56.90570300 16.92276100	
H 0 11.76962700 63.78269400 14.91231800	H 0 13.21388000 57.62835400 17.64646400	
H 0 10.92439000 61.89548700 12.65841100	H 0 14.29322700 55.36996200 17.81153100	
H 0 9.82940200 62.08951600 14.01864200	H 0 12.86717700 54.62712900 17.07376000	
H 0 9.23953100 62.37027900 12.38077500	H 0 14.32807000 56.66129200 15.76590900	
H -1 15.41789500 51.40125100 3.31792600	H 0 10.15991600 66.89687100 4.05019800	
H -1 8.46288000 61.01889500 3.48752800	C -1 10.41975000 67.50456600 4.92177400	
H -1 18.76091500 57.25115300 1.87951200	C 0 11.94178300 67.62290400 5.10565400	
H -1 19.49900500 52.57368100 8.71124300	C 0 12.71099900 66.32602700 5.18954300	
H -1 22.21784800 63.14304300 14.80892500	C 0 13.47770700 66.02997000 6.32165900	
H -1 19.93340300 56.70798600 10.41260200	C 0 12.73375300 65.43181100 4.10964900	
H -1 6.00269700 59.81685600 7.41884500	C 0 14.25639700 64.87470100 6.38494100	
H -1 11.67881500 57.43294600 15.10818800	C 0 13.52046400 64.28330300 4.16041500	
H 0 11.59963200 53.56286400 13.16877400	C 0 14.28333400 64.00609300 5.29536900	
H -1 9.59013200 65.85837900 13.78383200	H 0 9.93278700 67.07159400 5.79977300	
H -1 8.38391100 64.58804700 13.42586500	H 0 12.33761900 68.21090600 4.26602000	
H 0 14.93511300 52.33020000 4.74626700	H 0 12.14371000 68.21288100 6.00680100	
H -1 13.20186400 54.61273800 8.59404800	H 0 13.47488300 66.71622000 7.16185300	
C -1 13.92150400 69.63676000 15.14266100	H 0 12.15473200 65.65081800 3.21519600	
H -1 14.06769900 70.72210400 15.13460200	H 0 14.84933000 64.67527500 7.27060300	
H -1 12.89126700 69.40610800 14.84983200	H 0 13.56607700 63.61206800 3.30972600	
H 0 14.02339600 69.31641800 16.18763500	H 0 14.89923700 63.11859300 5.31395700	

## indene-Int<sub>IR,2S</sub>

H -1 3.60473500 -6.72566300 -2.37457700
H -1 10.44977300 2.53651400 1.18830700
H -1 7.91085400 -1.04105400 6.78538200
H -1 -10.1163040 5.55970500 3.81493200
H -1 -9.98977400 3.77732600 3.87287000
C 0 -3.12413300 1.25573100 0.22143800
C 0 -1.86886500 1.81219200 -0.01258000
C 0 -0.77517300 1.26120500 0.64401200
C 0 -0.98500300 0.22470600 1.62009000
C 0 -2.28973500 -0.25456700 1.92326900
C 0 -3.33847200 0.24055100 1.18993100
H 0 -3.96948300 1.59899600 -0.36729800
H 0 -1.71460000 2.58770100 -0.74923400
H 0 -2.44147200 -0.98345000 2.70571800
H 0 -4.33130100 -0.15493300 1.35373300
O 0 1.82620700 -2.14845000 -0.70451800
O 0 2.42395300 -0.22855700 1.02719100
H 0 5.83138100 3.93004800 -2.66680100
C -1 2.44314800 -4.67111600 4.10880900
C 0 1.07847300 -5.31539400 3.85870200
O 0 0.14107700 -5.07483300 4.62149800
C 0 2.33346600 -3.18595900 4.41192100
O 0 1.89868800 -2.41588900 3.29966700
H 0 2.77146200 -5.14231800 5.04884300
H 0 1.64473200 -3.05883000 5.25523600
H 0 3.30874300 -2.78692200 4.70093700
H 0 1.19305500 -2.88595300 2.79997300
N 0 0.98035200 -6.17645400 2.81692300
C 0 -0.09116600 -7.16120800 2.75503700
C 0 -1.55098200 -6.69263600 2.71692600
O 0 -2.42395600 -7.49599200 3.03278000
H 0 1.82320600 -6.37694000 2.27630200
H 0 0.07267700 -7.75845500 1.85342900
N 0 -1.81944800 -5.44539300 2.26348500

C -1 -3.19456700 -4.95042100 2.30709700 H 0 -1.84843500 -3.78945700 5.40780400 C 0 2.85660700 1.00290700 -2.67378600  
C 0 -3.19100900 -3.42669300 2.34190400 H 0 -0.21931300 0.14636100 4.90879600 O 0 1.83457900 0.61569400 -2.07614800  
S 0 -4.82001900 -2.70151800 2.79492000 H 0 -0.16937400 -2.29570900 4.42512800 C 0 4.64245400 -0.24166800 -1.48990000  
H 0 -1.06581100 -4.77225000 2.17079800 C -1 3.74168000 -5.67479600 -2.65034100 C 0 6.08302300 -0.57058500 -1.88653400  
H 0 -3.69370800 -5.37380600 3.18197700 N 0 1.28079600 -5.03396100 -2.02416200 C 0 6.32895000 0.33136300 -3.09586800  
H 0 -2.44615300 -3.07014300 3.05391500 C 0 -0.04689600 -4.86895500 -1.74486600 H 0 3.43452200 -0.94605900 -3.17848700  
H 0 -2.93691100 -3.00920600 1.36422800 O 0 -0.94248700 -5.30097000 -2.45353800 H 0 4.61352500 0.68674900 -0.91227700  
H 0 -4.61097700 -2.73923500 4.12734600 N 0 -0.39524300 -4.22318200 -0.52432500 H 0 4.13831300 -1.01883300 -0.92115000  
C -1 10.15774000 1.59169200 0.71813000 C 0 0.47730400 -3.67536300 0.35986900 H 0 6.78973500 -0.38172400 -1.07684100  
C 0 9.94585900 1.75987400 -0.79440500 C 0 1.88286300 -3.39573400 -0.20174600 H 0 6.16903900 -1.62171000 -2.17539700  
C 0 9.78811200 0.39888100 -1.48346700 O 0 0.08953500 -3.27325200 1.47364700 H 0 6.59268500 1.34636600 -2.79198900  
C 0 8.74467700 2.66368500 -1.08935600 C 0 4.21064100 -3.51981100 0.39895600 H 0 7.11564400 -0.03845000 -3.75527800  
H 0 10.94767900 0.86188800 0.93322300 N 0 2.89263800 -3.61608200 0.85691800 N 0 3.02994000 2.27563700 -3.05241000  
H 0 9.23827400 1.23979000 1.20177900 C 0 5.20625800 -2.84343300 1.10813400 C 0 2.24723400 3.34215500 -2.42506600  
H 0 10.84490000 2.23832800 -1.20945000 C 0 6.54165300 -2.86453400 0.70157900 C 0 0.73955300 3.17492300 -2.54709800  
H 0 9.61964700 0.51999900 -2.55828000 C 0 7.58636500 -2.06887100 1.44215400 O 0 -0.00893300 3.65939200 -1.69053200  
H 0 10.67389100 -0.23122900 -1.34125600 C 0 6.89178700 -3.61134300 -0.44028200 C 0 2.70194600 4.72379800 -2.95761400  
H 0 8.92644800 -0.14064000 -1.07485600 C 0 8.32113000 -3.66853700 -0.91674800 C 0 2.06265100 5.86786900 -2.14984700  
H 0 8.58437400 2.82065200 -2.16015500 C 0 5.88914000 -4.24648500 -1.17573400 C 0 2.48538700 4.87709000 -4.46633700  
H 0 7.82790400 2.21937200 -0.68154000 C 0 4.54492600 -4.18174700 -0.79686100 C 0 2.89834000 7.14921700 -2.19015300  
H 0 8.86540000 3.64819400 -0.62515500 C 0 2.18561600 -4.45098800 -1.28360100 H 0 3.94187000 2.55750500 -3.44027700  
C -1 7.68330800 -2.09507500 6.59516800 N 0 3.48756400 -4.75694000 -1.54119400 H 0 2.45350200 3.32848600 -1.35286800  
C 0 7.30585400 -2.29549800 5.12076900 H 0 -1.39033300 -4.16931000 -0.33825700 H 0 3.77784700 4.75237800 -2.77454100  
C 0 7.06481200 -3.77272600 4.79013700 H 0 8.28278400 -2.71643500 1.98927300 H 0 1.04857800 6.06463700 -2.51756200  
C 0 6.05746400 -1.46411700 4.82128000 H 0 8.18961000 -1.46725600 0.75465200 H 0 1.94062000 5.55385300 -1.10985000  
H 0 8.54692300 -2.69917700 6.89137800 H 0 7.12890600 -1.38680800 2.15958500 H 0 2.92520500 5.81345000 -4.82095000  
H -1 6.81982800 -2.39645900 7.19740300 H 0 9.00230500 -4.00321800 -0.12604800 H 0 2.96232000 4.06354500 -5.01770000  
H 0 8.12888200 -1.93293000 4.49001300 H 0 8.42733400 -4.35271300 -1.76268600 H 0 1.41809900 4.89164700 -4.71357400  
H 0 6.78250900 -3.90234700 3.74058100 H 0 8.67479600 -2.68246900 -1.24235500 H 0 2.43884600 7.93848600 -1.58550900  
H 0 7.95697100 -4.37921600 4.98065100 H 0 4.90169700 -2.25330800 1.96624700 H 0 3.90627000 6.96624200 -1.80016100  
H 0 6.25009700 -4.17754800 5.40379100 H 0 6.18191600 -4.77599000 -2.07311200 H 0 3.00917300 7.53471500 -3.20924900  
H 0 5.71864200 -1.56973700 3.78899000 H 0 4.75199800 -5.53364300 -3.02378000 N 0 0.24820100 2.53549500 -3.63595800  
H 0 5.23338400 -1.78377800 5.46948600 H 0 3.03067800 -5.45596500 -3.44489200 C -1 -1.16922800 2.28181200 -3.75760600  
H 0 6.22888600 -0.40073600 5.01098800 C -1 5.84146400 0.96843900 -6.00220400 C 0 -1.66861600 1.00234600 -3.05202900  
C -1 -3.94489400 -0.26471400 7.69723200 C 0 4.71861000 0.53155800 -5.08170400 O 0 -2.88624400 0.76049600 -3.03136500  
C 0 -2.92249800 -0.82721000 6.74466500 O 0 3.55659200 0.43883300 -5.49019000 C 0 -1.55883700 2.18221900 -5.23698700  
C 0 -2.88935100 -2.19525600 6.44511300 C 0 5.92728300 2.51076900 -6.06037800 C 0 -1.31970200 3.47215800 -6.01033400  
C 0 -1.95497600 0.00833000 6.17078300 C 0 6.39749400 3.05772800 -4.70655600 O 0 -0.75710700 1.10497600 -5.74230200  
C 0 -1.90120300 -2.72547800 5.61361000 O 0 5.44207600 3.41719900 -3.90360200 H 0 0.88267000 2.06568100 -4.27113300  
C 0 -0.97079300 -0.51263700 5.33346800 O 0 7.60328100 3.04997300 -4.44339300 H -1 -1.70252800 3.11574500 -3.29020600  
C 0 -0.94090900 -1.88055800 5.05675400 H 0 6.81427900 0.58135700 -5.68882900 H 0 -2.62214000 1.91246300 -5.26697900  
H 0 -4.74930800 -0.98101600 7.88557200 H 0 6.65743200 2.79494400 -6.82302900 H 0 -0.91819600 1.01676200 -6.68985400  
H 0 -4.39774800 0.65058800 7.30650200 H 0 4.94808700 2.91746100 -6.32690300 H 0 -1.60419900 3.34591400 -7.06101900  
H 0 -3.63208500 -2.85365700 6.88861000 N 0 5.01862800 0.31787800 -3.77154800 H 0 -1.92391600 4.28603700 -5.59757900  
H 0 -1.96929600 1.07200800 6.39392800 C 0 3.94165700 -0.03282200 -2.85389200 H 0 -0.26693700 3.76130300 -5.96793000

N 0 -0.73858400 0.21266400 -2.50879200	C -1 -5.62277000 2.87989200 5.67934900	C 0 -5.91629100 -2.17236500 -1.00178600
C 0 -1.06644100 -1.00165200 -1.78831500	C 0 -5.24189200 2.40666500 4.27286100	C 0 -6.54538400 -1.21335100 -0.20355100
C 0 -1.64364600 -2.10066200 -2.67078200	C 0 -3.81957400 2.85010600 3.90495700	H 0 -9.43040800 -5.27617600 0.12265700
O 0 -2.54687200 -2.82664500 -2.24997700	C 0 -5.41391100 0.89053100 4.13871300	H 0 -8.33523800 -4.89999800 -2.72476100
H 0 0.24816400 0.49080900 -2.51641100	H 0 -4.87819200 2.54130900 6.41115600	H 0 -9.82754600 -4.14614100 -2.14085300
H 0 -0.13614600 -1.36983400 -1.33540100	H -1 -5.63757200 3.97337300 5.72644400	H 0 -9.70893200 -2.46014300 -0.25378300
H 0 -1.81329200 -0.81348000 -1.01715600	H 0 -5.92683000 2.88914600 3.56694500	H 0 -6.19488600 -3.97637600 -2.16640600
N 0 -1.04857100 -2.22521400 -3.88319800	H 0 -3.57714300 2.59664700 2.86968200	H 0 -8.40034200 -0.58383900 0.69266400
C -1 -1.54888200 -3.10074400 -4.92771400	H 0 -3.69783300 3.93312800 4.00926800	H 0 -4.85140400 -2.10759800 -1.21474100
C 0 -1.95635000 -2.34319300 -6.19189100	H 0 -3.08194300 2.35689800 4.54996400	H 0 -5.98848500 -0.36946000 0.18801600
C 0 -3.06120400 -1.31351200 -5.91394100	H 0 -5.25612000 0.55801100 3.11205800	C -1 4.48136800 2.40388900 5.81019000
C 0 -4.27734900 -1.98023300 -5.27118300	H 0 -4.69394400 0.35327300 4.76604200	C 0 3.63934500 1.85725000 4.64542200
N 0 -4.74650600 -1.36830400 -4.15020800	H 0 -6.42086700 0.57628800 4.43514800	C 0 4.48493000 1.76236300 3.36751200
O 0 -4.78673100 -2.98764200 -5.75689900	C 0 6.66031900 6.11070700 0.38266900	C 0 3.00021400 0.51056000 5.01348900
H 0 -0.36932700 -1.51744800 -4.13086100	C 0 6.16101600 4.67530500 0.58334200	H 0 5.38926100 1.80067500 5.93570000
H 0 -2.43980300 -3.56945000 -4.50200500	C 0 5.55295500 4.02990400 -0.65385500	H 0 2.82924600 2.57432300 4.45592700
H 0 -1.08880500 -1.84019000 -6.63773800	O 0 6.11790700 4.43807500 -1.76264500	H 0 3.92664500 1.34595100 2.52406300
H 0 -2.32484400 -3.07513700 -6.91714700	O 0 4.65814300 3.18730400 -0.56890800	H 0 4.85835100 2.74648200 3.06683700
H 0 -2.68147400 -0.50834400 -5.28519700	H 0 5.80640800 6.80115300 0.37314300	H 0 5.35281600 1.11229800 3.52498100
H 0 -3.39246500 -0.86819600 -6.85995500	H 0 7.12743500 6.17922100 -0.60231100	H 0 2.53707900 0.02256600 4.15152000
H 0 -4.14000400 -0.73467200 -3.63849300	H 0 7.01074300 4.03558900 0.85670900	H 0 3.75156500 -0.18289100 5.40096700
H 0 -5.42974300 -1.88462800 -3.61165000	H 0 5.44238300 4.60336900 1.40391500	H 0 2.23855300 0.63186600 5.79249800
C -1 -4.45836900 -6.26048300 -4.92818900	C -1 -8.49732200 0.59499100 -4.28353900	H -1 -9.64876100 -6.44965700 -1.18587100
C 0 -4.94519500 -5.89957700 -3.53434500	C 0 -7.94758100 0.71692000 -2.85042900	H -1 -6.59175700 2.48663500 6.00383500
N 0 -3.99025300 -5.52348300 -2.64765500	C 0 -7.22103800 2.01280400 -2.58929000	H -1 -8.74423800 -0.45685400 -4.46173600
O 0 -6.13559000 -5.97602800 -3.22144100	C 0 -7.90753300 3.18020200 -2.23468200	H -1 -3.93361700 -7.22127800 -4.90913100
H 0 -3.78726200 -5.49480300 -5.32443100	C 0 -5.82947100 2.07990200 -2.74002200	H -1 5.62094700 0.56506900 -6.99714400
H 0 -5.32722200 -6.33819800 -5.58048000	C 0 -7.22488100 4.37991300 -2.02634700	H -1 -0.87597500 -3.93861200 -5.13859400
H 0 -4.30680300 -5.20395700 -1.74511400	C 0 -5.14397100 3.27593200 -2.53211800	H -1 -3.49108700 -0.01691600 8.66248400
H 0 -3.02372700 -5.32581100 -2.87696100	C 0 -5.83762100 4.43258600 -2.16926600	H -1 3.23688300 -4.91846800 3.39581500
C -1 -9.51276900 4.69472700 3.51479700	H 0 -9.38202700 1.21808800 -4.44483100	H 0 -0.04681200 -7.84111600 3.61264900
C 0 -9.39504600 4.71404500 1.97464500	H 0 -7.73448600 0.88186400 -5.01368200	H -1 4.79458900 3.43475900 5.61089100
C 0 -9.17641900 3.32928700 1.33377100	H 0 -8.76532300 0.59198400 -2.13205000	H -1 3.94026300 2.36590300 6.76170300
C 0 -8.33788200 5.73767200 1.54136100	H 0 -7.26113400 -0.11348400 -2.66871300	H 0 -8.02429200 -6.08420100 -0.58808700
C 0 -7.87633200 2.61145000 1.69394700	H 0 -8.98847100 3.14664700 -2.12196700	H -1 -3.73909200 -5.28574300 1.41882900
H 0 -8.53226200 4.76325900 3.99799600	H 0 -5.27231300 1.19823700 -3.03313000	C -1 7.65986100 6.51182600 1.46231500
H 0 10.36303900 5.06245600 1.58635100	H 0 -7.77688200 5.27514300 -1.75532600	H -1 8.03735800 7.53397800 1.34441200
H 0 10.02502100 2.68739800 1.60603000	H 0 -4.06593000 3.29084800 -2.65898700	H -1 7.23771900 6.39743100 2.46799700
H 0 -9.21780600 3.44773400 0.24511200	H 0 -5.30211200 5.35895200 -1.98961100	H 0 8.53384300 5.84940100 1.41845000
H 0 -8.24372000 5.78667500 0.45255400	C -1 -9.00159200 -5.64803600 -0.81471000	H 0 2.72449900 -2.99419800 1.64944400
H 0 -8.58852700 6.73982400 1.90646600	C 0 -8.83696500 -4.50801800 -1.83636900	C -1 0.21321300 5.31521600 5.81829900
H 0 -7.35434400 5.48117600 1.94764900	C 0 -8.03680000 -3.34675600 -1.27993600	C 0 -0.29492800 4.91323200 4.39901600
H 0 -7.79906200 1.66270800 1.15390600	C 0 -8.64482700 -2.38259800 -0.46572900	C 0 0.74892700 5.18008300 3.33577600
H 0 -6.99680800 3.20305700 1.42325900	C 0 -6.66277400 -3.22725200 -1.53725400	C 0 1.11769900 6.49838600 3.02748700
H 0 -7.82132000 2.39115900 2.76369600	C 0 -7.90884300 -1.32546800 0.06911200	C 0 1.40944700 4.14099800 2.67509100

C 0 2.10782000 6.76457600 2.08397800  
C 0 2.41504700 4.39491000 1.73678100  
C 0 2.76099300 5.71241000 1.43793400  
H -1 1.20083500 5.76754100 5.68311000  
H -1 0.29363000 4.43912100 6.47065300  
H 0 -0.44338700 6.04181600 6.30483900  
H 0 -0.57338600 3.85496200 4.37655300  
H 0 -1.20542600 5.46523300 4.14431100  
H 0 0.61723400 7.32113700 3.53246500  
H 0 1.12877400 3.11799200 2.90537700  
H 0 2.37129400 7.79217600 1.85034800  
H 0 2.93928200 3.58599400 1.23605200  
H 0 3.53120200 5.91424300 0.70272300  
C -1 5.39348400 -6.46284200 2.60177800  
C 0 4.56525000 -7.35423200 1.68820100  
O 0 3.36001300 -6.70979900 1.26238700  
H -1 6.25825600 -6.94026200 3.07441100  
H -1 4.75736900 -6.04475400 3.38876200  
H 0 5.77709400 -5.60812600 2.03084300  
H 0 5.15544900 -7.66065400 0.81298900  
H 0 4.24354800 -8.26469300 2.20338400  
H 0 3.53629100 -5.78630300 1.01554000  
H 0 -3.90750200 7.79701300 4.50645000  
C -1 -2.86925800 8.07027100 4.29766400  
C 0 -2.57882300 8.13565600 2.78972300  
C 0 -2.86496100 6.89213900 1.98174800  
C 0 -1.85732700 6.31473500 1.20098200  
C 0 -4.15593000 6.34766200 1.92246000  
C 0 -2.12308000 5.23288800 0.36257100  
C 0 -4.43153700 5.27231500 1.08042500  
C 0 -3.41785400 4.72078000 0.29586800  
H 0 -2.21578900 7.35989800 4.81112300  
H 0 -3.16641400 8.96398400 2.36991600  
H 0 -1.52870100 8.41325700 2.64596900  
H 0 -0.85362000 6.72457000 1.23760400  
H 0 -4.95553100 6.78767300 2.51376200  
H 0 -1.32674900 4.81450200 -0.24387000  
H 0 -5.43923800 4.87688200 1.00905200  
H 0 -3.65452000 3.90929500 -0.37829000  
H -1 -2.68588500 9.07772000 4.68651100  
C 0 0.24130600 -0.20914000 2.07609900  
C 0 1.36882900 0.56495800 1.47622000  
C 0 0.67501000 1.50622200 0.45498400  
H 0 1.00713100 1.20840500 -0.54378000  
H 0 0.92310500 2.56546300 0.54242000

H 0 0.42349200 -1.01812800 2.76601500  
H 0 1.77328600 1.17782000 2.30083200  
H 0 2.11712000 -0.91173400 0.34774000

### indene-Int<sub>1S,2R</sub>

H -1 2.58525100 -5.07724400 5.57883800  
H -1 -0.50584300 6.07316600 8.96305500  
H -1 -6.26393500 1.97615600 8.16823400  
H -1 -4.44282400 1.81714200 -11.17185700  
H -1 -4.49670600 0.19256700 -10.42683700  
C 0 -1.52201700 -1.00075400 -3.11076300  
C 0 -2.32420200 -0.85894100 -1.96989700  
C 0 -1.98445000 0.11879700 -1.05650400  
C 0 -0.86276400 0.97473200 -1.32621000  
C 0 -0.11722100 0.87476200 -2.53017200  
C 0 -0.43852600 -0.14343300 -3.40287600  
H 0 -1.74968000 -1.82026500 -3.78323600  
H 0 -3.16710900 -1.51868100 -1.81066200  
H 0 0.70341500 1.55826500 -2.69900800  
H 0 0.15134000 -0.30147500 -4.29883700  
O 0 1.27963800 -1.46078800 2.38069600  
O 0 -0.65726900 0.28370700 1.65059600  
H 0 3.04104400 5.68224000 3.83156500  
C -1 -3.95433100 -3.39475200 4.16131400  
C 0 -3.74859500 -4.53872100 3.16930500  
O 0 -4.63172500 -4.83180500 2.36175200  
C 0 -4.23334800 -2.05895300 3.47086800  
O 0 -3.16398000 -1.51148500 2.71509500  
H 0 -4.88987100 -3.65590000 4.67552400  
H 0 -5.11746500 -2.20046600 2.83588900  
H 0 -4.48205000 -1.30700500 4.22471400  
H 0 -2.68356800 -2.18389900 2.18847600  
N 0 -2.56557700 -5.20107500 3.23762200  
C 0 -2.41756500 -6.51027500 2.61688800  
C 0 -2.64857700 -6.63477400 1.10605900  
O 0 -3.01954800 -7.71415600 0.65329700  
H 0 -1.94168200 -4.99249900 4.01679200  
H 0 -1.39660700 -6.84818800 2.81870100  
N 0 -2.34205500 -5.57310800 0.32474700  
C -1 -2.51972000 -5.66236400 -1.12172900  
C 0 -2.57691300 -4.25522300 -1.71068600  
S 0 -3.13602500 -4.21802300 -3.46300200  
H 0 -2.09389400 -4.67914200 0.73734900  
H 0 -3.42469600 -6.23487200 -1.33539400  
H 0 -3.24498400 -3.62464600 -1.12536100

