

# “Supporting Information”

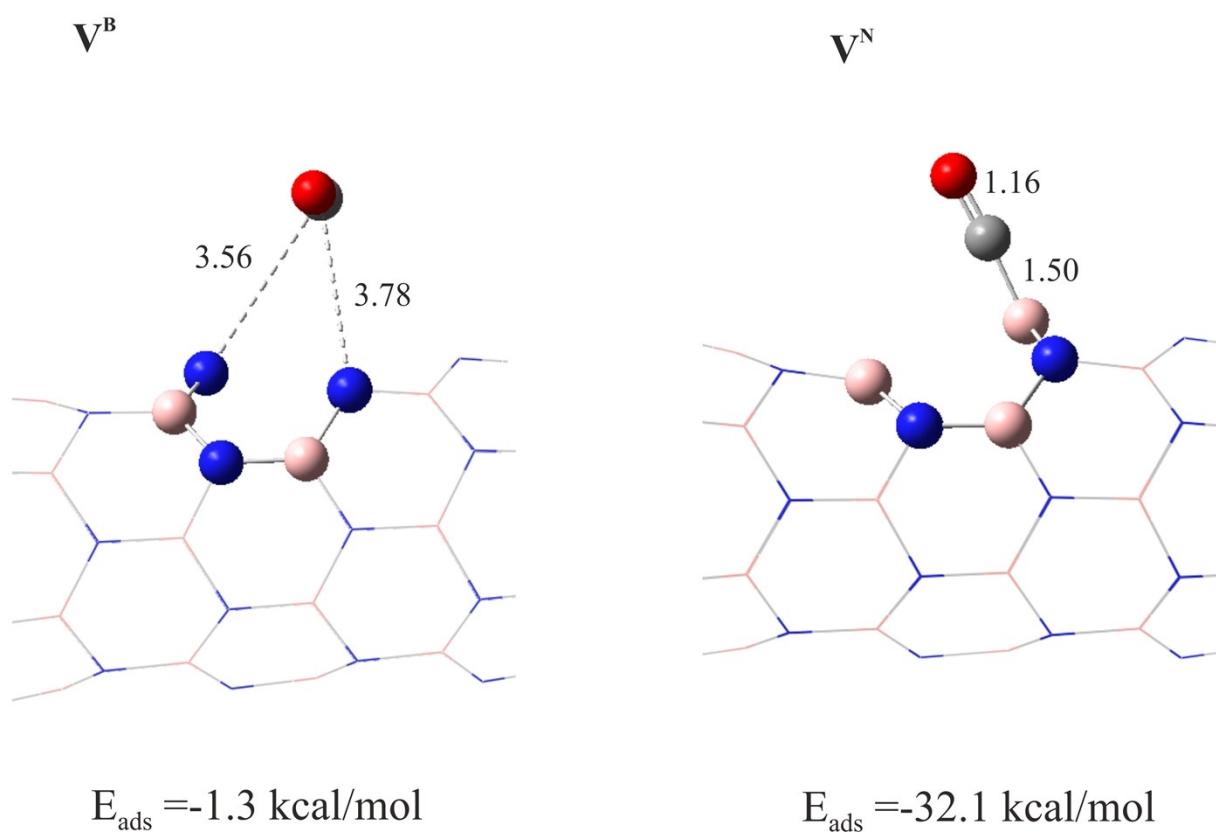
## **The healing of B- or N-vacancy defective BNNTs by using CO molecule: A DFT study**