H 0 -1.59011700 -3.78556100 -1.69348900  
H 0 -4.45238600 -4.14915100 -3.17517200  
C -1 -0.05799400 5.07438700 8.99120600  
C 0 1.41460000 5.10086800 8.55654200  
C 0 2.07443500 3.73158300 8.76024200  
C 0 1.55950900 5.55603900 7.10146700  
H 0 -0.16790200 4.69187700 10.01298500  
H 0 -0.64358100 4.42453000 8.32877500  
H 0 1.94297300 5.82342400 9.19551800  
H 0 3.12193200 3.75186000 8.44354300  
H 0 2.03522200 3.41360800 9.80873900  
H 0 1.56380800 2.96852100 8.16101100  
H 0 2.60397600 5.60943400 6.78068500  
H 0 1.04559900 4.85186200 6.43440500  
H 0 1.11006000 6.54336200 6.94820300  
C -1 -6.09157000 0.90442900 8.31177900  
C 0 -4.64942400 0.52619600 7.94754700  
C 0 -4.35485400 -0.94452600 8.26478000  
C 0 -4.42936000 0.80864000 6.46035400  
H 0 -6.33874000 0.65024800 9.34770200  
H -1 -6.74881400 0.33654100 7.64495600  
H 0 -3.95712900 1.14897700 8.52996900  
H 0 -3.33253400 -1.21341800 7.98121600  
H 0 -4.48192400 -1.15992700 9.33131700  
H 0 -5.03440900 -1.60261800 7.70887800  
H 0 -3.42917200 0.52782300 6.12535600  
H 0 -5.14615800 0.23373200 5.86234100  
H 0 -4.58204500 1.86638600 6.22757800  
C -1 -7.93460300 -1.39727600 -3.13744400  
C 0 -7.01275900 -1.86365200 -2.03901300  
C 0 -6.75853700 -3.22736400 -1.84254000  
C 0 -6.40773400 -0.94198000 -1.17329400  
C 0 -5.93585300 -3.66198700 -0.80180700  
C 0 -5.58725300 -1.37192800 -0.13016500  
C 0 -5.34637100 -2.73422700 0.05726300  
H 0 -8.19711200 -2.21901400 -3.80941000  
H 0 -7.46818300 -0.61357900 -3.74133400  
H 0 -7.22442200 -3.95417000 -2.50333000  
H 0 -6.59451800 0.12041800 -1.31249200  
H 0 -5.75669600 -4.72077900 -0.64210800  
H 0 -5.14586300 -0.65118900 0.54939300  
H 0 -4.73005600 -3.09242500 0.87041000  
C -1 2.87163800 -4.05135900 5.32413000  
N 0 2.11223900 -4.41067100 2.84056500  
C 0 1.82347100 -4.64613600 1.52429900



O 0 2.49410900 -5.38369900 0.81255800	H 0 1.14550600 2.09725500 4.07755000	H 0 0.85870000 -1.36297300 -1.34369900
N 0 0.64475400 -4.06650900 0.98324700	H 0 1.28188900 0.32229000 4.02235000	N 0 3.81333700 -2.50385700 -0.42142600
C 0 -0.16061100 -3.16601900 1.61815900	H 0 1.60361400 1.62230800 6.41311300	C -1 4.81084400 -3.53598700 -0.65698500
C 0 0.51889400 -2.46815300 2.81672700	H 0 2.75411700 0.34711000 5.99676400	C 0 6.05427900 -3.00638400 -1.37326400
O 0 -1.27584900 -2.87155200 1.15943600	H 0 3.10872600 3.36461000 5.56109900	C 0 5.71982400 -2.42065700 -2.75258600
C 0 -0.10030900 -1.73659100 5.03870000	H 0 4.23602800 2.25852000 6.34674800	C 0 5.02373200 -3.46463300 -3.62531100
N 0 -0.53609500 -2.12806600 3.78941900	N 0 3.23913600 3.26195200 1.77581200	N 0 3.85256700 -3.05945800 -4.18977700
C 0 -0.75393100 -0.74582400 5.78623600	C 0 2.62311200 4.03308900 0.70021200	O 0 5.50981500 -4.57915000 -3.80066100
C 0 -0.35538700 -0.40318000 7.07749200	C 0 2.61570800 3.27162400 -0.62197800	H 0 4.10041700 -1.64344200 0.02569200
C 0 -1.00835200 0.74042900 7.81192300	O 0 1.69647800 3.43461900 -1.43589000	H 0 4.31580800 -4.26686900 -1.30079000
C 0 0.70997100 -1.10897500 7.67187200	C 0 3.27402100 5.43002300 0.57587300	H 0 6.55569500 -2.24550500 -0.76129900
C 0 1.17029700 -0.78162000 9.06973800	C 0 2.51631800 6.29072100 -0.45251700	H 0 6.75077600 -3.84097200 -1.50056300
C 0 1.38128500 -2.07745800 6.92484300	C 0 4.77799800 5.36641000 0.29050800	H 0 5.10281700 -1.52845800 -2.64687000
C 0 1.03084600 -2.37141500 5.60105100	C 0 2.70086300 7.79084500 -0.21481800	H 0 6.64658300 -2.13121900 -3.26274700
C 0 1.44644000 -3.48438300 3.48389900	H 0 3.78227000 3.78197700 2.48313700	H 0 3.35722100 -2.27457700 -3.77958100
N 0 1.74424900 -3.29335500 4.79861900	H 0 1.57054700 4.18470400 0.95122100	H 0 3.28434100 -3.78744500 -4.60311800
H 0 0.44706000 -4.31316200 0.01978600	H 0 3.14191200 5.88863700 1.56010600	C -1 4.61601200 -7.50943800 -2.27684500
H 0 -1.56513700 0.39975800 8.69302300	H 0 2.83960400 6.02574100 -1.46662100	C 0 3.19382100 -7.29711200 -2.76811100
H 0 -0.26129400 1.45672600 8.17109400	H 0 1.44965700 6.04995700 -0.41385900	N 0 2.38114700 -6.58500700 -1.95066700
H 0 -1.69972700 1.28342700 7.16666400	H 0 5.21275800 6.36944200 0.31497700	O 0 2.79950700 -7.76721500 -3.83865600
H 0 0.35211300 -0.84326300 9.79696600	H 0 5.30000500 4.76785700 1.04029700	H 0 5.06295700 -6.57121800 -1.93967000
H 0 1.95861800 -1.46582600 9.39487400	H 0 4.97351700 4.94001700 -0.69923900	H 0 5.20516300 -7.90337900 -3.10394300
H 0 1.57123500 0.23809600 9.13278500	H 0 2.14495500 8.37858700 -0.95288100	H 0 1.45172100 -6.38766800 -2.28820400
H 0 -1.56494600 -0.20903600 5.30356200	H 0 2.34129900 8.07148700 0.78177900	H 0 2.66609200 -6.10950700 -1.10115700
H 0 2.20993700 -2.59054100 7.39531300	H 0 3.75244800 8.08924200 -0.27896500	C -1 -4.10593700 1.21067900 -10.32450400
H 0 3.28887100 -3.55391500 6.19534800	N 0 3.65443800 2.44347900 -0.88400900	C 0 -2.56134200 1.21860800 -10.32598100
H 0 3.62954700 -4.11651400 4.54538800	C -1 3.68132300 1.66963000 -2.10967100	C 0 -1.92097000 -0.01679600 -9.66268000
C -1 6.36950300 2.82124500 4.77198400	C 0 2.94817200 0.31566300 -2.03137800	C 0 -2.04041700 2.54019100 -9.74830200
C 0 5.37798800 2.09780800 3.85057200	O 0 2.89202500 -0.38964800 -3.04945300	C 0 -2.21341400 -0.21848700 -8.17649500
O 0 5.73384100 1.68756000 2.74237300	C 0 5.12952400 1.39108900 -2.52769700	H 0 -4.51590500 1.63054000 -9.39994900
C 0 6.43065800 4.31256300 4.37002100	C 0 5.92027900 2.65280000 -2.84723000	H 0 -2.24489700 1.17773700 -11.37833000
C 0 5.07188000 4.97702600 4.63881400	O 0 5.68797100 0.68198000 -1.41426200	H 0 -2.24944300 -0.90860600 -10.21315600
O 0 4.28768000 5.06423600 3.60707100	H 0 4.34307300 2.25025700 -0.16531500	H 0 -0.83517300 0.04526100 -9.79885200
O 0 4.79190200 5.30984200 5.79440100	H -1 3.18309500 2.27744400 -2.87167200	H 0 -0.94717300 2.57757300 -9.74320400
H 0 6.09067100 2.75848600 5.82574500	H 0 5.08005200 0.74087500 -3.40983100	H 0 -2.40708100 3.39381100 -10.32911800
H 0 7.18985800 4.81471200 4.97618000	H 0 6.61020200 0.47433600 -1.60903900	H 0 -2.38108800 2.68000600 -8.71796900
H 0 6.69986800 4.39174800 3.31359500	H 0 6.94424800 2.39583300 -3.14021100	H 0 -1.69458800 -1.10503000 -7.79908100
N 0 4.07038300 2.01434300 4.24098200	H 0 5.46206000 3.19524100 -3.68016300	H 0 -1.86972100 0.62824400 -7.57584700
C 0 3.07099100 1.36900000 3.37790900	H 0 5.96574400 3.31480800 -1.97929000	H 0 -3.28264200 -0.35463300 -7.99146500
C 0 2.68396400 2.09572000 2.10613000	N 0 2.42877000 -0.04294600 -0.84878400	C -1 -6.02106700 0.91510100 -5.92272000
O 0 1.81094100 1.56501700 1.37344400	C 0 1.71571000 -1.29819000 -0.67311500	C 0 -4.60047700 0.56869500 -5.46566700
C 0 1.80650200 1.24440300 4.26356500	C 0 2.56481200 -2.53241600 -0.95064100	C 0 -4.17891200 1.43822200 -4.27328000
C 0 2.35877500 1.31950100 5.68661200	O 0 2.08977500 -3.49172700 -1.56539300	C 0 -4.47095100 -0.92407100 -5.14691000
C 0 3.48929100 2.33961800 5.55746900	H 0 2.40936500 0.61284300 -0.06763400	H 0 -6.71437700 0.87529500 -5.07267100
H 0 3.41623200 0.37707200 3.06763100	H 0 1.38701700 -1.33124800 0.37633900	H -1 -6.06575000 1.93643200 -6.31588700

H 0 -3.92014900 0.79773500 -6.29352700	H 0 1.74617100 -5.91104600 -4.51779300	H 0 -4.43504300 3.53201100 -1.66004300
H 0 -3.13168900 1.27173600 -4.00875200	H 0 -1.23863100 -3.41753000 -7.58668600	H 0 -4.22188600 4.83007300 -2.80412800
H 0 -4.28904000 2.50409800 -4.49693200	H 0 0.88943500 -3.66809600 -3.84910900	H 0 -3.38529500 7.14076600 -1.76871600
H 0 -4.79056400 1.20617300 -3.39170800	H 0 -0.58486900 -2.39777800 -5.43189300	H 0 -2.86337500 3.32558500 0.09512100
H 0 -3.43464100 -1.20107800 -4.94704800	C -1 -5.50257000 3.98764300 3.70107100	H 0 -1.50067000 8.05222800 -0.44797700
H 0 -5.05693700 -1.19555300 -4.26128100	C 0 -4.38105500 3.15770500 3.05789400	H 0 -0.97225100 4.25608600 1.46551200
H 0 -4.81819600 -1.54212500 -5.98204600	C 0 -3.07164600 3.35614600 3.83520700	H 0 -0.28904400 6.59278700 1.16500100
C 0 0.06259400 8.09514800 4.10693000	C 0 -4.77335700 1.67742400 2.95940800	C -1 -2.26507800 -4.08492000 7.45592900
C 0 -0.18127500 6.58066500 4.10318300	H 0 -5.57961400 3.74730300 4.76935000	C 0 -1.41713200 -5.24697900 6.96144500
C 0 1.00855000 5.72372500 3.68279700	H 0 -4.22182500 3.53642400 2.03949700	O 0 -0.90077900 -4.99924700 5.65094000
O 0 2.16066900 6.28330400 3.95445500	H 0 -2.24803900 2.77017500 3.41746600	H -1 -2.68229800 -4.21981100 8.45937700
O 0 0.84949900 4.60739200 3.18378900	H 0 -2.76046600 4.40546100 3.82992900	H -1 -3.09022500 -3.89491800 6.76187800
H 0 0.02763800 8.47428000 3.07688300	H 0 -3.18784900 3.04733100 4.87986100	H 0 -1.65715600 -3.17210600 7.48570600
H 0 1.07522900 8.28123600 4.47193200	H 0 -3.93501700 1.04344200 2.65905700	H 0 -0.59189500 -5.44827500 7.65966700
H 0 -0.42407600 6.25253200 5.12231700	H 0 -5.12626000 1.30432100 3.92440800	H 0 -2.00760500 -6.16423200 6.87719400
H 0 -1.03793400 6.30743700 3.48076300	H 0 -5.58725200 1.53233500 2.23921600	H 0 -0.42226800 -4.15649600 5.67113200
C -1 3.73018700 -2.47357100 -8.40730100	H -1 0.54697700 -9.39938300 -6.84295500	H 0 -4.74219000 6.09256100 -6.09808900
C 0 2.36961900 -2.13568000 -7.76901500	H -1 -6.40804200 0.21824200 -6.67334500	C -1 -4.45117300 6.70393600 -5.23912400
C 0 2.14921400 -0.66357200 -7.52450600	H -1 3.88996900 -3.54948600 -8.28140800	C 0 -2.92471100 6.79263200 -5.08787500
C 0 1.73189000 0.19426200 -8.54954600	H -1 4.62809000 -8.22694600 -1.44964500	C 0 -2.18702400 5.47769000 -4.98008400
C 0 2.38912700 -0.11656700 -6.25662000	H -1 7.34693700 2.34243500 4.64804700	C 0 -1.32063300 5.23660100 -3.90796900
C 0 1.54871100 1.55789700 -8.31536100	H -1 5.06248300 -4.09265000 0.25170600	C 0 -2.29267000 4.50719000 -5.98709600
C 0 2.20294900 1.24479400 -6.01825500	H -1 -8.86821300 -0.98378700 -2.74200300	C 0 -0.56426700 4.06616500 -3.83703900
C 0 1.77781200 2.08957800 -7.04540400	H -1 -3.19212000 -3.36772600 4.94730900	C 0 -1.53404100 3.34125600 -5.92755600
H 0 3.77157900 -2.21088400 -9.46846900	H 0 -3.10556900 -7.23752000 3.06038100	C 0 -0.66657500 3.12144100 -4.85702000
H 0 4.54157400 -1.95421500 -7.88857900	H -1 -5.28077400 5.05774400 3.62295400	H 0 -4.92509600 6.28476900 -4.34707700
H 0 1.56475800 -2.53574200 -8.39540900	H -1 -6.48700000 3.78741600 3.26494300	H 0 -2.52914900 7.34481500 -5.95168400
H 0 2.29384500 -2.66336900 -6.81528000	H 0 0.04911400 -8.47921000 -5.41715200	H 0 -2.68839500 7.40336700 -4.20949400
H 0 1.54955600 -0.21323300 -9.54107500	H -1 -1.66905800 -6.18789500 -1.56684000	H 0 -1.22616300 5.97778700 -3.12174600
H 0 2.73326200 -0.75126400 -5.44846000	C -1 -0.94942100 8.83613600 4.98175900	H 0 -2.95080100 4.67773800 -6.83560800
H 0 1.22837100 2.20673400 -9.12522800	H -1 -0.80322100 9.92147200 4.97371500	H 0 0.11104300 3.91530300 -3.00120100
H 0 2.39201400 1.63557500 -5.02321300	H -1 -1.97965700 8.60546800 4.68894500	H 0 -1.59548300 2.60880300 -6.72432400
H 0 1.61474400 3.14517100 -6.85484000	H 0 -0.84397400 8.51046500 6.02434100	H 0 -0.06398800 2.22402500 -4.84385700
C -1 0.22013000 -8.41368400 -6.49570900	H 0 -1.23581200 -1.50755700 3.38766900	H -1 -4.82528700 7.72111700 -5.39732300
C 0 1.25280300 -7.31001400 -6.79019500	C -1 -5.77776500 5.23142200 -1.30579600	C 0 -0.59059500 1.73422700 -0.20181900
C 0 0.74838800 -5.93155400 -6.40844000	C 0 -4.40980400 4.62296500 -1.74563400	C 0 -1.42626200 1.25920000 0.95431200
C 0 -0.10030600 -5.21654400 -7.26341200	C 0 -3.24507800 5.15851600 -0.94038100	C 0 -2.57375700 4.07996400 0.27322400
C 0 1.09151000 -5.35206100 -5.17748000	C 0 -2.85474000 6.49907100 -1.06957400	H 0 -3.45056000 1.12341800 0.12651100
C 0 -0.58558900 -3.95837100 -6.90732900	C 0 -2.55033200 4.35681100 -0.02815400	H 0 -2.87360200 -0.37289400 0.87870800
C 0 0.60735800 -4.09168300 -4.81091100	C 0 -1.79504100 7.01403200 -0.32428100	H 0 0.19482000 2.47432700 -0.13677700
C 0 -0.22711200 -3.38981100 -5.68481200	C 0 -1.49458700 4.86623400 0.73503300	H 0 -1.75918200 2.06643700 1.61120000
H 0 -0.73970700 -8.19014800 -6.97504500	C 0 -1.11172700 6.19828700 0.58009200	H 0 0.28170500 0.54289400 1.77442400
H 0 2.16868600 -7.52585800 -6.23423100	H -1 -5.57801700 5.99574500 -0.54774100	
H 0 1.49816600 -7.31670800 -7.86011600	H -1 -6.42587100 4.45482600 -0.88616400	
H 0 -0.37919800 -5.65059700 -8.22105100	H 0 -6.30812900 5.69832300 -2.14034200	

E:IO<sub>1S,2R</sub>

H -1 17.45619800 55.72339500 15.73978000

H -1 14.36508500 66.87380000 19.12396800	H 0 14.63319300 65.46574800 20.15360200	N 0 14.31802300 58.60091600 13.99690900
H -1 8.60699600 62.77679000 18.32913900	H 0 14.27596100 65.24328800 18.43335400	C 0 14.09160000 60.02787600 15.96705700
H -1 10.42809900 62.61775500 -1.01097900	H 0 16.78511200 66.65625700 19.48238200	C 0 14.53558900 60.43793800 17.22402500
H -1 10.37421900 60.99319700 -0.26593100	H 0 18.03485500 64.57416900 18.85646900	C 0 13.85662500 61.56725700 17.95473500
C 0 13.30561600 59.81931400 6.70821300	H 0 16.87332000 64.27833900 20.16813900	C 0 15.67069400 59.81508900 17.78352900
C 0 12.45761600 59.82942600 7.82107600	H 0 16.50124700 63.76841600 18.51440000	C 0 16.18775900 60.22926100 19.13730000
C 0 12.76813800 60.66259800 8.88240100	H 0 17.61534800 66.39024400 17.11234900	C 0 16.35433800 58.85099700 17.04460600
C 0 13.92382100 61.46219300 8.83766900	H 0 16.08237100 65.62467900 16.68537400	C 0 15.94303300 58.47956900 15.75901400
C 0 14.70360900 61.53327900 7.69185100	H 0 16.11708000 67.32288600 17.17060900	C 0 16.31359000 57.31690700 13.65686900
C 0 14.39660500 60.68367200 6.62331800	C -1 8.77936100 61.70506800 18.47267500	N 0 16.62895100 57.53091400 14.96190500
H 0 13.09292800 59.13019600 5.90323600	C 0 10.22002900 61.33436900 18.09463400	H 0 15.24467900 56.46609200 10.20482000
H 0 11.57635300 59.19908400 7.83728700	C 0 10.52593600 59.86478000 18.40594500	H 0 13.35461300 61.22077100 18.86572000
H 0 15.54651200 62.20991600 7.65646900	C 0 10.41903600 61.62280200 16.60543200	H 0 14.58160600 62.32737300 18.26320400
H 0 15.02897900 60.67752200 5.74160200	H 0 8.53953300 61.44843900 19.50938300	H 0 13.11343600 62.05742200 17.32636600
O 0 16.11762700 59.36396600 12.58650700	H -1 8.12211100 61.13717300 17.80584800	H 0 15.40937700 60.17117200 19.90620800
O 0 14.30337700 60.92771400 11.16805600	H 0 10.91463700 61.96013600 18.67108300	H 0 17.02028200 59.59527200 19.45247900
H 0 17.93317700 66.48740900 14.06011900	H 0 11.54726200 59.60171600 18.11393100	H 0 16.54586700 61.26578500 19.12616400
C -1 10.91651600 57.40593900 14.32213600	H 0 10.40952000 59.64621400 19.47292000	H 0 13.23052100 60.50215300 15.50782600
C 0 11.15459600 56.24688500 13.35572000	H 0 9.84519900 59.20378400 17.85489300	H 0 17.23663100 58.40838100 17.48726200
O 0 10.26447500 55.87150300 12.59388900	H 0 11.41774700 61.35522500 16.25494500	H 0 18.15925600 57.23709100 16.36079500
C 0 10.65601800 58.74955400 13.64539700	H 0 9.70061600 61.04286000 16.01440400	H 0 18.50793000 56.68499400 14.71302800
O 0 11.78348300 59.33337800 13.00429300	H 0 10.25336800 62.67889500 16.37580100	C -1 21.24040900 63.62192500 14.93284700
H 0 9.97872400 57.14131700 14.82843300	C -1 6.93651400 59.40332800 7.02372500	C 0 20.24049100 62.84302800 14.08436400
H 0 9.83296600 58.61957600 12.93324200	C 0 7.78211900 58.80067600 8.11274300	O 0 20.58035000 62.31531300 13.02234900
H 0 10.33684100 59.47682700 14.39530200	C 0 8.04489000 57.42620200 8.14695600	C 0 21.30685400 65.09187300 14.45832100
H 0 12.13019400 58.75041700 12.30120700	C 0 8.30484800 59.60676100 9.13220000	C 0 19.98256600 65.80052800 14.77064500
N 0 12.38026400 55.65846300 13.39486000	C 0 8.79123500 56.86634400 9.18440200	O 0 19.13709000 65.83925200 13.78694700
C 0 12.57626800 54.34484600 12.79158100	C 0 9.04582100 59.04968400 10.17217900	O 0 19.78108200 66.20374800 15.92061400
C 0 12.35769400 54.18463200 11.28104800	C 0 9.29130900 57.67561200 10.20514000	H 0 20.98846300 63.61242100 15.99601600
O 0 12.09661800 53.06740100 10.84690200	H 0 6.67741800 58.66218800 6.26287100	H 0 22.10989700 65.60107600 14.99837800
H 0 12.99165400 55.88501000 14.17831200	H 0 7.46028700 60.22149000 6.52093500	H 0 21.51984800 65.11590700 13.38632000
H 0 13.60696800 54.04499100 13.00293600	H 0 7.64659200 56.79034700 7.36032600	N 0 18.93771200 62.81380700 14.49155000
N 0 12.55176800 55.26084600 10.48262400	H 0 8.11723100 60.67760400 9.11353500	C 0 17.94328100 62.11371600 13.67717700
C -1 12.35118200 55.13828900 9.03914200	H 0 8.97672100 55.79656200 9.21057200	C 0 17.62824200 62.70191400 12.31406900
C 0 12.25116800 56.52254300 8.40417900	H 0 9.42697700 59.69041400 10.96067200	O 0 16.89264700 62.03138900 11.56492800
S 0 11.76857700 56.45162900 6.63221300	H 0 9.83588800 57.21764300 11.02145000	C 0 16.64698600 62.18115800 14.52223000
H 0 12.67437600 56.18198300 10.88526600	C -1 17.74257200 56.74932800 15.48498500	C 0 17.15894200 62.37704700 15.94930500
H 0 11.45488600 54.54185600 8.85117200	N 0 16.92774600 56.36614800 13.02054200	C 0 18.35298600 63.30850800 15.75091500
H 0 11.53127900 57.14669000 8.93478200	C 0 16.63059800 56.11700600 11.70042600	H 0 18.25301000 61.07933100 13.50118400
H 0 13.21170300 57.04374200 8.42856800	O 0 17.27252600 55.35271500 11.00713100	H 0 16.06182900 63.05507100 14.22054900
H 0 10.44305900 56.35923400 6.86527600	N 0 15.46069800 56.72654600 11.16224500	H 0 16.04630700 61.28626100 14.38174100
C -1 14.81292600 65.87500700 19.15206100	C 0 14.66470400 57.62220400 11.79663300	H 0 16.40248200 62.80712400 16.60780200
C 0 16.31318600 65.91310100 18.82338800	C 0 15.31785100 58.28030100 13.02647400	H 0 17.48546300 61.42407200 16.37672900
C 0 16.97073100 64.55790900 19.11255300	O 0 13.55650700 57.95230500 11.36932500	H 0 18.03185300 64.34600500 15.64113300
C 0 16.55373800 66.33919400 17.37191000	C 0 14.76929800 59.05008400 15.23103800	H 0 19.07566400 63.26524700 16.56587700