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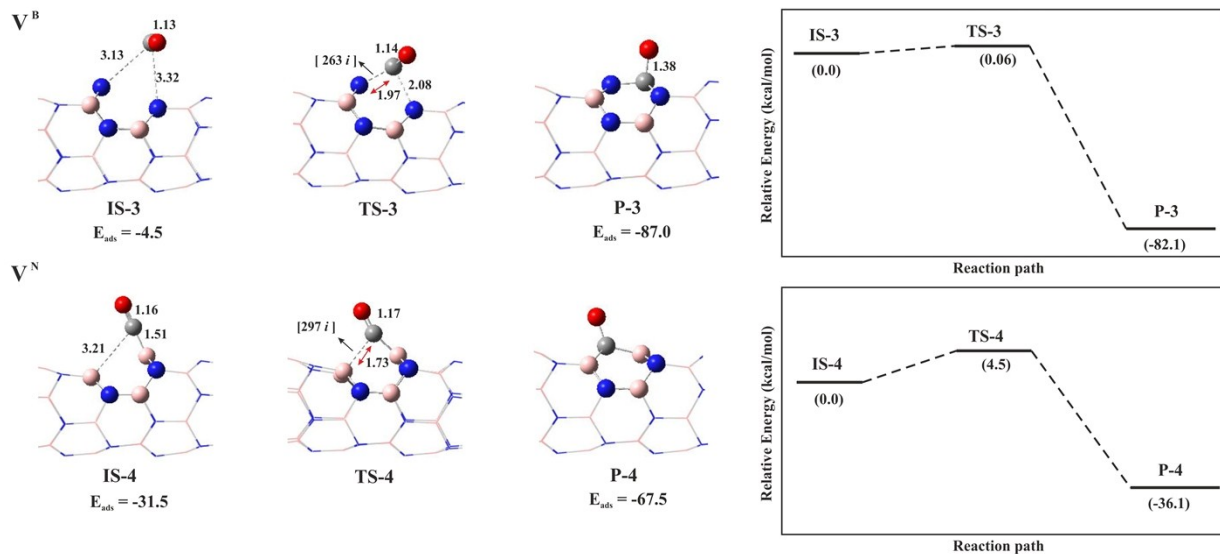
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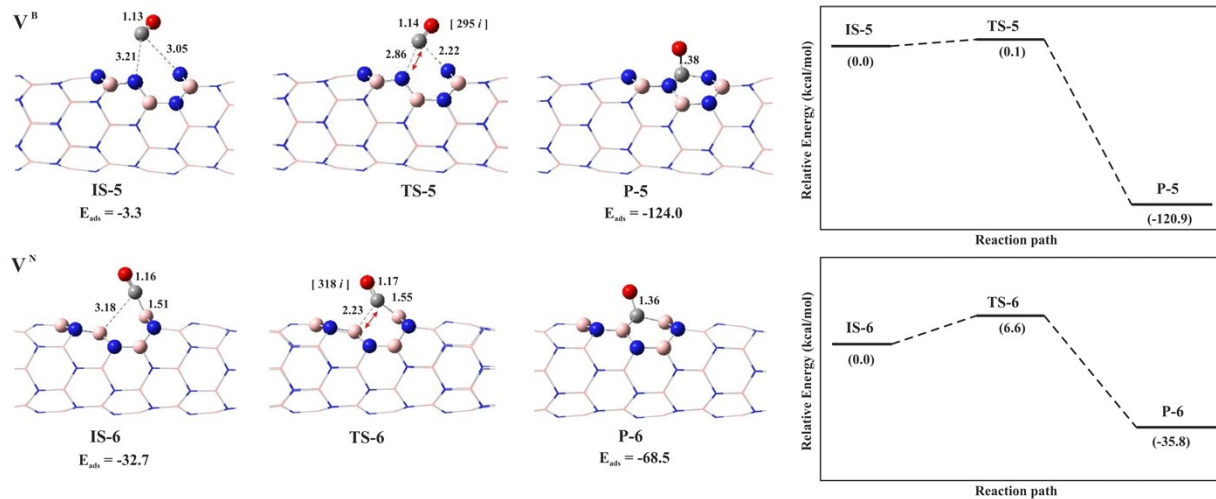
**Figure S1.** Optimized structures, corresponding binding distances and adsorption energies of CO molecule adsorbed over  $V^B$  and  $V^N$  by B3LYP/6-31G\*