N 0 18.05283200 63.93287200 11.99261300	N 0 18.78956200 57.77616900 5.94596400	H 0 9.86020900 59.23989000 4.20780800
C 0 17.35510100 64.66089900 10.93421700	O 0 20.37590700 56.20740600 6.42292900	C 0 14.93235000 68.86979000 14.29473300
C 0 17.37190900 63.93230500 9.59680500	H 0 18.94813100 59.21037300 9.97199600	C 0 14.71332300 67.35520900 14.39781100
O 0 16.44339300 64.06438500 8.79530100	H 0 19.22534500 56.51869400 8.84864500	C 0 15.90495400 66.49819100 13.98848700
C 0 17.89949900 66.10479100 10.80866500	H 0 21.40852300 58.58321500 9.43516300	O 0 17.05221500 67.08639500 14.21487900
C 0 17.07096200 66.91758300 9.79473700	H 0 21.64212700 56.98509200 8.71330100	O 0 15.75575400 65.36091400 13.53731000
C 0 19.39962900 66.15773900 10.50227700	H 0 20.03426600 59.29424300 7.50273600	H 0 14.87144100 69.18103400 13.24353900
C 0 17.09634200 68.41882900 10.08819600	H 0 21.57100400 58.64768900 6.92546000	H 0 15.94796800 69.09481500 14.62788000
H 0 18.52616400 64.50015500 12.70857700	H 0 18.33137100 58.61939300 6.27756500	H 0 14.51503900 67.09266500 15.44544700
H 0 16.29973300 64.73563500 11.20744800	H 0 18.21627500 57.07589400 5.49464500	H 0 13.83993100 67.02759000 13.82787700
H 0 17.74830800 66.54808700 11.79654600	C -1 19.48692500 53.29115600 7.88413400	C -1 18.60110900 58.32705900 1.75350900
H 0 17.43714400 66.72447300 8.77916100	C 0 18.07354500 53.42951500 7.34139200	C 0 17.21210100 58.67684400 2.31291600
H 0 16.03539000 66.56913300 9.80175900	N 0 17.21806900 54.16584200 8.09649300	C 0 16.99545700 60.15224000 2.54364300
H 0 19.74737200 67.19484700 10.49878200	O 0 17.71664900 52.87466500 6.30060900	C 0 16.62044000 61.01115900 1.50343100
H 0 19.97827200 65.62364800 11.25860800	H 0 19.87948000 54.24810000 8.23487500	C 0 17.19562200 60.70044300 3.81728900
H 0 19.61531500 65.72804900 9.51855000	H 0 20.12439400 52.92293900 7.08125000	C 0 16.43537300 62.37589600 1.73107600
H 0 16.49494300 68.97298900 9.35992200	H 0 16.29952000 54.33039800 7.71345800	C 0 17.00809200 62.06222000 4.04990200
H 0 16.69295400 68.62499700 11.08645500	H 0 17.49959300 54.76293100 8.86334200	C 0 16.62015900 62.90722400 3.00869200
H 0 18.11284000 68.82575900 10.05860300	C -1 10.76499000 62.01135700 -0.16364400	H 0 18.70533100 58.59538700 0.69774300
N 0 18.46904200 63.18883900 9.30191500	C 0 12.30901800 62.03242200 -0.15096800	H 0 19.38415500 58.84305300 2.31789200
C -1 18.55217400 62.47014900 8.05122700	C 0 12.95732300 60.80380800 0.51712200	H 0 16.43878400 58.28421700 1.64349500
C 0 17.86174900 61.09628600 8.04032200	C 0 12.80880700 63.35721200 0.43936900	H 0 17.07762600 58.15177900 3.26096800
O 0 17.86977200 60.43271000 6.99336400	C 0 12.65542400 60.60094600 2.00129600	H 0 16.46909400 60.60397000 0.50651400
C 0 20.01994000 62.24968400 7.66717700	H 0 10.34690500 62.42925100 0.75830300	H 0 17.50288400 60.06443100 4.63871400
C 0 20.79087000 63.54315900 7.44273100	H 0 12.63712300 61.99909200 -1.20018900	H 0 16.14520500 63.02522100 0.91009500
O 0 20.56205900 61.49290700 8.76091700	H 0 12.64330400 59.90802600 -0.03580600	H 0 17.16087700 62.45220800 5.05116700
H 0 19.15385200 62.99693500 10.02317200	H 0 14.04312400 60.87912500 0.38903700	H 0 16.45070300 63.96259800 3.19499500
H -1 18.05401800 63.07810200 7.28924700	H 0 13.90152500 63.40717000 0.45372200	C -1 15.09103100 52.38698400 3.66528100
H 0 20.01702000 61.64490600 6.75211700	H 0 12.43650300 64.21017800 -0.13908200	C 0 16.13370700 53.46618600 3.32463600
H 0 21.50491000 61.35747400 8.60506300	H 0 12.45666600 63.48416000 1.46770700	C 0 15.67307300 54.85420700 3.71209100
H 0 21.82882200 63.32535000 7.16662100	H 0 13.19704800 59.73288500 2.38975000	C 0 14.82286500 55.58795900 2.87576700
H 0 20.34421200 64.12095500 6.62765100	H 0 12.96341300 61.46051000 2.60327900	C 0 16.05373200 55.41900700 4.93769400
H 0 20.79435900 64.15764600 8.34583700	H 0 11.58909400 60.43125200 2.17456700	C 0 14.37789600 56.85732400 3.24283100
N 0 17.30116500 60.66809900 9.18134200	C -1 8.84987500 61.71585600 4.23811700	C 0 15.60243700 56.68613800 5.31798600
C 0 16.56063900 59.42331700 9.19245200	C 0 10.25082600 61.32618100 4.70263300	C 0 14.77460500 57.41282800 4.45890100
C 0 17.42254200 58.17104000 9.15571200	C 0 10.70681300 62.20255800 5.87645800	H 0 14.12289300 52.61106900 3.20442900
O 0 16.95559000 57.13067100 8.68048700	C 0 10.28117700 59.82893700 5.03081100	H 0 17.06326200 53.23231600 3.85056200
H 0 17.24131400 61.27852600 10.00177300	H 0 8.14888200 61.68015100 5.08301300	H 0 16.34237900 53.44257000 2.24722200
H 0 15.94278300 59.41135600 10.08800600	H -1 8.80508600 62.73704400 3.84496300	H 0 14.51484000 55.16091100 1.92390800
H 0 15.90359600 59.36205600 8.32574100	H 0 10.94247000 61.50643000 3.87297100	H 0 16.71333500 54.84733000 5.58018400
N 0 18.65901200 58.27906400 9.69839700	H 0 11.74112100 61.99785200 6.15617300	H 0 13.73037500 57.41961900 2.57581100
C -1 19.68193700 57.26463500 9.50379800	H 0 10.63906500 63.26550900 5.62117800	H 0 15.89985300 57.09773000 6.27955300
C 0 20.93319100 57.81238400 8.81523100	H 0 10.07918200 62.02214800 6.75928200	H 0 14.46319700 58.41504300 4.72059800
C 0 20.62978800 58.38495000 7.42306200	H 0 11.29187300 59.46967000 5.20684300	C -1 9.36829900 64.78814000 13.86200000
C 0 19.92531000 57.34414100 6.55243000	H 0 9.69662800 59.60813300 5.93103600	C 0 10.45814500 63.93990700 13.19040000

C 0 11.79080400 64.09406500 13.93490900	H 0 14.50185200 67.04388000 11.63184500	C 0 14.18839100 61.78375500 8.84614600
C 0 10.00322800 62.47609400 13.09251200	C -1 12.60577800 56.71563300 17.61677000	C 0 13.22479400 60.84443200 9.24985800
H 0 9.29930300 64.54229300 14.92964300	C 0 13.45392500 55.55130600 17.12866800	C 0 12.79519500 59.84612300 8.38591100
H 0 10.60657300 64.31841200 12.17078700	O 0 14.01957500 55.82230000 15.84111000	C 0 13.38140700 59.75595800 7.12032400
H 0 12.59945000 63.52994000 13.46187800	H -1 12.18867400 56.58085100 18.62029400	H 0 14.83001300 60.57758300 5.74822800
H 0 12.10929100 65.14054200 13.96060700	H -1 11.78068100 56.90579100 16.92280000	H 0 15.52298300 62.40779900 7.29107000
H 0 11.70647300 63.74357400 14.96977000	H 0 13.21444200 57.62802400 17.64999000	H 0 12.01932000 59.15570000 8.68316100
H 0 10.79756100 61.80827600 12.75134900	H 0 14.25266600 55.32363800 17.84881900	H 0 13.06622300 58.96036900 6.45750900
H 0 9.66892800 62.10839700 14.06699500	H 0 12.85522900 54.64465300 17.00366000	O 0 16.05051600 59.36094000 12.58261800
H 0 9.15823200 62.37692400 12.40128400	H 0 14.49545300 56.66322500 15.90261200	O 0 14.00193500 60.97131700 11.57514900
H -1 15.41792600 51.40128200 3.31786800	H 0 10.15717400 66.89629400 4.05130100	H 0 17.90659200 66.45666400 14.08131300
H -1 8.46291300 61.01883100 3.48757000	C -1 10.41976500 67.50457300 4.92179500	C -1 10.91653300 57.40587200 14.32217700
H -1 18.76089600 57.25115400 1.87954400	C 0 11.94357100 67.60729900 5.10667900	C 0 11.16161300 56.33317200 13.26278900
H -1 19.49902500 52.57365100 8.71121700	C 0 12.68927900 66.29721700 5.21093400	O 0 10.34977800 56.16161100 12.35381200
H -1 22.21785100 63.14304300 14.80895000	C 0 13.40161900 65.97495100 6.37137900	C 0 10.62346800 58.77532700 13.71862900
H -1 19.93326300 56.70801500 10.41265800	C 0 12.73324200 65.40780200 4.12769200	O 0 11.73759300 59.37901800 13.06695700
H -1 6.00266400 59.81686100 7.41876200	C 0 14.14171500 64.79559900 6.46229600	H 0 9.99122000 57.08532700 14.82168700
H -1 11.67884500 57.43283000 15.10816000	C 0 13.48363600 64.23657500 4.20518800	H 0 9.78550000 58.67216300 13.02044400
H 0 11.91245200 53.60167000 13.24470500	C 0 14.18802700 63.93060500 5.37047100	H 0 10.32899800 59.47367100 14.50477700
H -1 9.59022600 65.85835500 13.78376500	H 0 9.92996500 67.07392500 5.79943900	H 0 12.09840500 58.79163000 12.37325400
H -1 8.38388800 64.58810300 13.42589100	H 0 12.34918700 68.17815600 4.26014900	N 0 12.28860600 55.58796100 13.40716300
H 0 14.95043800 52.33489400 4.74860300	H 0 12.15150600 68.20556400 6.00115600	C 0 12.42753100 54.27982100 12.77837500
H -1 13.20187200 54.61273000 8.59407100	H 0 13.38474000 66.65827500 7.21414500	C 0 12.32297100 54.14839700 11.25450400
C -1 13.92160200 69.63668600 15.14276400	H 0 12.19746300 65.64675600 3.21153300	O 0 12.09609600 53.03568700 10.79025900
H -1 14.06762400 70.72211400 15.13455000	H 0 14.69087300 64.57054000 7.37000600	H 0 12.86053000 55.74440400 14.23697700
H -1 12.89127000 69.40615800 14.84978300	H 0 13.54511300 63.56851200 3.35295900	H 0 13.41018300 53.89188300 13.06202900
H 0 14.01650400 69.32459100 16.19128300	H 0 14.77133400 63.02215300 5.41533500	N 0 12.56248600 55.23689600 10.48453800
H 0 13.46407200 59.04122700 13.64733000	H -1 10.04562400 68.52174100 4.76354500	C -1 12.35132100 55.13847100 9.03915700
C -1 9.09319100 66.03205600 8.85513700	C 0 14.17260900 62.02169900 10.19287300	C 0 12.23245600 56.53081700 8.43613500
C 0 10.46048800 65.43175500 8.41484000	C 0 13.04241100 61.59897800 11.04538200	S 0 11.66640600 56.51567200 6.68663300
C 0 11.59795200 65.86261200 9.31578700	C 0 12.03854200 60.84040700 10.19372300	H 0 12.55795800 56.15589600 10.90948400
C 0 11.94336800 67.22079200 9.39968700	H 0 11.12753000 61.43974300 10.06562400	H 0 11.45682300 54.54014100 8.84591400
C 0 12.32416300 64.94756300 10.08358800	H 0 11.73867200 59.89818500 10.64552400	H 0 11.53104000 57.13647600 9.01142400
C 0 12.98255900 67.64932200 10.22199700	H 0 14.81342700 62.87048000 10.37826500	H 0 13.19357100 57.04999000 8.44009700
C 0 13.35592200 65.37258900 10.92532800	H 0 12.72982800 62.15031800 11.92342000	H 0 10.34979400 56.56930600 6.97395800
C 0 13.68931500 66.72385900 10.99269500	H 0 15.56296100 60.08079100 12.20105600	C -1 14.81300000 65.87498100 19.15217900
H -1 9.29288900 66.79638500 9.61314900		C 0 16.30536500 65.91827700 18.79062400
H -1 8.44503800 65.25545300 9.27469600		C 0 16.98046700 64.57119600 19.07653500
H 0 8.55824200 66.49524000 8.02094900		C 0 16.51125600 66.33507000 17.33110600
H 0 10.41210300 64.33911800 8.38443500		H 0 14.65602500 65.47467600 20.16106300
H 0 10.69909900 65.74176400 7.39255500		H 0 14.26250400 65.23594700 18.45044500
H 0 11.39513100 67.94511500 8.80159200		H 0 16.78628600 66.67056100 19.43252900
H 0 12.08444800 63.89194200 10.01269300		H 0 18.03805100 64.59434500 18.79517800
H 0 13.24566200 68.70253300 10.26138200		H 0 16.91026200 64.30104100 20.13673100
H 0 13.90348300 64.66594800 11.53847600		H 0 16.50369300 63.77201500 18.49732400

E:IO<sub>1R,2S</sub>

H 0 17.56766900 66.40024300 17.05405700	C 0 16.36917400 58.84978000 17.06291600	C 0 19.49282400 66.20775300 10.51179000
H 0 16.03824000 65.60755700 16.65917300	C 0 15.94504800 58.48140500 15.78082100	C 0 17.27918100 68.57070900 10.40999700
H 0 16.05534300 67.31004200 17.12941000	C 0 16.28580600 57.31892300 13.67364500	H 0 18.57216100 64.50379100 12.69175900
C -1 8.77935900 61.70508800 18.47257500	N 0 16.62062400 57.53223900 14.97502600	H 0 16.37491400 64.80460700 11.14483500
C 0 10.22252300 61.34233300 18.09713900	H 0 15.12209600 56.41280600 10.26500900	H 0 17.91759500 66.53022100 11.91254500
C 0 10.52958700 59.86762600 18.38169600	H 0 13.38511200 61.21220700 18.91775000	H 0 17.42991900 66.97243100 8.94785800
C 0 10.43018200 61.66163200 16.61592600	H 0 14.60447600 62.32600000 18.31268100	H 0 16.10621100 66.79952500 10.06454900
H 0 8.53895800 61.44744700 19.50896900	H 0 13.13034600 62.05582300 17.38459700	H 0 19.89110900 67.22047700 10.61923000
H -1 8.12210600 61.13715600 17.80586400	H 0 15.45339500 60.16116700 19.93727300	H 0 20.08044000 65.55573400 11.16287600
H 0 10.91201900 61.95780800 18.69078700	H 0 17.06042700 59.58879100 19.46572700	H 0 19.64516000 65.89536800 9.47255800
H 0 11.55470900 59.61332300 18.09357200	H 0 16.58095200 61.26016100 19.15065800	H 0 16.63892500 69.20740500 9.78988600
H 0 10.40441100 59.62727100 19.44301900	H 0 13.23674900 60.51212700 15.55724600	H 0 16.98452100 68.70824700 11.45677000
H 0 9.85549100 59.21615800 17.81139700	H 0 17.25418200 58.40386500 17.49686000	H 0 18.30600300 68.93891600 10.31070200
H 0 11.43167100 61.40525200 16.26497700	H 0 18.16788500 57.23572300 16.35716500	N 0 18.48180700 63.18102300 9.30291500
H 0 9.71694100 61.09257600 16.00877200	H 0 18.49868300 56.68645200 14.70373100	C -1 18.55249500 62.47039000 8.05113600
H 0 10.26184700 62.72161600 16.40722700	C -1 21.24016800 63.62251200 14.93331500	C 0 17.85724400 61.09950600 8.04320600
C -1 6.93626200 59.40298400 7.02353400	C 0 20.23957700 62.85457600 14.07807700	O 0 17.85760200 60.43283800 6.99829900
C 0 7.96548000 59.32899700 8.12086300	O 0 20.57459300 62.34501400 13.00550600	C 0 20.01750200 62.24044200 7.65653200
C 0 8.29084300 58.11392400 8.73496700	C 0 21.30354000 65.09977700 14.48081700	C 0 20.79386700 63.53286300 7.44825400
C 0 8.57542700 60.50146300 8.58630300	C 0 19.97625700 65.79863900 14.80447500	O 0 20.55694000 61.46816300 8.74175100
C 0 9.18718200 58.06719500 9.80555100	O 0 19.12131800 65.82185500 13.82878600	H 0 19.10334600 62.91248700 10.05566900
C 0 9.48122600 60.46234400 9.64157800	O 0 19.78010900 66.20550000 15.95398700	H -1 18.05383900 63.07798100 7.28927200
C 0 9.78281600 59.24555600 10.25511300	H 0 20.98659400 63.59966400 15.99611500	H 0 20.00989500 61.64478400 6.73556100
H 0 6.71475600 58.41452800 6.61178900	H 0 22.10533800 65.60295000 15.02809200	H 0 21.50069800 61.33713000 8.58797700
H 0 7.26429200 60.04638300 6.20320800	H 0 21.51456000 65.14146700 13.40896300	H 0 21.83396700 63.31583900 7.17946000
H 0 7.81953000 57.19869300 8.38535300	N 0 18.93951600 62.81821200 14.49181500	H 0 20.35471600 64.11828400 6.63449400
H 0 8.33346600 61.45028700 8.11558700	C 0 17.94081300 62.14340300 13.66417200	H 0 20.78851900 64.13873800 8.35731800
H 0 9.41386100 57.13068900 10.30592700	C 0 17.64915700 62.73134400 12.29523700	N 0 17.30662800 60.67848900 9.19022900
H 0 9.95402600 61.37802100 9.98239900	O 0 16.91856600 62.04536900 11.55478100	C 0 16.56057000 59.43872900 9.22464500
H 0 10.48244900 59.21717800 11.07773200	C 0 16.63791800 62.23168300 14.49549700	C 0 17.41856700 58.18058300 9.17745500
C -1 17.74267500 56.74911300 15.48497500	C 0 17.14372600 62.37673400 15.93052500	O 0 16.94273600 57.14004600 8.71401300
N 0 16.89360900 56.37119900 13.02720000	C 0 18.36343700 63.28251700 15.76715100	H 0 17.26275800 61.29365100 10.00719800
C 0 16.56237200 56.10440700 11.71826000	H 0 18.22966700 61.10272100 13.48804300	H 0 15.97299600 59.43292100 10.14086100
O 0 17.18516500 55.33027000 11.01914400	H 0 16.08433100 63.13049600 14.20668400	H 0 15.87969500 59.37683100 8.37618700
N 0 15.37958500 56.70791000 11.20090900	H 0 16.00991500 61.35990600 14.32744000	N 0 18.66470300 58.28639800 9.70248100
C 0 14.59778200 57.61026900 11.84062100	H 0 16.39381400 62.80766300 16.59582500	C -1 19.68172300 57.26458200 9.50367400
C 0 15.27254300 58.27376300 13.05589800	H 0 17.44158900 61.40417400 16.33364000	C 0 20.93014600 57.80157900 8.80251900
O 0 13.48777500 57.95135700 11.42458200	H 0 18.07211500 64.33213000 15.69668600	C 0 20.61667000 58.37118400 7.41107300
C 0 14.76786400 59.05632300 15.26647400	H 0 19.08197700 63.18674200 16.58195900	C 0 19.89394700 57.33340200 6.55191800
N 0 14.28965200 58.60093800 14.04234900	N 0 18.09156500 63.95426400 11.96665200	N 0 18.75313200 57.77156600 5.96001000
C 0 14.10111600 60.03630100 16.00861300	C 0 17.43953200 64.73356200 10.90784400	O 0 20.33540100 56.19329000 6.41866100
C 0 14.55583000 60.44097600 17.26345400	C 0 17.51036700 64.10130300 9.52220900	H 0 18.96290900 59.21839500 9.96347200
C 0 13.87991500 61.56508400 18.00510400	O 0 16.72216800 64.44023500 8.63679000	H 0 19.21528900 56.51987300 8.85369300
C 0 15.69436600 59.81389200 17.81063700	C 0 18.00723700 66.17394400 10.88540400	H 0 21.41631000 58.57161000 9.41498500
C 0 16.22423300 60.22309100 19.16101900	C 0 17.15488800 67.10116600 10.00025100	H 0 21.63283600 56.96936000 8.69703500