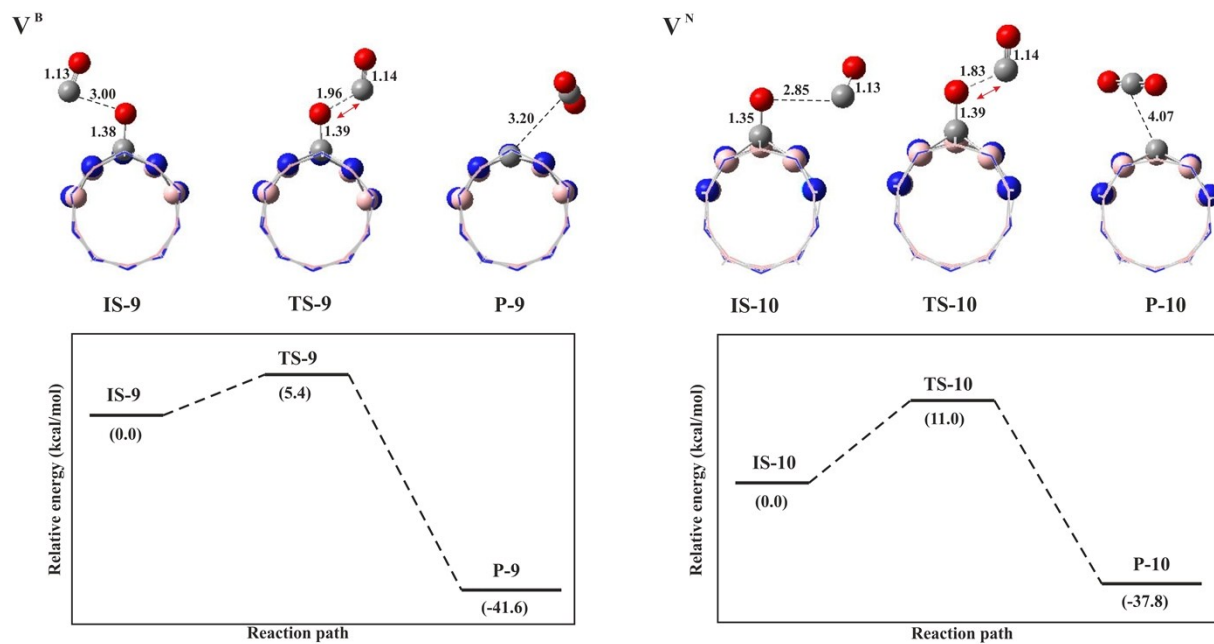
**Figure S2.** Optimized geometries of each step in the CO-vacancy recombination process over (5,0) BNNT. All energy values and distances are in kcal/mol and Å, respectively. For the transition state structures, the red arrow indicates the displacement vector along the imaginary frequency. The imaginary frequency value is shown within the bracket.



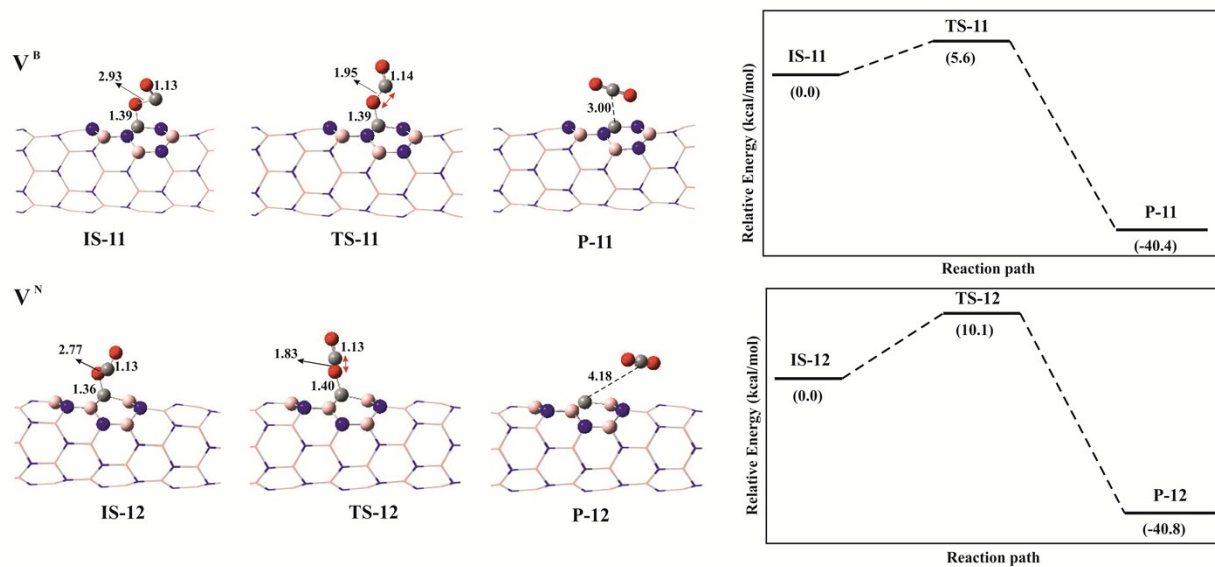
**Figure S3.** Optimized geometries of each step in the CO-vacancy recombination process over the long-length (6,0) BNNT. All energy values and distances are in kcal/mol and Å, respectively. For the transition state structures, the red arrow indicates the displacement vector along the imaginary frequency. The imaginary frequency value is shown within the bracket.