H 0 20.03000400 59.28589000 7.49385200	H 0 14.90578200 69.24130800 13.25071700	H 0 11.67373500 63.86515800 15.06071300
H 0 21.55480600 58.62376700 6.90255900	H 0 15.94784800 69.07330800 14.65297300	H 0 10.98862500 61.87864300 12.80586900
H 0 18.30477700 58.61913900 6.29478100	H 0 14.43664200 67.06798500 15.34386000	H 0 9.77550000 62.09810800 14.05967000
H 0 18.17011200 57.07434700 5.51657300	H 0 13.82860600 67.08877000 13.69883900	H 0 9.33497800 62.33855500 12.36989300
C -1 19.48682000 53.29112800 7.88417700	C -1 18.60141900 58.32720800 1.75400100	H -1 15.41785300 51.40131600 3.31770100
C 0 18.07419900 53.43112200 7.33969400	C 0 17.20190800 58.66596600 2.30166500	H -1 8.46289300 61.01874000 3.48766700
N 0 17.21884200 54.17163600 8.09074900	C 0 16.98449400 60.13992600 2.53965200	H -1 18.76062400 57.25107300 1.87919000
O 0 17.71789100 52.87436000 6.29959300	C 0 16.61916700 61.00422000 1.50057400	H -1 19.49910000 52.57363700 8.71120300
H 0 19.87984100 54.24808800 8.23426900	C 0 17.18606900 60.68253300 3.81549000	H -1 22.21764100 63.14274400 14.80846000
H 0 20.12430500 52.92264700 7.08141300	C 0 16.44834000 62.37044600 1.73024800	H -1 19.93334500 56.70810200 10.41268900
H 0 16.29935300 54.33272600 7.70870800	C 0 17.01564300 62.04606500 4.04914400	H -1 6.00275800 59.81700300 7.41883100
H 0 17.49623700 54.76676200 8.86032400	C 0 16.64012100 62.89747800 3.00830600	H -1 11.67885300 57.43287600 15.10814700
C -1 10.76454500 62.01018900 -0.16232000	H 0 18.71366600 58.60047900 0.70058200	H 0 11.67730200 53.58058800 13.16325300
C 0 12.30945600 62.02145500 -0.17280400	H 0 19.37503600 58.84431700 2.32978200	H -1 9.59004700 65.85840000 13.78388400
C 0 12.96299200 60.79039500 0.48544900	H 0 16.43796500 58.27788700 1.61843800	H -1 8.38389500 64.58800000 13.42592400
C 0 12.82729500 63.34660300 0.39944600	H 0 17.05654100 58.13268600 3.24464300	H 0 14.97178700 52.33406200 4.75156800
C 0 12.68937000 60.58590500 1.97468400	H 0 16.46631400 60.60039700 0.50250500	H -1 13.20177600 54.61259800 8.59404900
H 0 10.35768100 62.42867700 0.76393300	H 0 17.48436400 60.04210600 4.63673900	C -1 13.92237900 69.63582100 15.14423300
H 0 12.61843900 61.98106400 -1.22765300	H 0 16.16591800 63.02451100 0.91031000	H -1 14.06700500 70.72219200 15.13387400
H 0 12.63492200 59.89625600 -0.06203000	H 0 17.17522600 62.43209800 5.05087600	H -1 12.89134100 69.40678200 14.84904000
H 0 14.04663400 60.86060000 0.33671200	H 0 16.48433200 63.95473700 3.19561100	H 0 14.01883800 69.31873000 16.19076700
H 0 13.92049700 63.38386700 0.41221700	C -1 15.09114300 52.38698400 3.66550400	H 0 13.45582000 59.08087100 13.69622000
H 0 12.46405300 64.19661400 -0.18904900	C 0 16.10515600 53.48987700 3.31059500	C -1 9.09325600 66.03228100 8.85515900
H 0 12.47861400 63.49200900 1.42596100	C 0 15.62974500 54.86318400 3.73881700	C 0 10.47914300 65.44899600 8.44117000
H 0 13.23718600 59.71600300 2.34995100	C 0 14.74071400 55.59900600 2.94547900	C 0 11.59602700 66.07910400 9.24407000
H 0 13.01284200 61.44289000 2.57179700	C 0 16.03217400 55.40895500 4.96652100	C 0 11.94185700 67.42369300 9.04000000
H 0 11.62640800 60.41944400 2.16996200	C 0 14.26822100 56.84379200 3.36218900	C 0 12.26410900 65.37189700 10.24649100
C -1 8.85008200 61.71623300 4.23763200	C 0 15.55510900 56.65138100 5.39621700	C 0 12.92970900 68.03430600 9.80934000
C 0 10.28239200 61.37235400 4.66511400	C 0 14.67614200 57.37517200 4.58596700	C 0 13.25641000 65.97480200 11.02628200
C 0 10.75291800 62.26305600 5.82277800	H 0 14.11005000 52.59721200 3.22562200	C 0 13.58926300 67.31084300 10.80628100
C 0 10.41702900 59.88646900 5.01185200	H 0 17.05404000 53.26516900 3.80531200	H -1 9.29284200 66.79633600 9.61320800
H 0 8.17113000 61.67391400 5.09902000	H 0 16.28275800 53.48881600 2.22742300	H -1 8.44509100 65.25538100 9.27464700
H -1 8.80496600 62.73713100 3.84520500	H 0 14.41717300 55.19102400 1.99038000	H 0 8.56888800 66.49769000 8.01596800
H 0 10.93601500 61.57930400 3.81015100	H 0 16.72434900 54.83882700 5.57538000	H 0 10.49939700 64.36385600 8.58102000
H 0 11.79680800 62.06403900 6.07811500	H 0 13.58108500 57.40149000 2.73212300	H 0 10.66847200 65.61459900 7.37597600
H 0 10.67348400 63.32515100 5.56824800	H 0 15.86883800 57.04408500 6.36072900	H 0 11.43085900 67.99121000 8.26622800
H 0 10.15296400 62.07690700 6.72108100	H 0 14.31957300 58.34906000 4.89788100	H 0 12.00640500 64.33025600 10.40781200
H 0 11.45575100 59.62036600 5.21179300	C -1 9.36856200 64.78825300 13.86182300	H 0 13.19126800 69.07324500 9.62980200
H 0 9.84256800 59.63608900 5.91066200	C 0 10.50186700 63.97406500 13.22432500	H 0 13.78319900 65.41601300 11.79480700
H 0 10.05973400 59.25100800 4.19320400	C 0 11.79645200 64.18977500 14.02138200	H 0 14.36348700 67.78194300 11.40126700
C 0 14.93626800 68.88258800 14.28771600	C 0 10.13398100 62.49069200 13.10404400	C -1 12.60587200 56.71568700 17.61686700
C 0 14.68483200 67.37047300 14.31736900	H 0 9.28932700 64.54892100 14.93059400	C 0 13.44875300 55.54742900 17.13076400
C 0 15.87386100 66.50333000 13.92411400	H 0 10.66767000 64.36427700 12.21281700	O 0 13.95626000 55.78124800 15.81182300
O 0 17.02276100 67.05813700 14.21548300	H 0 12.64025700 63.63165300 13.60733900	H -1 12.18860300 56.58082800 18.62026000
O 0 15.71687700 65.38341800 13.43270200	H 0 12.08168300 65.24625700 14.03483500	H -1 11.78069400 56.90577500 16.92277900

H 0 13.21583700 57.62715600 17.64688400	H 0 11.79277500 59.21132500 8.12891300	C 0 10.54746200 59.88270500 18.35757700
H 0 14.27983600 55.35331400 17.82340400	H 0 15.58070800 62.37387000 7.38881800	C 0 10.47744800 61.73662400 16.64996200
H 0 12.85779600 54.62981700 17.05973900	H 0 15.05115000 60.61604200 5.69541900	H 0 8.53433400 61.44524100 19.50816100
H 0 14.38954800 56.64699800 15.80819600	O 0 15.68654000 59.41907600 12.67739100	H -1 8.12213400 61.13718500 17.80581300
H 0 10.11374200 66.88475700 4.07308800	O 0 14.77374900 59.31379300 11.50835300	H 0 10.90016000 61.96401100 18.74583600
C -1 10.41950700 67.50426300 4.92095600	H 0 17.94339900 66.52817400 14.06479300	H 0 11.58368300 59.64888000 18.09526600
C 0 11.94926100 67.60758000 5.03478600	C -1 10.91655900 57.40594500 14.32228800	H 0 10.39128100 59.60563600 19.40628400
C 0 12.69959300 66.30061400 5.13130800	C 0 10.98170800 56.20199600 13.38050700	H 0 9.90099300 59.24394600 17.74317500
C 0 13.53175500 66.03647300 6.22506700	O 0 10.02673000 55.97003800 12.63390700	H 0 11.50564500 61.55034600 16.33355300
C 0 12.63393500 65.35988500 4.09390300	C 0 10.69472800 58.74480500 13.61013900	H 0 9.82661100 61.14518700 15.99670700
C 0 14.28802600 64.86592800 6.29064900	O 0 11.84357600 59.30957900 13.01768400	H 0 10.25983600 62.79239300 16.46344200
C 0 13.39298600 64.19408800 4.14974800	H 0 9.97768300 57.22327000 14.86765900	C -1 6.93632100 59.40334500 7.02342600
C 0 14.21923900 63.94650100 5.24541600	H 0 9.89787700 58.59231900 12.86956200	C 0 7.80421800 58.76287200 8.07662900
H 0 9.96924400 67.09051400 5.82749900	H 0 10.32876400 59.47456800 14.34112800	C 0 7.83172200 57.37107800 8.22987500
H 0 12.31647000 68.15975900 4.15854700	H 0 12.27835000 58.63579400 12.39625900	C 0 8.60876400 59.54193900 8.91910200
H 0 12.19949100 68.22555700 5.90428900	N 0 12.06052200 55.39310200 13.43861600	C 0 8.62527700 56.77272600 9.20968400
H 0 13.59744800 66.75869100 7.03216000	C 0 12.06492500 54.12210000 12.73573700	C 0 9.39909500 58.94765100 9.90325500
H 0 12.00452800 65.55369700 3.22825500	C 0 11.96092700 54.10068800 11.19798200	C 0 9.40797000 57.55998900 10.05526000
H 0 14.94081600 64.69463900 7.14028700	O 0 11.50433800 53.08110600 10.67681400	H 0 6.66491900 58.68138700 6.24693400
H 0 13.36325500 63.48132200 3.33378200	H 0 12.77741000 55.56663000 14.13603800	H 0 7.46148600 60.22703500 6.53205600
H 0 14.80755400 63.04079500 5.26677500	H 0 12.99492400 53.60996200 13.00043700	H 0 7.22436300 56.75340200 7.57208700
H -1 10.04587700 68.52193000 4.76417100	N 0 12.44348300 55.14953100 10.50005700	H 0 8.61919600 60.62252800 8.79738400
C 0 12.85993000 61.10178700 10.66757700	C -1 12.35122200 55.13832500 9.03916600	H 0 8.63750800 55.69279200 9.32375100
C 0 13.63197200 62.28400200 11.10174200	C 0 12.32544200 56.55771100 8.47567200	H 0 10.01747500 59.56101300 10.54972500
C 0 14.46971500 62.78212100 9.94113100	S 0 11.67319500 56.60490100 6.75360400	H 0 9.99774400 57.08552000 10.82906900
H 0 15.51360300 62.79134700 10.23473100	H 0 12.76439800 55.99819200 10.98536400	C -1 17.74268200 56.74912500 15.48507100
H 0 14.19962600 63.79751500 9.64689500	H 0 11.44939100 54.58639700 8.76685900	N 0 16.80166400 56.44394600 13.04009700
H 0 11.92454300 60.79402500 11.11008200	H 0 11.71936700 57.21542900 9.09600600	C 0 16.45682900 56.27670700 11.68634400
H 0 13.29805500 62.95867300 11.88101800	H 0 13.32514600 56.99562000 8.42192600	O 0 17.10717500 55.49767500 10.99512700
H 0 15.46171100 60.05592900 12.20839200	H 0 10.37226500 56.58405400 7.11199400	N 0 15.38326300 56.97027100 11.17987400

## E:indene<sub>1S,2R</sub>(OO)

H -1 17.45622100 55.72339900 15.73982000	C 0 16.29902100 65.91771000 18.76306000	C 0 14.73304600 58.99605800 15.47987700
H -1 14.36507800 66.87379900 19.12394600	C 0 16.97268600 64.56186700 19.00738900	O 0 13.21744900 57.59734300 11.68384800
H -1 8.60698900 62.77679000 18.32914400	C 0 16.48321700 66.35939500 17.30752500	C 0 14.73304600 58.99605800 15.47987700
H -1 10.42809700 62.61777800 -1.01096100	H 0 14.67425800 65.47916200 20.16565000	N 0 14.17385100 58.48370400 14.30620300
H -1 10.37422000 60.99319800 -0.26594200	H 0 14.25119900 65.23229400 18.46336700	C 0 14.09532500 59.96258200 16.25860200
C 0 13.40328400 59.80570100 6.82576300	H 0 16.79532700 66.65585400 19.41072800	C 0 14.62862100 60.39488900 17.47509700
C 0 12.62778200 59.88687100 7.98862300	H 0 18.02792500 64.59183400 18.71816200	C 0 13.95500900 61.48558200 18.26875100
C 0 12.95698700 60.83390000 8.94267600	H 0 16.90919500 64.26119900 20.06021300	C 0 15.82897600 59.81840700 17.93034600
C 0 14.03107800 61.72629200 8.72908200	H 0 16.49127300 63.78158500 18.40765900	C 0 16.45221600 60.26335000 19.22932700
C 0 14.76602300 61.67812500 7.54603200	H 0 17.53636000 66.42116800 17.01662600	C 0 16.47731800 58.86633900 17.14032100
C 0 14.45610500 60.69633100 6.60022800	H 0 15.99739300 65.64568900 16.63069100	C 0 15.96606300 58.46116700 15.90315200
H 0 13.17529200 59.02756100 6.10987500	H 0 16.02943100 67.34050700 17.13017000	C 0 16.20034100 57.33455400 13.75365900
	C -1 8.77933800 61.70507300 18.47268500	N 0 16.60060800 57.53085400 15.05518700
	C 0 10.23212800 61.36283500 18.11320600	H 0 15.19744300 56.79358400 10.20058000



H 0 13.55802500 61.11350500 19.22190900	H 0 17.40240000 66.90826100 8.87394900	C 0 18.05716900 53.45407100 7.38744300
H 0 14.65481900 62.29246400 18.51186000	H 0 16.07178300 66.76837300 9.98562200	N 0 17.21831700 54.14614200 8.19376800
H 0 13.12716400 61.92581400 17.71253100	H 0 19.84665300 67.22533400 10.55806600	O 0 17.68125100 52.93817400 6.33001300
H 0 15.75329400 60.17727700 20.06977200	H 0 20.04199000 65.57740900 11.15251100	H 0 19.90659700 54.24022000 8.22508500
H 0 17.33708800 59.66646600 19.46631400	H 0 19.61994600 65.86380200 9.44930500	H 0 20.09175500 52.91002200 7.06230000
H 0 16.76402700 61.31425700 19.18394400	H 0 16.59301900 69.16569200 9.64463000	H 0 16.29134700 54.32564400 7.83792500
H 0 13.17582200 60.39348100 15.87701200	H 0 16.94411800 68.72028000 11.32529600	H 0 17.49575200 54.71408400 8.98757100
H 0 17.41091900 58.45828200 17.50579300	H 0 18.26379900 68.92164200 10.17133400	C -1 10.76497100 62.01132200 -0.16366200
H 0 18.22221900 57.21440200 16.34214700	N 0 18.46092100 63.18206200 9.29941600	C 0 12.30922600 62.02712800 -0.16551300
H 0 18.45106500 56.68820400 14.65937100	C -1 18.55226300 62.47031600 8.05121400	C 0 12.96093800 60.80914400 0.51875700
C -1 21.24046800 63.62192400 14.93289600	C 0 17.88903100 61.09006700 8.00794300	C 0 12.81626000 63.36224300 0.39375000
C 0 20.24892800 62.85974800 14.05008200	O 0 17.97113300 60.43134700 6.95711500	C 0 12.66454400 60.62523500 2.00625800
O 0 20.61696300 62.35721400 12.98507500	C 0 20.02567800 62.27641300 7.66521100	H 0 10.35494600 62.42942500 0.76129500
C 0 21.31020500 65.10363300 14.50053000	C 0 20.77644500 63.58595300 7.46569800	H 0 12.62618400 61.97320800 -1.21793900
C 0 19.98290000 65.80938500 14.81695200	O 0 20.58081200 61.51419500 8.74853300	H 0 12.64580400 59.90565400 -0.02157500
O 0 19.15458600 65.87729000 13.82482200	H 0 19.07830600 62.92383400 10.05888000	H 0 14.04626000 60.88401000 0.38506600
O 0 19.77385400 66.18769200 15.97627100	H -1 18.05401800 63.07805900 7.28922000	H 0 13.90918000 63.40596200 0.40988900
H 0 20.97527800 63.58402700 15.99262900	H 0 20.03380200 61.68437300 6.74252400	H 0 12.44951400 64.20393200 -0.20516800
H 0 22.10902900 65.59859800 15.06106500	H 0 21.50969600 61.33763900 8.55635800	H 0 12.46330700 63.51479500 1.41761200
H 0 21.53141900 65.15749800 13.43118000	H 0 21.82114200 63.39129600 7.19585500	H 0 13.20697400 59.76197600 2.40345300
N 0 18.93925000 62.81738500 14.43194200	H 0 20.32526800 64.17001000 6.65706000	H 0 12.97495600 61.49092200 2.59749700
C 0 17.95225000 62.12051800 13.59591100	H 0 20.75946700 64.18310100 8.38010600	H 0 11.59926000 60.45785300 2.18676500
C 0 17.62641100 62.73248400 12.24287200	N 0 17.27983100 60.65088300 9.11131100	C -1 8.84984200 61.71580300 4.23806700
O 0 16.88583500 62.08739800 11.48943400	C 0 16.55911300 59.39509200 9.06669700	C 0 10.25976800 61.34916800 4.70663100
C 0 16.65401600 62.14491500 14.44039500	C 0 17.44167300 58.16227800 9.03548100	C 0 10.70844300 62.23688100 5.87514700
C 0 17.16191400 62.30971300 15.87231700	O 0 17.03666900 57.13630700 8.48342300	C 0 10.33676500 59.86037900 5.05812300
C 0 18.33756300 63.27060000 15.69936700	H 0 17.15027500 61.26347700 9.92164700	H 0 8.15067800 61.67803300 5.08409700
H 0 18.28442600 61.09701300 13.39811300	H 0 15.91373700 59.35366700 9.94422600	H -1 8.80513100 62.73707000 3.84502700
H 0 16.06184700 63.02135300 14.16021000	H 0 15.93475500 59.35034900 8.17463900	H 0 10.94700800 61.53773600 3.87452200
H 0 16.05724100 61.25325900 14.26068000	N 0 18.64100100 58.26129900 9.67240900	H 0 11.73481800 62.01382500 6.17360800
H 0 16.39583600 62.70250200 16.54365400	C -1 19.68172900 57.26468700 9.50387100	H 0 10.66198500 63.29849000 5.60809000
H 0 17.50696200 61.35215600 16.27404900	C 0 20.94137300 57.82372900 8.83530200	H 0 10.06683100 62.07579900 6.75118500
H 0 17.99437600 64.30350100 15.60798900	C 0 20.66469600 58.39542200 7.43647200	H 0 11.35650100 59.55734500 5.28805900
H 0 19.05854100 63.22717400 16.51621300	C 0 19.99609100 57.34867600 6.54503400	H 0 9.72961800 59.62799900 5.93996600
N 0 18.08126600 63.96625900 11.94083200	N 0 18.85558400 57.76034900 5.93142600	H 0 9.97734600 59.23781400 4.22990500
C 0 17.40592500 64.73071800 10.89474100	O 0 20.47970000 56.22604700 6.40234600	C 0 14.93818700 68.89999100 14.27383700
C 0 17.45317300 64.06000800 9.52647900	H 0 18.89880600 59.18424400 9.99791400	C 0 14.70685200 67.38525900 14.28123700
O 0 16.62777600 64.34875300 8.65629900	H 0 19.24415100 56.51182200 8.84283700	C 0 15.92124600 66.53406500 13.92715100
C 0 17.96828100 66.17102800 10.83808600	H 0 21.39582700 58.60169900 9.46282200	O 0 17.06002100 67.13358600 14.17908600
C 0 17.12009700 67.06949300 9.92032200	H 0 21.66306500 57.00476500 8.74872200	O 0 15.79192500 65.38774900 13.49986000
C 0 19.45708700 66.20615500 10.47711100	H 0 20.05363100 59.29507400 7.50426000	H 0 14.90148700 69.27358600 13.24232200
C 0 17.23832900 68.55190100 10.28269100	H 0 21.61535400 58.67190000 6.96340200	H 0 15.94852400 69.09752300 14.63896700
H 0 18.54180800 64.51150100 12.67647400	H 0 18.37281500 58.58091700 6.28809000	H 0 14.42125400 67.06688900 15.29299000
H 0 16.34426500 64.80098800 11.14776900	H 0 18.28526000 57.03803100 5.51140000	H 0 13.88087100 67.09442600 13.62662100
H 0 17.86782200 66.55324100 11.85604300	C -1 19.48695100 53.29109100 7.88410600	C -1 18.60108400 58.32705700 1.75355100

C 0 17.25415400 58.69283600 2.39783800	H -1 8.46288000 61.01889100 3.48753200	C -1 10.41975300 67.50455900 4.92176000
C 0 17.03851300 60.17627600 2.57164400	H -1 18.76091100 57.25115200 1.87950800	C 0 11.94988400 67.61726200 5.03895600
C 0 16.64519800 60.98683600 1.49930400	H -1 19.49901800 52.57367400 8.71123700	C 0 12.70508700 66.31303700 5.12440900
C 0 17.25173100 60.77954800 3.81795100	H -1 22.21783200 63.14301300 14.80891600	C 0 13.44474300 65.99284300 6.26821800
C 0 16.45503700 62.35910600 1.66892000	H -1 19.93338000 56.70798300 10.41260600	C 0 12.72602500 65.42707200 4.03837700
C 0 17.05717300 62.14933300 3.99219400	H -1 6.00269200 59.81684000 7.41885100	C 0 14.18671300 64.81405800 6.34069800
C 0 16.65201900 62.94613700 2.92025300	H -1 11.67886900 57.43283600 15.10813500	C 0 13.47701400 64.25556300 4.09958200
H 0 18.63562400 58.58225700 0.68932900	H 0 11.22977600 53.49549000 13.06456900	C 0 14.20477400 63.94768900 5.24893800
H 0 19.42304900 58.84462200 2.25802100	H -1 9.59009100 65.85838600 13.78381200	H 0 9.97101500 67.08828700 5.82759500
H 0 16.43926700 58.26249800 1.80569600	H -1 8.38390400 64.58801100 13.42589800	H 0 12.31345900 68.18199200 4.16888200
H 0 17.19354400 58.21164700 3.37635100	H 0 14.91900100 52.32758500 4.74354500	H 0 12.19141000 68.22555300 5.91776800
H 0 16.48079400 60.53454200 0.52373900	H -1 13.20185900 54.61271200 8.59407000	H 0 13.44483700 66.67527900 7.11159900
H 0 17.56797800 60.18492300 4.66690300	C -1 13.92147000 69.63677600 15.14262500	H 0 12.16887600 65.66773200 3.13494300
H 0 16.14890000 62.97019500 0.82422000	H -1 14.06772300 70.72210100 15.13462600	H 0 14.75728800 64.59132900 7.23553400
H 0 17.21354100 62.58388100 4.97442600	H -1 12.89126500 69.40610200 14.84984300	H 0 13.51941300 63.58550400 3.24833500
H 0 16.47409500 64.00681900 3.06449400	H 0 14.02498700 69.31239800 16.18626600	H 0 14.77721000 63.03259600 5.28455200
C -1 15.09109000 52.38696600 3.66518500	H 0 13.31833300 58.95477100 13.97607800	H -1 10.04562700 68.52174500 4.76357000
C 0 16.14572600 53.46755900 3.36467700	C -1 9.09318900 66.03208900 8.85510300	C 0 14.19276300 62.54140600 9.93321300
C 0 15.67009100 54.85817500 3.73020500	C 0 10.48677000 65.46466600 8.44774900	C 0 13.27940400 62.16973300 10.85059900
C 0 14.83125400 55.57650000 2.86898300	C 0 11.59939800 66.14335500 9.21981900	C 0 12.38254500 61.08655900 10.31105200
C 0 16.02509700 55.44161100 4.95503600	C 0 11.83082300 67.52010200 9.07102700	H 0 11.33327900 61.41308100 10.26576700
C 0 14.36650000 56.84491000 3.21516500	C 0 12.38524800 65.43495700 10.13150700	H 0 12.40779900 60.19400700 10.93866400
C 0 15.55919500 56.71085900 5.31164300	C 0 12.81789000 68.16402100 9.81492800	H 0 14.95008000 63.29954100 10.04725500
C 0 14.73562300 57.41812000 4.43211300	C 0 13.37358800 66.07305900 10.88626400	H 0 13.20048900 62.55998100 11.85576500
H 0 14.13653900 52.62107000 3.18090300	C 0 13.58873300 67.44250600 10.73071900	
H 0 17.05413300 53.23599300 3.92708000	H -1 9.29289800 66.79635700 9.61317400	
H 0 16.39541300 53.44210400 2.29533400	H -1 8.44503700 65.25545400 9.27469700	
H 0 14.54336700 55.13580100 1.91644100	H 0 8.56805400 66.49855300 8.01623200	H -1 17.45622500 55.72339900 15.73982200
H 0 16.67151100 54.88137100 5.62122300	H 0 10.53425600 64.38670600 8.62520800	H -1 14.36507800 66.87379900 19.12395100
H 0 13.72092500 57.39164300 2.53287900	H 0 10.66125700 65.59585500 7.37467900	H -1 8.60700200 62.77679200 18.32914000
H 0 15.84060600 57.13351900 6.27331700	H 0 11.23196000 68.08814300 8.36233200	H -1 10.42809600 62.61777900 -1.01096000
H 0 14.39687900 58.41517400 4.68268800	H 0 12.24672800 64.36614700 10.23838300	H -1 10.37421700 60.99319800 -0.26593400
C -1 9.36836700 64.78828500 13.86197100	H 0 12.98922200 69.22884800 9.68081600	C 0 14.36069400 60.61140400 6.70747100
C 0 10.49467200 63.99288300 13.18078500	H 0 13.97383800 65.50727500 11.59339300	C 0 14.69556700 61.60261100 7.63946000
C 0 11.81870900 64.23727500 13.91765400	H 0 14.35815100 67.94277600 11.30919000	C 0 13.96571800 61.69361300 8.81345600
C 0 10.15158200 62.50157400 13.08086800	C -1 12.60587300 56.71572300 17.61678800	C 0 12.84997900 60.85332100 9.03635400
H 0 9.30880400 64.53359600 14.92794300	C 0 13.46054400 55.56301500 17.10881900	C 0 12.50081400 59.88499100 8.09785600
H 0 10.61202800 64.38293200 12.16077700	O 0 13.85964800 55.74476200 15.75063600	C 0 13.28519400 59.75317400 6.94945100
H 0 12.66349600 63.75587800 13.41982000	H -1 12.18862000 56.58080200 18.62026400	H 0 14.95438200 60.50000000 5.80527600
H 0 12.04652600 65.30691600 13.97479500	H -1 11.78066400 56.90575200 16.92281200	H 0 15.52915900 62.27301400 7.46962900
H 0 11.77469500 63.84991400 14.94235800	H 0 13.20557500 57.63336600 17.64492400	H 0 11.64290700 59.23990000 8.24405200
H 0 10.99191700 61.90169800 12.72372100	H 0 14.34740200 55.43920400 17.74880300	H 0 13.04315600 58.96525300 6.24853500
H 0 9.86321500 62.10355800 14.05797200	H 0 12.90516100 54.61938700 17.13244300	O 0 15.70440600 59.41999400 12.68081200
H 0 9.30726800 62.33782900 12.40117400	H 0 14.06109400 56.67933800 15.58076600	O 0 14.79586200 59.33389900 11.50576500
H -1 15.41788900 51.40124500 3.31793700	H 0 10.12188000 66.88216900 4.07289200	H 0 17.92038900 66.49238200 14.07089600