**Figure S4.** Optimized geometries along with their relative energy profile for extra O removal by CO molecule over the (5, 0) BNNT. All distances are in Å. For the transition state structures, the red arrow indicates the displacement vector along the imaginary frequency. The imaginary frequency value is shown within the bracket.



**Figure S5.** Optimized geometries along with their relative energy profile for extra O removal by CO molecule over the long-length (6, 0) BNNT. All distances are in Å. For the transition state structures, the red arrow indicates the displacement vector along the imaginary frequency. The imaginary frequency value is shown within the bracket.



**Table S1.** Atomic coordinates of the optimized structures at the M06-2X/6-31G\* level

<b>V<sup>B</sup></b>				<b>V<sup>N</sup></b>			
B	2.86068000	-2.12646800	1.16750700	B	-2.87374000	2.14428000	1.18947300
N	3.52616600	-2.67805200	-0.00268500	N	-3.55927700	2.62177500	0.00020100
N	1.41518800	-2.22513900	1.24425400	N	-1.42144300	2.29304200	1.24065500
B	0.70307600	-2.48603300	-0.00208600	B	-0.78573900	2.60344500	0.00021800
B	-1.45030900	-2.12433300	1.17508800	B	1.52662500	1.99610800	0.86971300
N	-0.73955500	-2.61099200	-0.00205200	N	2.92150000	2.31726200	1.21131000
N	-2.89677800	-2.21277600	1.23850300	B	3.67252200	2.62426600	0.00025000
B	-3.60822900	-2.48540900	-0.00149300	B	-2.80603000	0.02571600	2.33176000
B	2.86937600	0.04595300	2.18580400	N	-3.51239800	1.28666900	2.16520200
N	3.54232800	-1.23518100	2.08719000	N	-1.35918000	0.05011300	2.38800300
N	1.41613900	0.04398400	2.29264900	B	-0.66899900	1.24127200	1.92535500
B	0.70687600	-1.18386600	1.97224900	B	1.49768000	0.06717200	2.24523700
B	-1.46090000	0.01265100	2.22900900	N	0.75957900	1.26164200	1.86515500
N	-2.73596800	-1.23583500	2.08181800	N	2.93517600	0.12475800	2.39109200
N	-2.90562700	0.00376700	2.36039800	B	3.61407100	1.38283500	2.07314900
B	-3.60992800	-1.22480700	2.03250500	B	-2.78041800	-2.08443300	1.18807100
B	2.81967600	2.30717000	1.18709500	N	-3.46253600	-1.25728900	2.17127200
N	3.55672500	1.29511500	1.94305400	N	-1.33472700	-2.17620200	1.24778600
N	1.47270700	2.41593200	1.65000900	B	-0.63337800	-1.16693100	2.02800800
B	0.68451500	1.26350000	1.98910000	B	1.53878300	-2.04037500	1.18907100
B	-1.52069700	2.17989900	1.15351900	N	0.80668100	-1.21148300	2.13878300
N	-0.76207900	1.26305100	1.97381200	N	2.98884800	-2.07797700	1.24137500
N	-2.97598100	2.23156800	1.24816400	B	3.67773000	-1.07039800	2.04088700
B	-3.64790600	1.20810800	2.03313100	B	-2.78040700	-2.08423800	-1.18845100
B	2.81920100	2.30947600	-1.18337600	N	-3.45514500	-2.57744700	-0.00023400
N	3.37816000	2.94562300	0.00236600	N	-1.33471600	-2.17600000	-1.24816800
N	1.47187500	2.41868200	-1.64503300	B	-0.61523400	-2.41272000	-0.00020600
B	-1.52120400	2.18208700	-1.15041600	B	1.53879300	-2.04018700	-1.18940700
N	-0.94083900	2.85121900	0.00205900	N	0.83180600	-2.50877000	-0.00020800
N	-2.97652100	2.23387400	-1.24438900	N	2.98885900	-2.07778500	-1.24171200
B	-3.69911600	2.46396300	0.00225000	B	3.70633200	-2.31794300	-0.00018400
B	2.86870200	0.05012400	-2.18621200	B	-2.80600400	0.02610000	-2.33178500
N	3.55597200	1.29903000	-1.94170100	N	-3.46251300	-1.25693200	-2.17152100
N	1.41549500	0.04815600	-2.29302300	N	-1.35915400	0.05050600	-2.38800700
B	0.68384400	1.26704900	-1.98715500	B	-0.63335700	-1.16660000	-2.02821400
B	-1.46167300	0.01664100	-2.22911500	B	1.49770300	0.06753400	-2.24522200
N	-0.76281000	1.26677800	-1.97275700	N	0.80670200	-1.21114100	-2.13898900
N	-2.90642600	0.00783300	-2.36018600	N	2.93520100	0.12514800	-2.39105100
B	-3.64867300	1.21161200	-2.03072600	B	3.67774800	-1.07007200	-2.04105200
B	2.86035600	-2.12411100	-1.17155200	B	-2.87372400	2.14447400	-1.18914000
N	3.54179700	-1.23100400	-2.08953400	N	-3.51237300	1.28702500	-2.16501900
N	1.41481200	-2.22248800	-1.24806800	N	-1.42142500	2.29323900	-1.24027700
B	0.70626500	-1.18015900	-1.97424200	B	-0.66897700	1.24158100	-1.92514600
B	-1.45068900	-2.12198700	-1.17802200	B	1.52663800	1.99621100	-0.86934000
N	-0.73664500	-1.23193100	-2.08332700	N	0.75960200	1.26194000	-1.86493300
N	-2.89722900	-2.21013200	-1.24112600	N	2.92151400	2.31742900	-1.21086100
B	-3.61059700	-1.22115600	-2.03361400	B	3.61409700	1.38316200	-2.07286200
H	4.54944000	-1.18498800	1.97716800	H	-4.51912700	1.20251700	2.07070700
H	4.53289300	-2.54835400	-0.00266100	H	-4.56218200	2.46774000	0.00018100
H	4.55081800	1.22626300	1.75275700	H	-4.47203000	-1.21849100	2.07986800
H	4.54887800	-1.18083400	-1.97924600	H	-4.51910300	1.20285500	-2.07054200
H	4.39204100	2.85088900	0.00218000	H	-4.46180300	-2.45124200	-0.00022700
H	4.55027600	1.23023400	-1.75251100	H	-4.47200800	-1.21815000	-2.08012700
H	-4.78389200	-1.31516400	2.20990900	H	4.77124800	1.51847000	2.32645500
H	-4.82501500	1.25547300	2.20784800	H	4.85736600	-1.12338600	2.19882400
H	-4.78176100	-2.68648300	-0.00148800	H	4.82377000	2.92597000	0.00027600
H	-4.88274100	2.58792200	0.00264400	H	4.88756700	-2.47002500	-0.00018900
H	-4.78463900	-1.31127900	-2.21062000	H	4.77127800	1.51883900	-2.32612600