## E:indene<sub>1R,2S</sub> (OO)

C -1 10.91653300 57.40593600 14.32228400	H 0 10.39631300 59.62413800 19.44730200	H 0 13.17648400 60.39893200 15.87056800
C 0 10.99348900 56.20665100 13.37669400	H 0 9.90055300 59.23292700 17.79235000	H 0 17.38966100 58.43229700 17.51638900
O 0 10.03954500 55.96952800 12.63100200	H 0 11.51319800 61.53692900 16.34738200	H 0 18.22192300 57.21732000 16.34059800
C 0 10.68640100 58.74251000 13.60141300	H 0 9.84595000 61.08878700 16.00979300	H 0 18.44956700 56.68819800 14.65799800
O 0 11.82405100 59.34185700 13.02007900	H 0 10.24000000 62.75333500 16.44716200	C -1 21.24047000 63.62193100 14.93288400
H 0 9.97640300 57.21910800 14.86338200	C -1 6.93635200 59.40335200 7.02350800	C 0 20.24865900 62.84803000 14.06392500
H 0 9.90169200 58.56705000 12.85256700	C 0 7.70693700 58.56392700 8.01167500	O 0 20.60759800 62.35092400 12.99318200
H 0 10.29398800 59.46567800 14.32500200	C 0 7.52983800 57.17596900 8.05823500	C 0 21.29953400 65.09867100 14.48237100
H 0 12.26298800 58.70758700 12.36693300	C 0 8.63195500 59.14561000 8.89007900	C 0 19.96988700 65.79774400 14.80355800
N 0 12.08022300 55.40835200 13.43548800	C 0 8.24090600 56.39111400 8.96757000	O 0 19.12613300 65.83930000 13.82234700
C 0 12.10170600 54.13387900 12.74029200	C 0 9.33773500 58.36365600 9.80510100	O 0 19.77255800 66.19486500 15.95833600
C 0 12.00678400 54.10062600 11.20307600	C 0 9.14379300 56.98112400 9.85324500	H 0 20.98046900 63.59513800 15.99416500
O 0 11.58157900 53.06485700 10.68662500	H 0 6.67509400 58.81966600 6.13495200	H 0 22.09961600 65.60531600 15.03030000
H 0 12.79393000 55.59068100 14.13381600	H 0 7.53672600 60.25328500 6.68714200	H 0 21.51089100 65.14070700 13.41053800
H 0 13.03492500 53.63248600 13.01382100	H 0 6.83196400 56.70717700 7.36795500	N 0 18.94608700 62.78770300 14.46436600
N 0 12.45435200 55.16102500 10.49995300	H 0 8.80793200 60.21767200 8.84941100	C 0 17.96265900 62.07847700 13.63828800
C -1 12.35122000 55.13832600 9.03915900	H 0 8.09383600 55.31508400 8.98774500	C 0 17.64942800 62.65939200 12.27069100
C 0 12.29957200 56.55370000 8.46938600	H 0 10.05489300 58.82529400 10.47708700	O 0 16.96341200 61.96104800 11.50945700
S 0 11.56633300 56.59445000 6.78101300	H 0 9.68163700 56.38180000 10.57828400	C 0 16.65865300 62.13485500 14.47131700
H 0 12.75778400 56.01984400 10.97995900	C -1 17.74268400 56.74912500 15.48507300	C 0 17.16180500 62.29907100 15.90500600
H 0 11.45264100 54.57448100 8.78049200	N 0 16.79600800 56.44374600 13.03432100	C 0 18.35303800 63.24188400 15.73601000
H 0 11.72481400 57.21308000 9.11686700	C 0 16.44828000 56.27914400 11.67960800	H 0 18.28506200 61.04742300 13.46597700
H 0 13.29474200 56.99262400 8.36655000	O 0 17.09231000 55.49419600 10.98864800	H 0 16.08699500 63.02232400 14.18212700
H 0 10.28549700 56.50384900 7.19603200	N 0 15.38110000 56.98156800 11.17267500	H 0 16.04644200 61.25330600 14.29345200
C -1 14.81292300 65.87502000 19.15209200	C 0 14.46907200 57.88083100 11.86420800	H 0 16.39819500 62.70620200 16.57039700
C 0 16.30236800 65.91566500 18.77644000	C 0 15.11088800 58.23834000 13.25262200	H 0 17.48915700 61.33768300 16.31182200
C 0 16.97205000 64.55998800 19.03286600	O 0 13.21866700 57.62553000 11.67433700	H 0 18.02850900 64.28155100 15.65431400
C 0 16.49867400 66.35075700 17.32070700	C 0 14.72807300 58.99600300 15.47522500	H 0 19.07410900 63.17742400 16.55197800
H 0 14.66500300 65.47637000 20.16326500	N 0 14.17231100 58.49376100 14.29685700	N 0 18.03273700 63.91413200 11.97005800
H 0 14.25644200 65.23444900 18.45714900	C 0 14.09129700 59.96182800 16.25615700	C 0 17.33359200 64.65661500 10.92061900
H 0 16.79363200 66.65606300 19.42536700	C 0 14.61950200 60.38536900 17.47796500	C 0 17.39190800 63.99033800 9.55138600
H 0 18.02934400 64.58603000 18.75069200	C 0 13.94897100 61.47769800 18.27211400	O 0 16.54823500 64.24776100 8.69004900
H 0 16.90112000 64.26571200 20.08696800	C 0 15.81302400 59.79899500 17.93815300	C 0 17.86873700 66.10833700 10.85544000
H 0 16.49306600 63.77678800 18.43501300	C 0 16.42958800 60.23177400 19.24444500	C 0 17.00829300 66.98156800 9.92529500
H 0 17.55363300 66.41046800 17.03622400	C 0 16.46162400 58.84861800 17.14615300	C 0 19.35840000 66.17178800 10.50114100
H 0 16.01667800 65.63473900 16.64363500	C 0 15.95811400 58.45429500 15.90212300	C 0 17.10650500 68.47099000 10.26358100
H 0 16.04762200 67.33162800 17.13567000	C 0 16.19618500 57.33351200 13.74986600	H 0 18.48376800 64.47510300 12.70033400
C -1 8.77934200 61.70506500 18.47267200	N 0 16.59714300 57.52793600 15.05305200	H 0 16.27177200 64.70471500 11.17649200
C 0 10.23281700 61.35789500 18.12310300	H 0 15.18273500 56.79193100 10.19847600	H 0 17.75484100 66.49701400 11.86938600
C 0 10.54893800 59.88242600 18.39326900	H 0 13.54255300 61.10489700 19.22098100	H 0 17.29262200 66.80874200 8.88130100
C 0 10.47976500 61.70669900 16.65491500	H 0 14.65357000 62.27794700 18.52352100	H 0 15.96449900 66.66729100 9.99666500
H 0 8.52884100 61.44765800 19.50768800	H 0 13.12848800 61.92698800 17.71228800	H 0 19.72550000 67.19934000 10.58012400
H -1 8.12212100 61.13718500 17.80582600	H 0 15.72440800 60.14408400 20.07950800	H 0 19.95336900 65.55962200 11.18264600
H 0 10.89843200 61.97050100 18.74730800	H 0 17.30940700 59.62827500 19.48364400	H 0 19.53312600 65.82884900 9.47568200
H 0 11.58420800 59.64400700 18.13129000	H 0 16.74772500 61.28127700 19.20871200	H 0 16.44478100 69.06372500 9.62244400

H 0 16.81992000 68.65195200 11.30619000	H 0 17.47754800 54.70656200 8.96057400	C 0 16.53208500 62.85003100 3.04044300
H 0 18.12448100 68.85555600 10.13596500	C -1 10.76497400 62.01132300 -0.16367200	H 0 18.78938700 58.61503000 0.71451800
N 0 18.44037400 63.16496000 9.30720500	C 0 12.31046900 62.00690000 -0.18658900	H 0 19.32681000 58.83979900 2.39231800
C -1 18.55225100 62.47031900 8.05123200	C 0 12.95289700 60.77124500 0.47520000	H 0 16.45280500 58.29154800 1.45347000
C 0 17.88897300 61.08913300 7.98127400	C 0 12.85161200 63.32976000 0.36849600	H 0 16.94985700 58.08569500 3.11428300
O 0 17.95610800 60.45859200 6.91226900	C 0 12.71228200 60.59399300 1.97356500	H 0 16.50323700 60.65040100 0.44169600
C 0 20.02959900 62.28661800 7.68100200	H 0 10.36726900 62.43137900 0.76540100	H 0 17.32930800 59.94259600 4.59668200
C 0 20.77256000 63.60060800 7.49857600	H 0 12.60790700 61.95364700 -1.24484200	H 0 16.15718200 63.05482400 0.92820700
O 0 20.57560000 61.51963700 8.76558800	H 0 12.59077000 59.87792700 -0.05252900	H 0 16.97958800 62.30848400 5.08682200
H 0 19.06826700 62.91686000 10.06129800	H 0 14.03416900 60.81406100 0.29971800	H 0 16.35005100 63.89635200 3.26273200
H -1 18.05402400 63.07805300 7.28921100	H 0 13.94501300 63.35361200 0.36240500	C -1 15.09109200 52.38695900 3.66518100
H 0 20.05004700 61.70106600 6.75416500	H 0 12.48736800 64.18025400 -0.21948200	C 0 16.13045400 53.47757200 3.34625300
H 0 21.50830200 61.35097000 8.58510600	H 0 12.52531600 63.48575300 1.40038800	C 0 15.65704300 54.86139600 3.74265500
H 0 21.82575500 63.41194300 7.23946400	H 0 13.21891100 59.69623900 2.34009200	C 0 14.77018900 55.57692300 2.92819100
H 0 20.33290000 64.18791100 6.68857900	H 0 13.10792100 61.43257500 2.55205100	C 0 16.06125500 55.43954300 4.95479000
H 0 20.74766300 64.19195900 8.41646700	H 0 11.64850100 60.49283700 2.20469300	C 0 14.30126800 56.83368900 3.31013900
N 0 17.28840100 60.63035000 9.08057300	C -1 8.84987500 61.71575800 4.23807600	C 0 15.59123600 56.69673500 5.34784500
C 0 16.56427200 59.37657700 9.03614100	C 0 10.26338200 61.35122400 4.69872500	C 0 14.71377400 57.39906200 4.51735300
C 0 17.44693700 58.14618600 9.01767100	C 0 10.68162800 62.18860200 5.91427200	H 0 14.12606900 52.61218100 3.19777700
O 0 17.05544400 57.11860200 8.45969100	C 0 10.36740900 59.84864400 4.97531800	H 0 17.05548000 53.24564400 3.88083500
H 0 17.20558700 61.21713700 9.91414700	H 0 8.15342400 61.67269600 5.08575200	H 0 16.35097000 53.46531400 2.27021900
H 0 15.91151600 59.34006700 9.90954300	H -1 8.80511700 62.73707100 3.84503000	H 0 14.44480900 55.14228300 1.98500600
H 0 15.94783400 59.33021600 8.13980000	H 0 10.95444200 61.59413200 3.88246600	H 0 16.74510800 54.88347900 5.58605700
N 0 18.63664400 58.25280100 9.66930100	H 0 11.71068600 61.97790900 6.21073000	H 0 13.61450800 57.37539000 2.66543700
C -1 19.68173000 57.26468200 9.50386700	H 0 10.60845000 63.26055200 5.70099300	H 0 15.90666500 57.10978700 6.30307100
C 0 20.94245600 57.83057000 8.84252700	H 0 10.03827500 61.96572100 6.77516600	H 0 14.36268800 58.38345500 4.80030700
C 0 20.66957300 58.41138700 7.44726000	H 0 11.39121300 59.55567600 5.20038100	C -1 9.36833200 64.78823100 13.86201500
C 0 20.00754900 57.37225900 6.54153000	H 0 9.75661200 59.55754700 5.83715400	C 0 10.49489900 63.96022600 13.22868900
N 0 18.88901200 57.80124900 5.90028600	H 0 10.02967400 59.26233700 4.11233800	C 0 11.79997600 64.19726600 14.00202400
O 0 20.48009100 56.24386600 6.40890500	C 0 14.93537100 68.88762600 14.28318900	C 0 10.11309800 62.47582100 13.15507200
H 0 18.88523400 59.17543100 10.00195200	C 0 14.69328600 67.37505900 14.31657500	H 0 9.28779400 64.55179700 14.93179400
H 0 19.25248200 56.51036800 8.83924300	C 0 15.89443800 66.51142200 13.95128100	H 0 10.64936800 64.32191500 12.20481100
H 0 21.39387600 58.60526800 9.47634700	O 0 17.03993300 67.10153700 14.19264000	H 0 12.64813000 63.66789400 13.56120300
H 0 21.66566200 57.01334900 8.75274600	O 0 15.75045900 65.36632200 13.52485100	H 0 12.05824800 65.26131900 14.01980400
H 0 20.05682300 59.30955800 7.51968600	H 0 14.89893200 69.24559900 13.24614700	H 0 11.70752300 63.85958300 15.04055000
H 0 21.62115000 58.69569400 6.98038300	H 0 15.94726300 69.08476300 14.64411500	H 0 10.95731100 61.83401800 12.89339400
H 0 18.41097700 58.62965900 6.24543800	H 0 14.42582100 67.07450300 15.33859900	H 0 9.72641100 62.12888500 14.11749100
H 0 18.31961800 57.08947100 5.46150700	H 0 13.85128000 67.08247200 13.68386400	H 0 9.32502700 62.31360400 12.41121700
C -1 19.48694500 53.29109200 7.88410500	C -1 18.60108400 58.32705600 1.75355100	H -1 15.41788800 51.40124400 3.31793900
C 0 18.06031900 53.44076700 7.37418700	C 0 17.16480500 58.65184400 2.20508400	H -1 8.46286600 61.01891000 3.48752200
N 0 17.20868600 54.12885900 8.17069100	C 0 16.92972100 60.11644200 2.48260800	H -1 18.76091100 57.25115200 1.87950800
O 0 17.69874100 52.91836100 6.31486000	C 0 16.60607000 61.01707800 1.46070300	H -1 19.49902300 52.57367500 8.71123800
H 0 19.89457600 54.24389900 8.22943900	C 0 17.06762600 60.61202100 3.78581100	H -1 22.21783000 63.14300700 14.80892700
H 0 20.10279100 52.91585500 7.06777900	C 0 16.40896100 62.37185600 1.73487600	H -1 19.93338200 56.70798700 10.41260800
H 0 16.28507500 54.30207100 7.80291200	C 0 16.87110500 61.96341900 4.06413900	H -1 6.00266800 59.81684700 7.41878600

H -1 11.67887500 57.43286800 15.10812900  
H 0 11.27148700 53.50022700 13.06869700  
H -1 9.59010400 65.85838600 13.78385500  
H -1 8.38392400 64.58804700 13.42583600  
H 0 14.93868700 52.32973400 4.74667900  
H -1 13.20186100 54.61271100 8.59407500  
C -1 13.92146600 69.63679200 15.14254900  
H -1 14.06772800 70.72210100 15.13466900  
H -1 12.89126300 69.40608900 14.84985900  
H 0 14.02071100 69.31685500 16.18817000  
H 0 13.31736000 58.96494400 13.96586300  
C -1 9.09314600 66.03208100 8.85507900  
C 0 10.48125700 65.45653600 8.43978600  
C 0 11.59263400 66.10518100 9.23600400  
C 0 11.90939100 67.45859300 9.04299600  
C 0 12.27972400 65.39789500 10.22510600  
C 0 12.88612100 68.08174500 9.81732200  
C 0 13.26070000 66.01419000 11.00765500  
C 0 13.56194500 67.36111800 10.80556300  
H -1 9.29288000 66.79639700 9.61313800  
H -1 8.44509300 65.25543700 9.27475100  
H 0 8.56615600 66.49863700 8.01720700  
H 0 10.51371300 64.37421500 8.59189200  
H 0 10.66406900 65.61390200 7.37210100  
H 0 11.38444800 68.02379800 8.27605400  
H 0 12.05312200 64.34764700 10.37310000  
H 0 13.12591500 69.12831200 9.64910200  
H 0 13.79744300 65.45001700 11.76533100  
H 0 14.32756900 67.84311000 11.40333100  
C -1 12.60588800 56.71574000 17.61679100  
C 0 13.46066800 55.56162800 17.11267500  
O 0 13.87098700 55.74552900 15.75835600  
H -1 12.18861100 56.58079500 18.62025900  
H -1 11.78066500 56.90572700 16.92280900  
H 0 13.20618300 57.63298200 17.64506000  
H 0 14.34203700 55.43366200 17.75951700  
H 0 12.90225500 54.61965700 17.12969500  
H 0 14.08002000 56.67939200 15.59674300  
H 0 10.09624400 66.87824800 4.08544100  
C -1 10.41976200 67.50458600 4.92176300  
C 0 11.95225000 67.58973300 5.01143200  
C 0 12.66719100 66.26491500 5.12739000  
C 0 13.46797500 65.97875700 6.23868100  
C 0 12.57326900 65.31395400 4.10207600  
C 0 14.15963700 64.77078900 6.33735400

C 0 13.26865800 64.11150300 4.19117400  
C 0 14.06003500 63.83811700 5.30633700  
H 0 9.98317100 67.10013300 5.83895200  
H 0 12.31681900 68.11809200 4.11903300  
H 0 12.22399500 68.21771900 5.86731800  
H 0 13.55021800 66.70719900 7.03888200  
H 0 11.96438900 65.52352100 3.22499700  
H 0 14.77799200 64.57091100 7.20587000  
H 0 13.20571300 63.38279100 3.39152400  
H 0 14.58421600 62.89613500 5.36728200  
H -1 10.04562200 68.52174200 4.76356000  
C 0 12.28131000 61.18839800 10.34186100  
C 0 13.02130600 62.15989400 10.91315000  
C 0 14.17062600 62.55691800 10.02754700  
H 0 15.11634800 62.31833400 10.52786800  
H 0 14.21676800 63.62372900 9.78897100  
H 0 11.44607800 60.67756000 10.80208100  
H 0 12.88021700 62.55667100 11.90806200

### indene-TS<sub>1R,2S</sub>(OO)

H -1 17.45637700 55.72341600 15.74005600  
H -1 14.36507400 66.87379700 19.12391800  
H -1 8.60693700 62.77682700 18.32947900  
H -1 10.42812500 62.61773700 -1.01100000  
H -1 10.37419500 60.99320900 -0.26596300  
C 0 14.39538700 60.84456500 6.67022600  
C 0 14.80243500 61.78278000 7.62877600  
C 0 14.23164200 61.75105900 8.88987200  
C 0 13.23802500 60.79763200 9.21004000  
C 0 12.79629400 59.89779500 8.24061600  
C 0 13.39525700 59.91891500 6.97920200  
H 0 14.86341800 60.83033600 5.69075600  
H 0 15.57513500 62.50893300 7.40772700  
H 0 12.00629600 59.19190800 8.45388500  
H 0 13.07639300 59.19069100 6.24455400  
O 0 15.94566400 59.32464600 12.55211100  
O 0 14.65435200 60.23293000 11.74672400  
H 0 17.92766400 66.50213500 14.12724800  
C -1 10.91671000 57.40581900 14.32196800  
C 0 11.05326000 56.29200000 13.28301300  
O 0 10.18793900 56.15221400 12.41759600  
C 0 10.62584100 58.76972900 13.70141700  
O 0 11.71779300 59.37204700 13.03625000  
H 0 9.99093900 57.12907700 14.85121000

H 0 9.77434700 58.64719700 13.01955000  
H 0 10.32732900 59.46846100 14.48900400  
H 0 12.18292200 58.72882800 12.45672400  
N 0 12.10802100 55.44964900 13.40758800  
C 0 12.11357700 54.15545300 12.74411400  
C 0 12.03709400 54.08527400 11.21065700  
O 0 11.64671500 53.03367400 10.70471500  
H 0 12.74839100 55.58519700 14.18773200  
H 0 13.03556400 53.64567400 13.03935600  
N 0 12.47331900 55.14403300 10.49651200  
C -1 12.35161600 55.13851600 9.03967600  
C 0 12.30174800 56.56580300 8.50255100  
S 0 11.66459600 56.65427800 6.77679500  
H 0 12.67429200 56.02581700 10.96395300  
H 0 11.44994800 54.58188100 8.77373600  
H 0 11.66294900 57.18788100 9.12837100  
H 0 13.28888800 57.03334400 8.48450500  
H 0 10.36855800 56.79209700 7.12578500  
C -1 14.81293900 65.87501900 19.15213100  
C 0 16.30475700 65.91118200 18.78629700  
C 0 16.96627800 64.54996200 19.03602400  
C 0 16.51294900 66.35431300 17.33497100  
H 0 14.65729100 65.47336800 20.16108500  
H 0 14.25973600 65.23707200 18.45203300  
H 0 16.79564400 66.64442300 19.44372500  
H 0 18.02592900 64.57475900 18.76286900  
H 0 16.88520700 64.24601000 20.08673300  
H 0 16.49009200 63.77402600 18.42622700  
H 0 17.57025100 66.41253200 17.05916500  
H 0 16.03523400 65.64244600 16.65062700  
H 0 16.06562000 67.33690600 17.15037200  
C -1 8.77948100 61.70530900 18.47205400  
C 0 10.22360000 61.35715700 18.07988700  
C 0 10.52973100 59.87126600 18.30008900  
C 0 10.44041200 61.74155000 16.61385200  
H 0 8.54900700 61.44155200 19.50951200  
H -1 8.12207200 61.13700400 17.80602700  
H 0 10.91307700 61.94446500 18.70180300  
H 0 11.55741500 59.63249000 18.00984100  
H 0 10.39475400 59.58230700 19.34866800  
H 0 9.86294900 59.24601400 17.69313400  
H 0 11.43834200 61.47952400 16.25723500  
H 0 9.72103500 61.21573100 15.97592600  
H 0 10.29710200 62.81416100 16.45248200  
C -1 6.93656700 59.40371000 7.02328400

C 0 7.95920400 59.23066200 8.11797400	O 0 20.61406500 62.37452000 12.98572800	C 0 20.01600600 62.25809800 7.63792800
C 0 8.21110200 57.97462800 8.68397800	C 0 21.30503200 65.10318400 14.50223700	C 0 20.77040600 63.56065800 7.40680300
C 0 8.66000000 60.33950900 8.60993200	C 0 19.98482700 65.80302400 14.85395200	O 0 20.58990400 61.50708300 8.71943200
C 0 9.12976100 57.82749900 9.72635900	O 0 19.13033000 65.85919600 13.88366300	H 0 19.09850900 62.89359200 10.05291200
C 0 9.58958500 60.19922800 9.63727000	O 0 19.80269400 66.18499700 16.01633800	H -1 18.05374200 63.07815500 7.28947700
C 0 9.82263500 58.94249800 10.19800900	H 0 20.97930700 63.58706500 15.99432500	H 0 20.00242800 61.65448300 6.72243600
H 0 6.69710300 58.44766500 6.54793100	H 0 22.11630900 65.59520900 15.04710800	H 0 21.51794000 61.33762200 8.51706200
H 0 7.29308300 60.08383200 6.24547600	H 0 21.50122600 65.16091900 13.42835900	H 0 21.81108800 63.35757200 7.12713200
H 0 7.67290200 57.10593600 8.31143000	N 0 18.96782600 62.76131800 14.48817600	H 0 20.31126100 64.13291900 6.59423300
H 0 8.48119300 61.31866600 8.17337100	C 0 17.99287800 62.09295400 13.63042800	H 0 20.76588700 64.17263500 8.31174800
H 0 9.31165500 56.86024800 10.18405300	C 0 17.77498900 62.68741200 12.25774300	N 0 17.30835000 60.64609500 9.14578900
H 0 10.14865700 61.05938800 9.98953500	O 0 17.16536200 61.96983800 11.46037400	C 0 16.54437600 59.41247100 9.19549100
H 0 10.54852500 58.83098300 10.99085300	C 0 16.66106900 62.19523200 14.40525800	C 0 17.40889200 58.16177600 9.14384300
C -1 17.74213300 56.74941100 15.48443500	C 0 17.12214500 62.29546100 15.86094100	O 0 16.97239700 57.12333400 8.63432400
N 0 16.94057700 56.41614000 13.01332700	C 0 18.36898400 63.18127600 15.76818900	H 0 17.28625200 61.24074200 9.97929700
C 0 16.60340500 56.15058300 11.70473600	H 0 18.26861900 61.04773700 13.46452200	H 0 15.94585400 59.44660200 10.11657400
O 0 17.25389600 55.40186200 10.99316200	H 0 16.14568000 63.11761800 14.11925300	H 0 15.86852500 59.35393500 8.34148200
N 0 15.39513100 56.70196400 11.20899800	H 0 16.02323500 61.34565900 14.16674200	N 0 18.64596200 58.26480000 9.69717900
C 0 14.55088900 57.51640500 11.91018300	H 0 16.35995700 62.72427400 16.51468200	C -1 19.68219900 57.26476800 9.50385100
C 0 15.25475500 58.26749500 13.05963500	H 0 17.38405900 61.30678600 16.24956300	C 0 20.94080800 57.83347200 8.84394900
O 0 13.36997800 57.65854400 11.58332800	H 0 18.10420700 64.24084500 15.73877300	C 0 20.66175600 58.43452100 7.45942000
C 0 14.76736300 59.05081200 15.28757600	H 0 19.06478100 63.03019700 16.59651200	C 0 19.99216700 57.41022800 6.54466000
N 0 14.25990400 58.59231500 14.08203000	N 0 18.13550200 63.95764900 11.98173000	N 0 18.85652000 57.84311200 5.93995100
C 0 14.11864200 60.03688200 16.04074300	C 0 17.45671500 64.71710600 10.92826100	O 0 20.46996100 56.28795500 6.37694300
C 0 14.56779000 60.41720100 17.30551700	C 0 17.50877400 64.08403600 9.54121000	H 0 18.91075100 59.18250500 10.03157900
C 0 13.90053200 61.54192900 18.05605800	O 0 16.69848700 64.41998700 8.67426600	H 0 19.24187300 56.52093900 8.83546900
C 0 15.68713100 59.76242400 17.85461000	C 0 18.01053900 66.16286400 10.89540500	H 0 21.39815600 58.59664100 9.48695300
C 0 16.21246300 60.14160800 19.21615000	C 0 17.15422100 67.08042400 10.00479000	H 0 21.65938800 57.01391900 8.73926800
C 0 16.35206600 58.79747200 17.09539100	C 0 19.49686600 66.20643100 10.52499800	H 0 20.05025500 59.33140700 7.54983300
C 0 15.93855700 58.45770600 15.80269200	C 0 17.26165800 68.55218600 10.41213600	H 0 21.61091100 58.72368300 6.99071800
C 0 16.28398500 57.32673200 13.67556600	H 0 18.54003800 64.51937000 12.73735800	H 0 18.37694100 58.66521900 6.30224000
N 0 16.61694900 57.52478100 14.98494000	H 0 16.39370700 64.77918100 11.17493900	H 0 18.29503300 57.14191500 5.47573500
H 0 15.13167700 56.39214000 10.28104500	H 0 17.91750400 66.52369500 11.92131900	C -1 19.48677300 53.29134100 7.88421400
H 0 13.39741200 61.18904200 18.96519100	H 0 17.43632700 66.95269800 8.95400100	C 0 18.07208600 53.38419800 7.33223900
H 0 14.63016400 62.29535500 18.37234700	H 0 16.10882400 66.76807900 10.06223000	N 0 17.22229800 54.20011400 7.99943800
H 0 13.15799400 62.04483400 17.43585900	H 0 19.88969500 67.22237100 10.62931400	O 0 17.72035000 52.71700600 6.35418900
H 0 15.43760300 60.07566000 19.98952000	H 0 20.08349000 65.55684000 11.17903300	H 0 19.85470800 54.25546200 8.24102500
H 0 17.03905200 59.49057300 19.51429600	H 0 19.65247300 65.88910200 9.48777200	H 0 20.13917700 52.93120100 7.08931200
H 0 16.58386500 61.17431300 19.22981400	H 0 16.61698300 69.18226400 9.78906900	H 0 16.29834600 54.31445300 7.61047800
H 0 13.26246300 60.52826500 15.58956500	H 0 16.96158800 68.68799300 11.45774900	H 0 17.48776500 54.85599000 8.72580900
H 0 17.22425800 58.32815100 17.53189500	H 0 18.28585500 68.93033000 10.31750700	C -1 10.76495200 62.01137800 -0.16357800
H 0 18.17787300 57.23478700 16.35329500	N 0 18.49889500 63.19159900 9.29448600	C 0 12.31008700 62.03608400 -0.16504200
H 0 18.48930800 56.68388200 14.69490400	C -1 18.55257700 62.47011400 8.05094000	C 0 12.97510100 60.81227700 0.49486000
C -1 21.24028200 63.62187800 14.93290000	C 0 17.86671800 61.08701200 8.01987900	C 0 12.81100300 63.36330300 0.41892500
C 0 20.25891300 62.84957500 14.06866100	O 0 17.89485500 60.44901100 6.95206400	C 0 12.70562400 60.60976000 1.98503300

H 0 10.35277300 62.42857400 0.76094500	H 0 17.47996000 60.06900900 4.62794200	C -1 13.92176200 69.63662000 15.14277900
H 0 12.62599200 62.00408800 -1.21866700	H 0 16.20115300 63.02928500 0.86796300	H -1 14.06752400 70.72212700 15.13444400
H 0 12.65655200 59.91341600 -0.05110800	H 0 17.19444400 62.45792200 5.01811200	H -1 12.89124800 69.40616400 14.84985100
H 0 14.05783100 60.89472700 0.34531600	H 0 16.52267800 63.97462100 3.14835700	H 0 14.02401300 69.31500000 16.18742600
H 0 13.90389400 63.41391900 0.42883700	C -1 15.09099300 52.38682900 3.66572200	H 0 13.56038100 59.21951300 13.68252400
H 0 12.43463800 64.21495400 -0.15955300	C 0 15.86534500 53.53582300 2.99525000	C -1 9.09341400 66.03208000 8.85525100
H 0 12.46461800 63.49173300 1.44859000	C 0 15.55888800 54.87452100 3.63533900	C 0 10.47871300 65.43495700 8.45583900
H 0 13.27673900 59.75739300 2.36472200	C 0 14.64642000 55.77300800 3.07310000	C 0 11.59811700 66.04383900 9.27320800
H 0 13.00519600 61.47759700 2.57892200	C 0 16.15713700 55.20547200 4.86082600	C 0 11.89234800 67.41047900 9.14145100
H 0 11.64757500 60.41554100 2.18098600	C 0 14.33879400 56.97604700 3.71468400	C 0 12.32837700 65.29477200 10.20031900
C -1 8.84970700 61.71521300 4.23864800	C 0 15.84242000 56.39851500 5.51437700	C 0 12.88794000 68.00827100 9.91014200
C 0 10.27427300 61.35590100 4.67012500	C 0 14.93875200 57.29314500 4.93278900	C 0 13.32495300 65.88954900 10.98207200
C 0 10.76631100 62.26385300 5.80482400	H 0 14.01340700 52.48478800 3.49814500	C 0 13.60493200 67.24762200 10.83688000
C 0 10.36586900 59.87363500 5.04455800	H 0 16.93830200 53.33350900 3.08852500	H -1 9.29286700 66.79634500 9.61319300
H 0 8.16753800 61.67529300 5.09760500	H 0 15.63527600 53.57202400 1.92281100	H -1 8.44494600 65.25546000 9.27456500
H -1 8.80510600 62.73704300 3.84495900	H 0 14.16907800 55.52767900 2.12652800	H 0 8.57454300 66.49476300 8.01071300
H 0 10.92952700 61.52907800 3.80901200	H 0 16.85659900 54.50154500 5.30046200	H 0 10.48406400 64.34919500 8.58695000
H 0 11.80077000 62.03907300 6.07405800	H 0 13.62292300 57.66064300 3.26869600	H 0 10.68269600 65.60628600 7.39362700
H 0 10.71821900 63.32016500 5.51794300	H 0 16.28555500 56.63234200 6.47913800	H 0 11.33495300 68.00555200 8.42127500
H 0 10.15632400 62.12305800 6.70478000	H 0 14.71274000 58.22503800 5.43504100	H 0 12.12582200 64.23301700 10.30694800
H 0 11.39537400 59.57506500 5.23652300	C -1 9.36843700 64.78773700 13.86205200	H 0 13.10985100 69.06476500 9.78530000
H 0 9.79800900 59.66041600 5.95628100	C 0 10.47935800 64.01439200 13.13308800	H 0 13.89049300 65.30482300 11.70086500
H 0 9.97312100 59.23626900 4.24283400	C 0 11.82378700 64.22658100 13.83947500	H 0 14.38535100 67.70624800 11.43335500
C 0 14.93149100 68.89082800 14.27769600	C 0 10.15185000 62.52703800 12.96915800	C -1 12.60587200 56.71571500 17.61671100
C 0 14.69725200 67.37729500 14.31754700	H 0 9.32517400 64.51751800 14.92429400	C 0 13.46582500 55.57135000 17.10212900
C 0 15.90487200 66.53089500 13.93749800	H 0 10.56722400 64.44702900 12.12788400	O 0 13.86048600 55.77495300 15.74383900
O 0 17.04127200 67.10495600 14.24927500	H 0 12.64523400 63.76298400 13.28993700	H -1 12.18864100 56.58078800 18.62027000
O 0 15.77386200 65.41418800 13.43881700	H 0 12.05830600 65.29157200 13.93874600	H -1 11.78066300 56.90568800 16.92283000
H 0 14.88425300 69.24525900 13.23973400	H 0 11.81050100 63.79115600 14.84578400	H 0 13.20281300 57.63603300 17.64482500
H 0 15.94524200 69.09270700 14.63051900	H 0 10.95830000 61.99296000 12.46174600	H 0 14.35410300 55.44304100 17.73815600
H 0 14.44789000 67.07900500 15.34483100	H 0 10.00391800 62.04530800 13.94039500	H 0 12.91621900 54.62453500 17.10892200
H 0 13.85108400 67.07668000 13.69476400	H 0 9.23436500 62.38462200 12.38622500	H 0 14.15806000 56.69076900 15.62592500
C -1 18.60128900 58.32715800 1.75389300	H -1 15.41797000 51.40141100 3.31754300	H 0 10.13632900 66.88478700 4.06612900
C 0 17.20234100 58.67421100 2.29765100	H -1 8.46290100 61.01912300 3.48730700	C -1 10.41969300 67.50445300 4.92177900
C 0 16.99548400 60.15196400 2.52347800	H -1 18.76070900 57.25109500 1.87928700	C 0 11.94666700 67.63476800 5.05717500
C 0 16.64019600 61.01031000 1.47565500	H -1 19.49907800 52.57353000 8.71111100	C 0 12.72623700 66.34591300 5.14911700
C 0 17.19758900 60.70240700 3.79565500	H -1 22.21787600 63.14311100 14.80889400	C 0 13.49533100 66.06287300 6.28323900
C 0 16.47924100 62.37979300 1.69366900	H -1 19.93308900 56.70789500 10.41263300	C 0 12.75076500 65.44525800 4.07530600
C 0 17.03828700 62.06918900 4.01724600	H -1 6.00264300 59.81677600 7.41880000	C 0 14.27487800 64.90906700 6.35652700
C 0 16.67289800 62.91512400 2.96841300	H -1 11.67866500 57.43304900 15.10832000	C 0 13.53697900 64.29701600 4.13736800
H 0 18.71743400 58.60051900 0.70036800	H 0 11.27239400 53.54006800 13.08175400	C 0 14.29763300 64.02950500 5.27553700
H 0 19.37419600 58.84274500 2.33204600	H -1 9.59012000 65.85838800 13.78392700	H 0 9.96331300 67.08183600 5.82079600
H 0 16.43714600 58.28509900 1.61586200	H -1 8.38391100 64.58830100 13.42574900	H 0 12.31168900 68.20766700 4.19283700
H 0 17.05271000 58.14897100 3.24435200	H 0 15.27368100 52.41239900 4.74428200	H 0 12.16900400 68.24638100 5.93894700
H 0 16.48529700 60.59873200 0.48066100	H -1 13.20157500 54.61249400 8.59378600	H 0 13.49016800 66.75585500 7.11810600

H 0 12.16975800 65.65686900 3.17974500	O 0 11.55074500 53.04938700 10.71560600	H 0 6.68906300 58.88183300 6.09387600
H 0 14.87103900 64.71471400 7.24153700	H 0 12.81643700 55.67041000 14.08126400	H 0 7.56883800 60.25586300 6.75973800
H 0 13.58029600 63.61452200 3.29552800	H 0 13.07548800 53.68050400 13.00979500	H 0 6.88050700 56.67534300 7.11390100
H 0 14.90110200 63.13503100 5.31066800	N 0 12.43478100 55.13712300 10.49755100	H 0 8.64412200 60.07296100 9.05259600
H -1 10.04568700 68.52177200 4.76359300	C -1 12.35142800 55.13824700 9.03939700	H 0 8.04064600 55.16715600 8.69982300
C 0 12.89837400 60.93897200 10.62036800	C 0 12.29692700 56.57060600 8.50280300	H 0 9.78830400 58.56767100 10.64225700
C 0 13.68174100 61.92440600 11.17660400	S 0 11.65944300 56.65366900 6.77840500	H 0 9.47184500 56.11846300 10.51286900
C 0 14.53532400 62.56850400 10.11643600	H 0 12.76370200 55.98211500 10.96074800	C -1 17.74253600 56.74914000 15.48492800
H 0 15.58022200 62.51667200 10.40596400	H 0 11.45316700 54.58293000 8.75966300	N 0 17.03572100 56.31325600 13.01802300
H 0 14.30379700 63.62675200 9.96171600	H 0 11.65724300 57.19241600 9.12895600	C 0 16.77220900 56.04372900 11.69247800
H 0 12.14377400 60.37730800 11.14021100	H 0 13.28370600 57.03859600 8.48321100	O 0 17.49641800 55.33158100 11.00899800
H 0 13.58748900 62.31526000 12.17788300	H 0 10.35955700 56.53393500 7.12352900	N 0 15.57282300 56.54328800 11.14814800

## indene-TS<sub>1S,2R</sub> (OO)

H -1 17.45630700 55.72339600 15.73989200	C 0 16.27951200 65.90060800 18.69466900	C 0 15.34750700 58.14794900 12.96294200
H -1 14.36523200 66.87387500 19.12420100	C 0 16.93355700 64.52136600 18.84635400	O 0 13.56435000 57.58063500 11.38536300
H -1 8.60701300 62.77678700 18.32909200	C 0 16.41082500 66.39349800 17.25042100	C 0 14.75434600 59.00878600 15.12916200
H -1 10.42817600 62.61803500 -1.01080900	H 0 14.71661600 65.49327200 20.17566500	N 0 14.29773900 58.55670900 13.89378100
H -1 10.37418900 60.99323700 -0.26622300	H 0 14.21814200 65.22499700 18.49760100	C 0 14.08579700 60.01512700 15.83953200
C 0 13.80552400 60.58218800 6.99606300	H 0 16.82308300 66.60087500 19.34661200	C 0 14.49464800 60.41881500 17.11002900
C 0 12.90289300 60.09520500 7.95314500	H 0 17.97821300 64.55087200 18.52157600	C 0 13.82722700 61.57814400 17.80476700
C 0 12.96445800 60.60658100 9.24107300	H 0 16.89924600 64.16482400 19.88317100	C 0 15.57501700 59.57663800 17.72571600
C 0 13.89945600 61.60979700 9.57788600	H 0 16.41788000 63.78323100 18.22074600	C 0 16.04449600 60.15386900 19.10227400
C 0 14.75390000 62.13428900 8.61112700	H 0 17.45342100 66.44477600 16.92239200	C 0 16.25170000 58.76484500 17.01789100
C 0 14.71788200 61.58718000 7.32723300	H 0 15.88690100 65.71031000 16.57039800	C 0 15.89253900 58.41485600 15.71015400
H 0 13.78686000 60.18912300 5.98394100	H 0 15.96666000 67.38746700 17.12627200	C 0 16.34031700 57.22988200 13.63429500
H 0 12.18575000 59.32654800 7.68355200	C -1 8.77915700 61.70508600 18.47253500	N 0 16.62027900 57.47893600 14.93951500
H 0 15.44794300 62.92682700 8.85722300	C 0 10.21044100 61.38745900 18.00419900	H 0 15.41885400 56.33418400 10.16760200
H 0 15.42805500 61.92652300 6.58280000	C 0 10.49223300 59.88073000 18.00308600	H 0 13.28320100 61.26281500 18.70387600
O 0 16.07705700 59.19961200 12.47008500	C 0 10.39619300 61.97923000 16.60148700	H 0 14.56370300 62.32192400 18.12835900
O 0 14.75996800 60.23946500 11.91422000	H 0 8.58399700 61.42357300 19.51111800	H 0 13.12319800 62.08168500 17.14279600
H 0 17.98871000 66.61265400 14.03416100	H -1 8.12205400 61.13704500 17.80601300	H 0 15.23431200 60.11641800 19.84056600
C -1 10.91615300 57.40508900 14.32280700	H 0 10.92853900 61.87056100 18.67997200	H 0 16.84518100 59.49511300 19.45015400
C 0 10.93555700 56.15947300 13.44396800	H 0 11.50610200 59.66579900 17.65357800	H 0 16.43276800 61.18027400 19.11291500
O 0 9.94332600 55.84413700 12.78472900	H 0 10.37335800 59.44651200 19.00225000	H 0 13.23934900 60.48735300 15.35422900
C 0 11.04389900 58.66405200 13.46155500	H 0 9.79743500 59.35775900 17.33281700	H 0 17.09357500 58.28657500 17.50111400
O 0 11.19120800 59.83530600 14.26388400	H 0 11.32676700 61.65986800 16.13098100	H 0 18.13693600 57.25236700 16.36300500
H 0 9.93828200 57.40721000 14.82122500	H 0 9.57248600 61.66939500 15.94478800	H 0 18.51868500 56.68516900 14.72387700
H 0 11.93882800 58.59512700 12.84692500	H 0 10.38540700 63.07323600 16.62285100	C -1 21.24093000 63.62205000 14.93270700
H 0 10.17513200 58.74786100 12.79737600	C -1 6.93637300 59.40333300 7.02376000	C 0 20.26830600 62.94153300 13.95626300
H 0 10.36942600 59.97943900 14.74830000	C 0 7.65269700 58.48470100 7.98496600	O 0 20.67041900 62.54620900 12.85809600
N 0 12.09699100 55.45653200 13.39475200	C 0 7.50974900 57.09446900 7.89575000	C 0 21.33437600 65.12854800 14.60417300
C 0 12.12429100 54.15392500 12.74830000	C 0 8.49282400 58.99851700 8.98250100	C 0 19.98541400 65.81349500 14.87755000
C 0 11.98951700 54.08435100 11.21601900	C 0 8.16510000 56.24257800 8.78860000	O 0 19.24453000 65.98958100 13.83309200
	C 0 9.14063000 58.15032100 9.88010700	O 0 19.68543600 66.08067600 16.04909100
	C 0 8.97746300 56.76579100 9.79606700	H 0 20.93585000 63.51557600 15.97640500



H 0 22.09422900 65.58540200 15.24605900	H 0 21.50573900 61.27182500 8.44991200	H 0 12.76075900 63.56382500 1.14231300
H 0 21.62271700 65.25318900 13.55710700	H 0 21.79670600 63.23109500 6.97124800	H 0 13.37111000 59.85229600 2.36229400
N 0 18.94608300 62.87447000 14.29157200	H 0 20.29693000 64.03808200 6.48626100	H 0 13.52436500 61.59756800 2.37418900
C 0 17.96169800 62.27709600 13.37005200	H 0 20.83241700 64.10859500 8.17943800	H 0 11.91366300 60.85007200 2.34379500
C 0 17.62843900 63.05014600 12.10583700	N 0 17.32113700 60.71121700 9.29790900	C -1 8.84989500 61.71596800 4.23799900
O 0 16.77840300 62.56986600 11.34103700	C 0 16.55789500 59.47292600 9.34172000	C 0 10.25482000 61.38753700 4.75673900
C 0 16.66423100 62.15326600 14.20514700	C 0 17.41323300 58.22042900 9.21736100	C 0 10.58394400 62.25912400 5.97633900
C 0 17.17059400 62.15399200 15.64767500	O 0 16.94148400 57.19583000 8.70633400	C 0 10.41201700 59.89749400 5.07563800
C 0 18.32301600 63.15916700 15.59733700	H 0 17.16929400 61.38315600 10.05800900	H 0 8.13455400 61.67764200 5.07106900
H 0 18.30982100 61.29149900 13.04373700	H 0 16.00222500 59.47122600 10.28580700	H -1 8.80497200 62.73703000 3.84493700
H 0 16.04790200 63.04130200 14.03499700	H 0 15.84819100 59.43846000 8.51324000	H 0 10.97534300 61.64141800 3.96970000
H 0 16.09673600 61.27715700 13.89423900	N 0 18.67289800 58.29373100 9.71905600	H 0 11.60245800 62.08814500 6.32980400
H 0 16.39963400 62.44275500 16.36494200	C -1 19.68142700 57.26488700 9.50391000	H 0 10.48757000 63.32394500 5.74147000
H 0 17.54023100 61.16299800 15.93192600	C 0 20.93462900 57.80150900 8.80963700	H 0 9.90090300 62.02789600 6.80453500
H 0 17.95535700 64.18863100 15.62462400	C 0 20.63273300 58.37442200 7.41626100	H 0 11.43146100 59.66134900 5.38751900
H 0 19.04030100 63.03953500 16.40973700	C 0 19.91415300 57.33170100 6.56273200	H 0 9.75073500 59.59118700 5.89407600
N 0 18.24016800 64.21607700 11.83319200	N 0 18.71448600 57.72653600 6.06542900	H 0 10.17599500 59.27453200 4.20497200
C 0 17.68960000 65.03062900 10.75570500	O 0 20.40172800 56.21910900 6.36218000	C 0 14.94061400 68.93033900 14.24666900
C 0 17.68817100 64.30550200 9.40760500	H 0 18.96722900 59.20459200 10.04824800	C 0 14.74192200 67.41099000 14.20316900
O 0 16.93711500 64.67691900 8.50236800	H 0 19.20353200 56.52778300 8.85433200	C 0 15.97962200 66.60180700 13.82221900
C 0 18.41990800 66.39149000 10.70173200	H 0 21.41507200 58.57172300 9.42682600	O 0 17.10356000 67.20172000 14.14140900
C 0 17.72046900 67.36884100 9.74173300	H 0 21.64035100 56.97044600 8.70800600	O 0 15.88014400 65.48739000 13.31488300
C 0 19.91338600 66.23093400 10.39307800	H 0 20.03908200 59.28410300 7.50107400	H 0 14.89227300 69.33366000 13.22672400
C 0 18.11287600 68.82724900 9.99178400	H 0 21.57411400 58.62668300 6.91318500	H 0 15.94961300 69.13382400 14.61275400
H 0 18.73555800 64.70726700 12.58497200	H 0 18.25379700 58.54836900 6.44897000	H 0 14.46167300 67.05297000 15.20267500
H 0 16.63241900 65.21817100 10.96433200	H 0 18.12420900 57.00500400 5.67340900	H 0 13.92871600 67.12062500 13.53215200
H 0 18.33242800 66.79965700 11.71377400	C -1 19.48691500 53.29112900 7.88408300	C -1 18.60119600 58.32712600 1.75383700
H 0 17.93462400 67.08719800 8.70505500	C 0 18.06280600 53.42596200 7.37163300	C 0 17.51029400 58.75215500 2.75311200
H 0 16.63634400 67.26382400 9.85067100	N 0 17.23783600 54.20154000 8.11431800	C 0 17.16491400 60.22438600 2.75049300
H 0 20.44226300 67.18038300 10.51708900	O 0 17.68290700 52.83260200 6.35752300	C 0 16.72788800 60.86457100 1.58287500
H 0 20.37882500 65.50399700 11.06343600	H 0 19.88759300 54.24587200 8.23043800	C 0 17.24987700 60.97879000 3.92924800
H 0 20.06387700 65.89348000 9.36130800	H 0 20.10821600 52.91582400 7.07183400	C 0 16.37964200 62.21537800 1.59050300
H 0 17.57463900 69.50185500 9.31667700	H 0 16.30170800 54.34484000 7.76713100	C 0 16.89522200 62.32865300 3.93955000
H 0 17.87713500 69.12151700 11.02106500	H 0 17.52267600 54.76145600 8.91143300	C 0 16.45371400 62.95379100 2.77269300
H 0 19.18451000 68.99532400 9.83908400	C -1 10.76479100 62.01089900 -0.16362800	H 0 18.31158800 58.51871600 0.71530800
N 0 18.55738100 63.27104400 9.25097300	C 0 12.30941600 61.96246000 -0.28076900	H 0 19.54397700 58.84736500 1.94898100
C -1 18.55311500 62.47000200 8.05116500	C 0 12.97373900 60.76875100 0.43592200	H 0 16.60261700 58.16752700 2.55623400
C 0 17.85519800 61.10235000 8.13396400	C 0 12.93147300 63.31290600 0.09226300	H 0 17.83555600 58.47008200 3.75751000
O 0 17.86536100 60.38502800 7.11811600	C 0 12.93619200 60.77389700 1.96357200	H 0 16.65165600 60.29661200 0.65859900
C 0 19.99727300 62.20188500 7.59524000	H 0 10.41492200 62.44030700 0.77902900	H 0 17.58510700 60.51782800 4.85277200
C 0 20.77672300 63.47384900 7.29242300	H 0 12.51752300 61.80178200 -1.34986800	H 0 16.04527600 62.69060100 0.67278100
O 0 20.59012000 61.47110100 8.68011100	H 0 12.50119500 59.84849400 0.06564000	H 0 16.95629600 62.89201300 4.86630900
H 0 19.13751400 62.98835500 10.03054100	H 0 14.02305400 60.72079400 0.11818300	H 0 16.15626900 63.99738100 2.79090400
H -1 18.05414000 63.07819700 7.28924900	H 0 14.01369300 63.31147700 -0.06912900	C -1 15.09100800 52.38699100 3.66511900
H 0 19.93631800 61.56892500 6.70198500	H 0 12.50157600 64.12044100 -0.51179000	C 0 15.98728700 53.53802500 3.17228400

C 0 15.55884400 54.87450600 3.74880100  
C 0 14.65541400 55.70973600 3.08199400  
C 0 16.02503700 55.27161700 5.01101400  
C 0 14.22151000 56.90501000 3.66292600  
C 0 15.58938400 56.46046600 5.60164800  
C 0 14.68563700 57.28272600 4.92320900  
H 0 14.05241000 52.53799100 3.35081900  
H 0 17.01848900 53.33198400 3.47671900  
H 0 15.96953400 53.58387100 2.07569700  
H 0 14.28243700 55.41949300 2.10170600  
H 0 16.72415400 54.61937100 5.52240700  
H 0 13.51027900 57.53600800 3.13673100  
H 0 15.95040300 56.74590100 6.58746700  
H 0 14.34652400 58.20476200 5.38145400  
C -1 9.36859400 64.78909800 13.86176600  
C 0 10.39774700 64.03341400 12.99823500  
C 0 11.80209100 64.05338000 13.60959200  
C 0 9.92468600 62.61120000 12.68251500  
H 0 9.37531500 64.47365800 14.90964300  
H 0 10.45598100 64.57038200 12.04082000  
H 0 12.52743500 63.57957600 12.94524600  
H 0 12.14406400 65.07771200 13.79161400  
H 0 11.82236700 63.51606300 14.56474800  
H 0 10.57352800 62.14304600 11.94097700  
H 0 9.94454200 61.97164300 13.56958900  
H 0 8.90221300 62.61646200 12.28570800  
H -1 15.41794900 51.40124800 3.31798700  
H -1 8.46287900 61.01882600 3.48759400  
H -1 18.76076300 57.25110300 1.87927800  
H -1 19.49904100 52.57366200 8.71122600  
H -1 22.21788200 63.14306100 14.80913600  
H -1 19.93355600 56.70789700 10.41250400  
H -1 6.00253100 59.81679900 7.41851300  
H -1 11.67898900 57.43267600 15.10801700  
H 0 11.31442500 53.51920900 13.12068500  
H -1 9.58986700 65.85842800 13.78375900  
H -1 8.38372100 64.58778100 13.42641900  
H 0 15.11182500 52.36256100 4.75884100  
H -1 13.20177200 54.61278100 8.59382400  
C -1 13.92118400 69.63685700 15.14217500  
H -1 14.06786700 70.72208400 15.13492300  
H -1 12.89121900 69.40615100 14.84996700  
H 0 14.03721500 69.30041600 16.18006500  
H 0 13.84086000 59.31441400 13.36598900  
C -1 9.09290200 66.03219000 8.85499100

C 0 10.44055800 65.40340700 8.38199100  
C 0 11.64815700 65.87810200 9.16380600  
C 0 12.00225100 67.23617900 9.14898600  
C 0 12.44010800 64.99335600 9.90577100  
C 0 13.10773800 67.69825900 9.86134800  
C 0 13.54498700 65.45277700 10.62813700  
C 0 13.87896900 66.80595400 10.60987100  
H -1 9.29290000 66.79662600 9.61290100  
H -1 8.44518800 65.25543000 9.27488600  
H 0 8.54996800 66.50374300 8.02964300  
H 0 10.38684900 64.31269000 8.44032400  
H 0 10.60873700 65.62953000 7.32340900  
H 0 11.40335300 67.93500300 8.56835600  
H 0 12.20327600 63.93373900 9.91483700  
H 0 13.36902400 68.75288600 9.83309700  
H 0 14.14709000 64.76693200 11.21214100  
H 0 14.73768300 67.15282400 11.17351000  
C -1 12.60582100 56.71579900 17.61680600  
C 0 13.45155200 55.55992700 17.10224000  
O 0 13.89943000 55.79349100 15.76588500  
H -1 12.18865200 56.58068800 18.62026200  
H -1 11.78068200 56.90590200 16.92280300  
H 0 13.21117800 57.63051400 17.64429600  
H 0 14.31181900 55.38550300 17.76597600  
H 0 12.87355000 54.63122800 17.06175200  
H 0 14.28739000 56.68098600 15.72702800  
H 0 10.10030500 66.89998800 4.06856300  
C -1 10.41985100 67.50453600 4.92158300  
C 0 11.94682300 67.54372800 5.05007300  
C 0 12.59580200 66.18067200 5.04214000  
C 0 13.51484700 65.81203600 6.03016500  
C 0 12.30409400 65.26852000 4.01971300  
C 0 14.13921000 64.56465400 5.99780100  
C 0 12.91196500 64.01839600 3.99313500  
C 0 13.83248600 63.66423600 4.97786300  
H 0 9.95226700 67.08919800 5.81854800  
H 0 12.35188400 68.14074100 4.22021700  
H 0 12.22356700 68.07140400 5.96932900  
H 0 13.73950600 66.50037400 6.83959400  
H 0 11.59848900 65.53633000 3.23747000  
H 0 14.85132500 64.30782000 6.77373700  
H 0 12.65872500 63.31022000 3.21412400  
H 0 14.29555500 62.68838400 4.94646400  
H -1 10.04557100 68.52174600 4.76370900  
C 0 13.81295000 61.87170100 11.01500900

C 0 12.83799900 61.07010000 11.55381800  
C 0 12.18044000 60.23720500 10.47629800  
H 0 11.11486600 60.48908700 10.36587100  
H 0 12.24836100 59.16933900 10.69014300  
H 0 14.41427200 62.60053100 11.53438800  
H 0 12.48234300 61.10018800 12.57267300

## E:IO<sub>1R,2S</sub> (OO)

H -1 17.45651300 55.72335500 15.73995000  
H -1 14.36506000 66.87378700 19.12380600  
H -1 8.60705100 62.77679100 18.32906500  
H -1 10.42805600 62.61770700 -1.01099400  
H -1 10.37409400 60.99328300 -0.26631900  
C 0 14.48836200 61.41427700 7.01509400  
C 0 14.61914500 62.23975100 8.13944100  
C 0 13.88255200 61.94149500 9.28105900  
C 0 13.04269200 60.81148600 9.29998300  
C 0 12.86647300 60.02593100 8.16880800  
C 0 13.60341200 60.33459200 7.02094300  
H 0 15.09467600 61.60223200 6.13617000  
H 0 15.30433500 63.08101700 8.13181000  
H 0 12.19232400 59.17906400 8.17126100  
H 0 13.49467000 59.71378600 6.13938100  
O 0 16.31284400 59.10879800 12.37321300  
O 0 13.67613100 60.38209800 11.58379400  
H 0 17.97417400 66.58227200 14.05652100  
C -1 10.91638400 57.40508000 14.32248800  
C 0 10.94931900 56.12046300 13.50048500  
O 0 9.94675500 55.71668200 12.90828700  
C 0 11.08581100 58.60233200 13.38079100  
O 0 11.25641700 59.83093700 14.08338100  
H 0 9.93269000 57.44879500 14.80454200  
H 0 11.97819800 58.47127800 12.76823600  
H 0 10.21502500 58.65113600 12.71606300  
H 0 10.49060400 59.95916100 14.65666700  
N 0 12.15647100 55.50529300 13.39824600  
C 0 12.24740400 54.20069100 12.76259700  
C 0 12.03925000 54.12030500 11.24012800  
O 0 11.58246400 53.08357600 10.76065200  
H 0 12.88825800 55.77257700 14.05237900  
H 0 13.24455300 53.80439400 12.97694700  
N 0 12.45003100 55.17103300 10.49640200  
C -1 12.35280000 55.13968900 9.04024000  
C 0 12.31528300 56.56570800 8.49295700

S 0 11.83901200 56.64667200 6.71790500	H 0 9.78555800 57.02648700 10.96401600	C 0 16.77340400 61.87042100 14.27000200
H 0 12.84629100 56.00401500 10.92798200	C -1 17.74209000 56.74904200 15.48476100	C 0 17.26706600 62.02415100 15.71151100
H 0 11.45023200 54.58472100 8.77424400	N 0 17.09512100 56.22915800 13.00181800	C 0 18.32447600 63.12324700 15.59038200
H 0 11.61440200 57.17382300 9.06545100	C 0 16.87709500 55.95673200 11.67472400	H 0 18.46596800 61.16167400 13.07676900
H 0 13.29235900 57.04488900 8.57303900	O 0 17.62146800 55.23685300 11.00937900	H 0 16.03534300 62.64732000 14.05154000
H 0 10.50894300 56.59160800 6.94175100	N 0 15.70511000 56.45994200 11.07529900	H 0 16.34883700 60.90183600 14.01272500
C -1 14.81302000 65.87492100 19.15218900	C 0 14.86926400 57.39862400 11.63380100	H 0 16.46538300 62.29189800 16.40171000
C 0 16.27886500 65.89804000 18.69256500	C 0 15.50176200 58.15527800 12.81563300	H 0 17.72276900 61.09456300 16.06909700
C 0 16.92561000 64.51395800 18.83023600	O 0 13.77763800 57.65868900 11.12337300	H 0 17.86085200 64.11157700 15.51734100
C 0 16.41032200 66.40146100 17.25196700	C 0 14.76513800 59.00849800 14.97098400	H 0 19.03657600 63.14438200 16.41468800
H 0 14.71813500 65.49408600 20.17644300	N 0 14.39448300 58.59586800 13.70726800	N 0 18.18680800 64.07507800 11.90119400
H 0 14.21728900 65.22440500 18.49962000	C 0 14.09592600 60.03554500 15.65838100	C 0 17.56820600 64.88530600 10.85774100
H 0 16.82695500 66.59004900 19.34957300	C 0 14.43563400 60.40846800 16.95768200	C 0 17.61012400 64.22089800 9.47911700
H 0 17.97112600 64.54251000 18.50819100	C 0 13.79814000 61.60868600 17.61108000	O 0 16.85370500 64.60925800 8.57979000
H 0 16.88782400 64.14573100 19.86276000	C 0 15.43598300 59.68823100 17.63954300	C 0 18.20753000 66.29376400 10.84586600
H 0 16.40779700 63.78529200 18.19531400	C 0 15.82135000 60.04129500 19.05377000	C 0 17.32253900 67.30934900 10.10813400
H 0 17.45388700 66.45160500 16.92606000	C 0 16.12149000 58.68316200 16.95840300	C 0 19.65210800 66.26114300 10.33447600
H 0 15.88618500 65.72448500 16.56658700	C 0 15.85180200 58.37212300 15.61830600	C 0 17.69623300 68.75972300 10.42476700
H 0 15.96927300 67.39824400 17.13657000	C 0 16.38186000 57.17349100 13.57123900	H 0 18.68850400 64.57655500 12.64240100
C -1 8.77922800 61.70492500 18.47276900	N 0 16.62100100 57.44263100 14.88494500	H 0 16.50272000 64.99263100 11.08719700
C 0 10.20642700 61.36789200 18.00742000	H 0 15.60156100 56.26443800 10.08508600	H 0 18.23850100 66.60086200 11.89259800
C 0 10.49512800 59.86516700 18.09846300	H 0 13.18991000 61.33600400 18.48205400	H 0 17.35651400 67.12432000 9.02847400
C 0 10.37486700 61.86354300 16.56544900	H 0 14.55933500 62.31067700 17.97037400	H 0 16.28268100 67.14481600 10.41105600
H 0 8.58197500 61.42793400 19.51217900	H 0 13.16359000 62.15038900 16.90918400	H 0 20.14352100 67.22534000 10.49177700
H -1 8.12193300 61.13719100 17.80600600	H 0 14.95930000 60.03258100 19.73226100	H 0 20.23495200 65.50441400 10.86769800
H 0 10.93046300 61.89699700 18.64078800	H 0 16.56169200 59.33800700 19.44597800	H 0 19.68812900 66.03337000 9.26285200
H 0 11.50588700 59.63338300 17.75006700	H 0 16.25795500 61.04691800 19.11431400	H 0 17.01347300 69.46003600 9.93009900
H 0 10.39258700 59.49521000 19.12478600	H 0 13.30935800 60.55728100 15.12543400	H 0 17.64084900 68.93907000 11.50418800
H 0 9.79358000 59.29836500 17.47236600	H 0 16.90339200 58.15783800 17.49136700	H 0 18.71196400 69.00396500 10.09575200
H 0 11.30979000 61.52346300 16.11818900	H 0 18.10060200 57.27709900 16.36389300	N 0 18.51956900 63.23687400 9.27762800
H 0 9.55017500 61.49492600 15.94020000	H 0 18.53930600 56.68218200 14.74572600	C -1 18.55354400 62.46972300 8.05035800
H 0 10.35004200 62.95611900 16.50792100	C -1 21.24068600 63.62235100 14.93307600	C 0 17.83960800 61.10307200 8.09504200
C -1 6.93614000 59.40304200 7.02345400	C 0 20.29322300 62.91549800 13.96624500	O 0 17.85199600 60.40664500 7.06561900
C 0 7.76415300 58.74221700 8.09640200	O 0 20.70237100 62.52624100 12.86764300	C 0 20.00640200 62.21833100 7.62772000
C 0 7.94489000 57.35414500 8.12392100	C 0 21.32607200 65.12760600 14.60911900	C 0 20.77805000 63.50090700 7.34562100
C 0 8.36342700 59.50897700 9.10361500	C 0 19.97521000 65.79902800 14.89761400	O 0 20.57898200 61.49251400 8.72440300
C 0 8.67936100 56.74442400 9.14356300	O 0 19.20095900 65.90914600 13.86759900	H 0 19.11069700 62.94684900 10.04717600
C 0 9.09162600 58.90294400 10.12543800	O 0 19.70202500 66.11486700 16.06254800	H -1 18.05350500 63.07832300 7.28977200
C 0 9.24896300 57.51510400 10.15823500	H 0 20.93887400 63.50910200 15.97715200	H 0 19.96886300 61.58757100 6.73135300
H 0 6.67578200 58.69636700 6.23021500	H 0 22.08960300 65.58646500 15.24461100	H 0 21.49194000 61.27122100 8.50447600
H 0 7.47838900 60.23189000 6.55977900	H 0 21.60096100 65.25641800 13.55882200	H 0 21.81239400 63.27161000 7.06376400
H 0 7.49712500 56.74510100 7.34225300	N 0 18.98439400 62.78697700 14.31822900	H 0 20.32003200 64.05283700 6.51837000
H 0 8.25316200 60.59057400 9.08872500	C 0 18.04366300 62.11174000 13.41849200	H 0 20.79256200 64.14242000 8.22985000
H 0 8.80401600 55.66577700 9.15772700	C 0 17.64728200 62.87394800 12.17261600	N 0 17.28850400 60.71730100 9.24836100
H 0 9.52953500 59.52149000 10.90208300	O 0 16.80932900 62.35231900 11.41974500	C 0 16.55329400 59.46608000 9.34915000

C 0 17.42226000 58.22799300 9.15853400	C 0 10.58599700 62.23452300 5.98286600	H 0 14.10847500 52.59636500 3.22784000
O 0 16.97914900 57.23377400 8.56909400	C 0 10.29678100 59.85521700 5.16888400	H 0 17.05145500 53.26724800 3.80613400
H 0 17.19168400 61.37258000 10.02885400	H 0 8.11901700 61.68951200 5.05864800	H 0 16.27505400 53.50081200 2.23179200
H 0 16.13359900 59.43411000 10.36474800	H -1 8.80482600 62.73710600 3.84515300	H 0 14.44714200 55.23595700 1.99506500
H 0 15.76264400 59.41913400 8.59906000	H 0 10.97313500 61.51403400 4.00620000	H 0 16.69462300 54.79845200 5.60900200
N 0 18.65971400 58.28025600 9.71372800	H 0 11.59188000 62.02703800 6.35295800	H 0 13.63760200 57.45193800 2.75518700
C -1 19.68090700 57.26472000 9.50383500	H 0 10.54420700 63.29276300 5.70674700	H 0 15.88113700 57.01878900 6.40351400
C 0 20.93208300 57.81699500 8.81619400	H 0 9.88397600 62.06469900 6.80955700	H 0 14.37615300 58.36362700 4.94161800
C 0 20.62857400 58.40426200 7.43000000	H 0 11.29945800 59.57350900 5.49515000	C -1 9.36858500 64.78811500 13.86137300
C 0 19.95066600 57.36239800 6.54151400	H 0 9.61897300 59.62153300 5.99654200	C 0 10.42687600 64.07837500 13.00149100
N 0 18.77551900 57.75888400 5.98555900	H 0 10.02756100 59.21298200 4.32214100	C 0 11.81371700 64.22117800 13.64655700
O 0 20.45315600 56.25492300 6.35284200	C 0 14.94763200 68.91533600 14.26384800	C 0 10.01722800 62.63289200 12.69606600
H 0 18.91450400 59.14836600 10.16540800	C 0 14.73454700 67.39620900 14.22401100	H 0 9.38097000 64.46851100 14.90758600
H 0 19.21284300 56.52521300 8.84983400	C 0 15.97442800 66.54827800 13.93537900	H 0 10.45216000 64.61622900 12.04184100
H 0 21.40538300 58.58461500 9.44232100	O 0 17.10309400 67.20092200 14.10386800	H 0 12.63165700 63.98536200 12.96442400
H 0 21.64491200 56.99297300 8.70608200	O 0 15.87286700 65.36275400 13.63309300	H 0 11.97747100 65.25065300 13.98402100
H 0 20.00892000 59.29543300 7.52402600	H 0 14.92374100 69.31655300 13.24290200	H 0 11.90838600 63.56886700 14.52242300
H 0 21.56776200 58.69377100 6.94200500	H 0 15.95220900 69.11006200 14.64621300	H 0 10.61797700 62.19810900 11.89684900
H 0 18.28359400 58.55460600 6.38386300	H 0 14.38014400 67.04955500 15.20381500	H 0 10.13542700 61.98452700 13.56724300
H 0 18.20735500 57.03036400 5.57380700	H 0 13.95927900 67.10649700 13.50727600	H 0 8.96819100 62.59316300 12.37888100
C -1 19.48694600 53.29102400 7.88402900	C -1 18.60131300 58.32712200 1.75413300	H -1 15.41831000 51.40170700 3.31702600
C 0 18.06040100 53.46203100 7.39026100	C 0 17.29729100 58.68371000 2.49234700	H -1 8.46275000 61.01887500 3.48761600
N 0 17.23965700 54.16593400 8.20308700	C 0 17.04110300 60.16337500 2.65230600	H -1 18.76068700 57.25106900 1.87908700
O 0 17.67793700 52.96063600 6.32789500	C 0 16.62285000 60.95052200 1.57114600	H -1 19.49901200 52.57373100 8.71128700
H 0 19.90835700 54.23834600 8.22721900	C 0 17.21955800 60.78389000 3.89606200	H -1 22.21778100 63.14294400 14.80878400
H 0 20.09050500 52.90802200 7.06204400	C 0 16.38073600 62.31576700 1.72722900	H -1 19.93388300 56.70806200 10.41251500
H 0 16.31011700 54.35874000 7.86223000	C 0 16.97594800 62.14847000 4.05550100	H -1 6.00264900 59.81699600 7.41858500
H 0 17.53284300 54.64798300 9.05020100	C 0 16.55122900 62.92098200 2.97378400	H -1 11.67886800 57.43260600 15.10813800
C -1 10.76511900 62.01121000 -0.16329500	H 0 18.55794700 58.57273900 0.68812700	H 0 11.50582600 53.51192900 13.17780000
C 0 12.30533300 61.91478600 -0.34098600	H 0 19.45536100 58.84913700 2.19627800	H -1 9.59003300 65.85841200 13.78402100
C 0 12.95917800 60.70802900 0.36341200	H 0 16.45306700 58.21544700 1.97381500	H -1 8.38363200 64.58848200 13.42630000
C 0 13.00430700 63.24470200 -0.03745200	H 0 17.32500700 58.22499900 3.48342100	H 0 14.97103500 52.33225400 4.75236300
C 0 12.95436500 60.71090300 1.89123500	H 0 16.47609200 60.48416900 0.59923600	H -1 13.20093900 54.61189100 8.59328700
H 0 10.44814100 62.44592600 0.78750300	H 0 17.54739500 60.20851200 4.75404600	C -1 13.92179400 69.63619700 15.14340400
H 0 12.45321900 61.72273000 -1.41514200	H 0 16.04800800 62.90678800 0.87901000	H -1 14.06738500 70.72214500 15.13433500
H 0 12.46224500 59.79669300 0.00277800	H 0 17.11336500 62.59833800 5.03429400	H -1 12.89128000 69.40661700 14.84938000
H 0 14.00045000 60.64035500 0.02281900	H 0 16.33576600 63.97626500 3.10534700	H 0 14.02834800 69.30650900 16.18469900
H 0 14.06794300 63.19415100 -0.29240000	C -1 15.09054600 52.38669100 3.66641400	H 0 13.84940400 59.28937100 13.19396000
H 0 12.55916900 64.05973000 -0.62036900	C 0 16.10066300 53.49486400 3.31605900	C -1 9.09297400 66.03206700 8.85495800
H 0 12.93415900 63.51920300 1.01718500	C 0 15.63156300 54.86803900 3.75596200	C 0 10.40564700 65.35840900 8.40614500
H 0 13.41745200 59.79843300 2.27884400	C 0 14.76565100 55.62720600 2.95946500	C 0 11.65263800 66.21773300 8.44008500
H 0 13.53125600 61.54803400 2.28746000	C 0 16.02625700 55.39211900 4.99578700	C 0 11.61592800 67.61397400 8.35541700
H 0 11.93776700 60.76237200 2.29310800	C 0 14.31013000 56.87612900 3.38557600	C 0 12.90125700 65.59293100 8.55701100
C -1 8.85027000 61.71577300 4.23780300	C 0 15.57032000 56.63939400 5.43231500	C 0 12.79544400 68.36279600 8.39323900
C 0 10.22839600 61.33887700 4.78971000	C 0 14.71511700 57.38669700 4.61890400	C 0 14.08155000 66.33104800 8.61503000

C 0 14.02824000 67.72544700 8.53225400  
H -1 9.29289700 66.79664600 9.61288100  
H -1 8.44517900 65.25546400 9.27493200  
H 0 8.56957100 66.51884000 8.02603300  
H 0 10.59388200 64.48648000 9.04259900  
H 0 10.28068600 64.94876300 7.39514200  
H 0 10.66257100 68.12641300 8.26486100  
H 0 12.95014400 64.50889900 8.58513000  
H 0 12.74548700 69.44669800 8.32781800  
H 0 15.03444700 65.81836300 8.70736400  
H 0 14.94443700 68.30623300 8.57716600  
C -1 12.60584600 56.71589700 17.61689900  
C 0 13.45155000 55.55938100 17.10217400  
O 0 13.93324800 55.81105800 15.78302300  
H -1 12.18863100 56.58067800 18.62025200  
H -1 11.78066500 56.90584400 16.92279900  
H 0 13.21354900 57.62904600 17.64474400  
H 0 14.29234600 55.36228300 17.78448100  
H 0 12.86331200 54.63879700 17.03200900  
H 0 14.41966400 56.65107100 15.79436000  
H 0 9.81543000 66.82517100 4.31353500  
C -1 10.41990700 67.50479600 4.92159200  
C 0 11.89853000 67.46476900 4.51070700  
C 0 12.47112500 66.07055500 4.46413900  
C 0 13.54934500 65.70338200 5.27334500  
C 0 11.91908300 65.11113600 3.60727300  
C 0 14.05975000 64.40532900 5.24216600  
C 0 12.42427300 63.81560200 3.57493700  
C 0 13.49514400 63.45499600 4.39355500  
H 0 10.29726200 67.22941000 5.97072800  
H 0 12.00051700 67.93242200 3.52109900  
H 0 12.48002400 68.07483700 5.20959100  
H 0 13.97761300 66.43341900 5.95079800  
H 0 11.08472300 65.37809800 2.96292700  
H 0 14.88428000 64.13929300 5.89443200  
H 0 11.97146100 63.08143800 2.92175600  
H 0 13.87791700 62.44243600 4.37604100  
H -1 10.04541900 68.52167700 4.76361700  
C 0 12.55691700 60.59298300 10.68749800  
C 0 13.10709600 61.69174600 11.51361900  
C 0 13.87804500 62.65006200 10.62339700  
H 0 14.88613500 62.82477500 11.00250900  
H 0 13.36199700 63.61749000 10.56862900  
H 0 11.66474200 60.02334300 10.91664000  
H 0 12.64669200 62.01699300 12.4350610

## E:IO<sub>1S,2R</sub> (OO)

H -1 17.45630500 55.72339500 15.73988400  
H -1 14.36523600 66.87387700 19.12420500  
H -1 8.60700400 62.77678300 18.32907300  
H -1 10.42817400 62.61803400 -1.01080900  
H -1 10.37418900 60.99323700 -0.26621900  
C 0 14.07814300 60.61283900 6.85221300  
C 0 13.11131900 60.03613800 7.68679200  
C 0 12.97153500 60.52457400 8.98085300  
C 0 13.80063200 61.56662600 9.43456600  
C 0 14.72523000 62.17191800 8.59673400  
C 0 14.86708600 61.67195300 7.30060000  
H 0 14.21495500 60.24293700 5.84074300  
H 0 12.49213100 59.22140200 7.32588500  
H 0 15.34182900 62.98906700 8.94645400  
H 0 15.62345200 62.08671100 6.64664500  
O 0 16.37988900 59.08301400 12.37044000  
O 0 13.85492400 60.57920900 11.63890300  
H 0 17.96894500 66.57644100 14.01035300  
C -1 10.91590800 57.40535600 14.32304400  
C 0 10.97016000 56.12295500 13.49972800  
O 0 9.97314700 55.69217100 12.91716800  
C 0 11.10608300 58.61267600 13.40277000  
O 0 11.17855900 59.83817000 14.13155600  
H 0 9.92803100 57.44259300 14.79605700  
H 0 12.04809000 58.51606900 12.86414100  
H 0 10.29412000 58.64075800 12.66741100  
H 0 10.36172000 59.94089600 14.63547000  
N 0 12.19114200 55.53650700 13.39458800  
C 0 12.31413300 54.23107200 12.76684000  
C 0 12.09197800 54.13703700 11.24848700  
O 0 11.66151300 53.08454900 10.77928900  
H 0 12.91382900 55.81603200 14.05369000  
H 0 13.32538300 53.86723900 12.97228600  
N 0 12.46029600 55.19597000 10.49320100  
C -1 12.35146900 55.13825000 9.03940800  
C 0 12.26205300 56.54926100 8.45941500  
S 0 11.80597400 56.55659900 6.67572300  
H 0 12.84943200 56.03832300 10.91290900  
H 0 11.45954900 54.55613800 8.79518700  
H 0 11.51951000 57.13798600 8.99964700  
H 0 13.21552200 57.07498300 8.54075200  
H 0 10.47548000 56.49028800 6.88926300

C -1 14.81273400 65.87485100 19.15175400  
C 0 16.26928600 65.88994300 18.66313900  
C 0 16.91052300 64.50092700 18.7728800  
C 0 16.37588600 66.40018200 17.22332800  
H 0 14.73668700 65.50122500 20.18024800  
H 0 14.20276700 65.22098300 18.51575300  
H 0 16.83567500 66.57420800 19.31268000  
H 0 17.95206900 64.52980700 18.44286500  
H 0 16.88311500 64.12012600 19.80563400  
H 0 16.38257500 63.78223400 18.13881600  
H 0 17.41227100 66.43923900 16.87461400  
H 0 15.82836900 65.73140100 16.54772200  
H 0 15.94270700 67.40182000 17.12171100  
C -1 8.77916400 61.70507500 18.47257200  
C 0 10.20641800 61.36503300 18.01031600  
C 0 10.48488600 59.85945400 18.08483300  
C 0 10.38686000 61.87828400 16.57624300  
H 0 8.57942700 61.42817600 19.51167500  
H -1 8.12204900 61.13706200 17.80600300  
H 0 10.93037800 61.88106600 18.65455800  
H 0 11.49664800 59.62607800 17.74063600  
H 0 10.37179500 59.47692600 19.10550100  
H 0 9.78520100 59.30495800 17.44573600  
H 0 11.31121900 61.52045400 16.12144500  
H 0 9.55382600 61.54094300 15.94425700  
H 0 10.38812100 62.97186200 16.53807100  
C -1 6.93639900 59.40340700 7.02370400  
C 0 7.68394600 58.64308400 8.09107500  
C 0 7.99306600 57.28612100 7.94661400  
C 0 8.06896300 59.28735600 9.27387000  
C 0 8.65295900 56.58688100 8.96150300  
C 0 8.72233700 58.59100200 10.28749000  
C 0 9.01763100 57.23289900 10.14361800  
H 0 6.69127300 58.76344900 6.17163100  
H 0 7.52810300 60.24350400 6.64650100  
H 0 7.70449800 56.76985000 7.03407900  
H 0 7.84664100 60.34420400 9.40233200  
H 0 8.87709500 55.53149000 8.83624800  
H 0 8.99993200 59.11517800 11.19605500  
H 0 9.50509800 56.68249900 10.94228900  
C -1 17.74254000 56.74914500 15.48493900  
N 0 17.06389200 56.20616100 13.01938700  
C 0 16.84713400 55.94023200 11.69019300  
O 0 17.58377400 55.21347200 11.02501300  
N 0 15.68129800 56.45930100 11.09069200

C 0 14.87051700 57.42036000 11.64571300	H 0 16.49773600 62.16246700 16.31971600	C -1 19.68144600 57.26489600 9.50390600
C 0 15.52479800 58.17021700 12.81890300	H 0 17.82529800 61.05682700 15.94830200	C 0 20.93851300 57.79934000 8.81268100
O 0 13.77959700 57.69868500 11.14413200	H 0 17.76975000 64.08518500 15.44604800	C 0 20.64253000 58.37423400 7.41894900
C 0 14.79478300 59.04538600 14.97426800	H 0 19.00538800 63.18728100 16.32637300	C 0 19.94364200 57.32558000 6.55622000
N 0 14.43464700 58.67351800 13.69407600	N 0 18.16841800 64.17051700 11.82662000	N 0 18.73859300 57.70339900 6.05514400
C 0 14.12684300 60.06881600 15.66701000	C 0 17.61040500 64.99383300 10.76276500	O 0 20.45044900 56.22317600 6.34919100
C 0 14.44664000 60.41160100 16.97918600	C 0 17.63546200 64.28188100 9.40796100	H 0 18.95036000 59.16436400 10.15401100
C 0 13.80860100 61.60513800 17.64395000	O 0 16.88480600 64.64302700 8.49733800	H 0 19.20036200 56.52948700 8.85469100
C 0 15.42465900 59.66395100 17.66505600	C 0 18.31984000 66.36598600 10.72657700	H 0 21.41713300 58.56899800 9.43216600
C 0 15.78565900 59.98326800 19.09375100	C 0 17.61694700 67.34014100 9.76449700	H 0 21.64460900 56.96827400 8.71238100
C 0 16.10609500 58.65906300 16.97917000	C 0 19.81934700 66.23585000 10.43371800	H 0 20.03698500 59.27630900 7.50270500
C 0 15.85472100 58.37567900 15.62902800	C 0 17.91973200 68.80515100 10.08960400	H 0 21.58524800 58.63823500 6.92426200
C 0 16.37144900 57.16838800 13.58374200	H 0 18.69825200 64.64472200 12.56477400	H 0 18.25917600 58.50462700 6.45754900
N 0 16.61900900 57.44353000 14.89345900	H 0 16.54921200 65.16216100 10.96612000	H 0 18.15910900 56.96847400 5.67163600
H 0 15.58164700 56.27417200 10.09788100	H 0 18.21352000 66.76540500 11.73958000	C -1 19.48691700 53.29112600 7.88408100
H 0 13.19519500 61.32178600 18.50781600	H 0 17.89964500 67.11018300 8.73114700	C 0 18.05934800 53.45508400 7.39172900
H 0 14.56945900 62.30069700 18.01638900	H 0 16.53601100 67.17694500 9.81000300	N 0 17.24029000 54.17117400 8.19580800
H 0 13.17804200 62.15578200 16.94535500	H 0 20.32114600 67.20168600 10.54417600	O 0 17.67421600 52.93864100 6.33755600
H 0 14.91115800 59.96169800 19.75594000	H 0 20.29912700 65.53572500 11.12183600	H 0 19.90549200 54.23955700 8.22724000
H 0 16.51654100 59.26863300 19.48309100	H 0 19.98742600 65.88441100 9.40940900	H 0 20.09162800 52.90957700 7.06236500
H 0 16.22349300 60.98586000 19.18523900	H 0 17.39534300 69.48001500 9.40382900	H 0 16.30294200 54.34188500 7.86495100
H 0 13.35907800 60.61435000 15.12907300	H 0 17.60348800 69.04711400 11.11087300	H 0 17.52814000 54.65046800 9.04593400
H 0 16.86865900 58.10926600 17.51587700	H 0 18.98996600 69.02758200 10.01691900	C -1 10.76479500 62.01090300 -0.16363300
H 0 18.10456500 57.27681600 16.36335900	N 0 18.52455600 63.26449500 9.25751600	C 0 12.30997300 61.96887100 -0.27281600
H 0 18.53595300 56.68305300 14.74179900	C -1 18.55311300 62.47001400 8.05117100	C 0 12.97524800 60.77103200 0.43606400
C -1 21.24092900 63.62205000 14.93270600	C 0 17.86511600 61.09663200 8.13775300	C 0 12.92285500 63.31809500 0.11946500
C 0 20.29451300 62.95135200 13.92258700	O 0 17.88633700 60.36657100 7.13230800	C 0 12.92627300 60.76012400 1.96331400
O 0 20.72795300 62.58460500 12.82596800	C 0 20.00446900 62.21802200 7.61510700	H 0 10.41031200 62.43958100 0.77780900
C 0 21.31903000 65.13515600 14.63635200	C 0 20.77250600 63.49838200 7.31634300	H 0 12.52588400 61.82041100 -1.34201500
C 0 19.94978000 65.79119200 14.88598300	O 0 20.59108300 61.49829000 8.70853900	H 0 12.51037400 59.85215700 0.05297500
O 0 19.22189600 65.95041500 13.82884100	H 0 19.11514900 63.00193800 10.03709600	H 0 14.02698700 60.73181400 0.12540800
O 0 19.62579500 66.05453300 16.05169700	H -1 18.05414300 63.07819200 7.28924300	H 0 14.00618200 63.32428000 -0.03397800
H 0 20.92175500 63.48483500 15.96851200	H 0 19.95972700 61.58197700 6.72278700	H 0 12.49318000 64.13032700 -0.47834500
H 0 22.05301800 65.59436000 15.30583700	H 0 21.50522500 61.28790800 8.48266200	H 0 12.74282600 63.55598100 1.17113800
H 0 21.63111500 65.28373300 13.59922900	H 0 21.79916800 63.26635600 7.00936100	H 0 13.36608500 59.83838100 2.35627200
N 0 18.96723800 62.85203800 14.22647100	H 0 20.29654200 64.05415700 6.50196600	H 0 13.50371400 61.58500400 2.38688100
C 0 18.02742100 62.18910600 13.30467300	H 0 20.81080900 64.13711900 8.20159800	H 0 11.90015500 60.82353800 2.33587100
C 0 17.55618000 63.00624600 12.11061200	N 0 17.32538400 60.72716800 9.30483500	C -1 8.84986800 61.71592300 4.23802800
O 0 16.65358000 62.54829400 11.39002200	C 0 16.57612800 59.48291900 9.40183500	C 0 10.25992200 61.37895800 4.73965700
C 0 16.80536500 61.80530200 14.17461400	C 0 17.42903600 58.24120000 9.19767100	C 0 10.60905200 62.22727800 5.97005800
C 0 17.30625500 61.96222600 15.61431100	O 0 16.96622700 57.24438600 8.62678700	C 0 10.41913300 59.88317500 5.03141200
C 0 18.29337800 63.12570200 15.50528600	H 0 17.17956400 61.41186300 10.05094900	H 0 8.14034600 61.67690800 5.07566200
H 0 18.50460100 61.29665100 12.88683500	H 0 16.16559800 59.44429500 10.42027400	H -1 8.80497400 62.73703300 3.84494400
H 0 15.98944600 62.50759900 13.98386100	H 0 15.78133800 59.44836600 8.65623400	H 0 10.97114300 61.64401100 3.94799700
H 0 16.46790500 60.80752500 13.89769100	N 0 18.67836800 58.29190700 9.72120100	H 0 11.63354600 62.04722800 6.30263700

H 0 10.51274900 63.29666200 5.75689000	H 0 15.82880300 56.94049800 6.49293700	H 0 11.42334600 67.93534300 8.51119900
H 0 9.93893400 61.98168300 6.80458400	H 0 14.25286800 58.27670900 5.10394600	H 0 12.16659600 63.97529700 9.98527200
H 0 11.44546800 59.64113300 5.31552200	C -1 9.36858700 64.78908700 13.86175100	H 0 13.36891300 68.78035900 9.78986500
H 0 9.77472400 59.56665500 5.85995600	C 0 10.36315900 64.03041800 12.95825300	H 0 14.10025200 64.84196800 11.31194300
H 0 10.16243600 59.27501400 4.15625800	C 0 11.75808800 63.91436900 13.57835500	H 0 14.69943100 67.21722300 11.20510400
C 0 14.93944700 68.92336900 14.24954700	C 0 9.79314000 62.66920000 12.53598600	C -1 12.60585200 56.71578200 17.61678200
C 0 14.72559600 67.40617100 14.20590000	H 0 9.38681800 64.46097700 14.90482800	C 0 13.45363800 55.56191900 17.10040400
C 0 15.95183900 66.57420500 13.83136200	H 0 10.46318800 64.62798600 12.04167700	O 0 13.94970400 55.82768700 15.78895500
O 0 17.08663900 67.17970500 14.09671800	H 0 12.45826400 63.42812500 12.89678400	H -1 12.18863500 56.58063600 18.62024800
O 0 15.83161200 65.43838500 13.37853900	H 0 12.17270600 64.89847800 13.81987900	H -1 11.78061400 56.90618200 16.92290000
H 0 14.89910100 69.32816900 13.22970100	H 0 11.72953400 63.32180600 14.49884000	H 0 13.21283200 57.62939000 17.64621200
H 0 15.94907600 69.11716500 14.61911700	H 0 10.33355300 62.27124700 11.67573700	H 0 14.28728600 55.35582700 17.78865800
H 0 14.43704200 67.05234700 15.20420400	H 0 9.86664700 61.92757800 13.33785400	H 0 12.86437600 54.64342700 17.01426300
H 0 13.90883200 67.12555000 13.53462500	H 0 8.73955600 62.75811900 12.24567900	H 0 14.44846300 56.66006600 15.82068200
C -1 18.60119500 58.32712600 1.75383600	H -1 15.41795100 51.40124800 3.31798800	H 0 10.10673800 66.90132300 4.06535900
C 0 17.52450600 58.75326200 2.76780200	H -1 8.46289200 61.01884100 3.48757400	C -1 10.41985600 67.50453800 4.92158500
C 0 17.18539900 60.22644100 2.77079500	H -1 18.76076400 57.25110300 1.87927800	C 0 11.94546400 67.55424900 5.05761600
C 0 16.71908300 60.86425300 1.61318100	H -1 19.49904000 52.57366500 8.71122800	C 0 12.61220300 66.19997000 5.05810600
C 0 17.30991300 60.98561900 3.94313300	H -1 22.21788200 63.14306100 14.80913700	C 0 13.56081000 65.86558600 6.03049900
C 0 16.38265000 62.21792100 1.62308700	H -1 19.93354300 56.70789100 10.41250400	C 0 12.31812300 65.26708400 4.05539600
C 0 16.96897300 62.33915100 3.95496800	H -1 6.00252100 59.81674800 7.41854100	C 0 14.21597300 64.64359000 5.99941100
C 0 16.49980600 62.96239600 2.79791600	H -1 11.67926700 57.43218000 15.10774700	C 0 12.95719400 64.03232500 4.02999000
H 0 18.29741700 58.51800500 0.71917500	H 0 11.59885900 53.52218800 13.19433400	C 0 13.91016000 63.71501900 4.99598700
H 0 19.54734100 58.84612500 1.93560300	H -1 9.58987000 65.85842800 13.78376600	H 0 9.94895700 67.08641600 5.81557200
H 0 16.61286200 58.17254000 2.58017200	H -1 8.38371900 64.58779300 13.42641800	H 0 12.34927300 68.15241500 4.22790900
H 0 17.86151300 58.46809500 3.76742000	H 0 14.98211700 52.33367700 4.75237200	H 0 12.21327900 68.08908300 5.97546000
H 0 16.61163800 60.29160400 0.69490500	H -1 13.20175900 54.61277800 8.59380200	H 0 13.78670400 66.57055400 6.82520300
H 0 17.66504700 60.52512200 4.85962000	C -1 13.92118400 69.63685700 15.14217400	H 0 11.58902100 65.50697000 3.28595400
H 0 16.02552800 62.69111900 0.71295200	H -1 14.06786700 70.72208400 15.13492300	H 0 14.95343800 64.40677500 6.76126700
H 0 17.06462800 62.90816100 4.87539800	H -1 12.89121900 69.40615100 14.84996700	H 0 12.70553500 63.30827700 3.26487100
H 0 16.21402800 64.00919600 2.81835400	H 0 14.03538800 69.30161200 16.18063900	H 0 14.40008900 62.75292600 4.96220500
C -1 15.09100500 52.38699300 3.66511800	H 0 13.97679600 59.42966100 13.18692700	H -1 10.04556700 68.52174400 4.76370900
C 0 16.08555500 53.50741200 3.30755100	C -1 9.09289700 66.03219500 8.85497200	C 0 13.57394500 61.78231800 10.88862100
C 0 15.60799200 54.86758200 3.77992000	C 0 10.44493400 65.40659200 8.38802400	C 0 12.49115300 60.85502600 11.28855400
C 0 14.72926200 55.63786700 3.00862800	C 0 11.64509000 65.89658600 9.17186300	C 0 12.01402200 60.08023700 10.06822300
C 0 15.99980500 55.36147900 5.03302900	C 0 12.00691500 67.25151200 9.12401300	H 0 10.97688200 60.33728600 9.81888900
C 0 14.24639300 56.86100100 3.47952100	C 0 12.41715900 65.03138700 9.95656400	H 0 12.06071700 59.00530000 10.24959800
C 0 15.51898700 56.58288000 5.51306900	C 0 13.10022200 67.72884500 9.84465000	H 0 13.84326400 62.70216100 11.39123000
C 0 14.63876900 57.33523900 4.73178300	C 0 13.50913900 65.50547000 10.68962300	H 0 11.84516400 61.01846100 12.14019000
H 0 14.10261700 52.58949400 3.23734700	C 0 13.85036700 66.85616800 10.63615000	
H 0 17.04797500 53.28276400 3.77612400	H -1 9.29289800 66.79662200 9.61290600	
H 0 16.23870500 53.53049600 2.22042100	H -1 8.44519300 65.25543200 9.27489800	
H 0 14.41591600 55.27315500 2.03221900	H 0 8.55254500 66.50293800 8.02778900	
H 0 16.68099100 54.76036900 5.62428000	H 0 10.39719400 64.31593400 8.45471700	
H 0 13.55832200 57.44086300 2.87263900	H 0 10.61524600 65.62627000 7.32856000	