H	-4.82583900	1.25922400	-2.20498000	H	4.85738500	-1.12303800	-2.19899100
<b>IS-1</b>				<b>IS-2</b>			
B	-2.52468400	-2.59546300	-1.30366800	B	-2.93028400	1.89878100	1.18716800
N	-3.10676600	-3.31211100	-0.17922900	N	-3.62627100	2.39611500	0.00014200
N	-1.07890600	-2.51289700	-1.38906400	N	-1.49427600	2.10862500	1.25349500
B	-0.32844600	-2.77988100	-0.16683200	B	-1.04976000	2.74715500	0.00014400
B	1.75487700	-2.07981900	-1.31531500	B	1.59356300	1.82510500	0.87271900
N	1.11855300	-2.73254500	-0.17703300	N	2.99575600	2.05286900	1.21339700
N	3.20081100	-1.99062800	-1.38624800	B	3.75412300	2.33674400	0.00028300
B	3.95125800	-2.26361300	-0.16995000	B	-2.80596200	-0.24081100	2.27668500
B	-2.79944700	-0.36948700	-2.16022600	N	-3.55572400	0.98796000	2.12317800
N	-3.31737800	-1.72438100	-2.15054700	N	-1.35620000	-0.16876200	2.28849000
N	-1.35753600	-0.19220600	-2.27578300	B	-0.69394900	1.04400800	1.82683800
B	-0.50580100	-1.34756700	-2.04264700	B	1.49127900	-0.11720600	2.22406800
B	1.50599400	0.11011400	-2.22400400	N	0.76247500	1.07901100	1.79631600
N	0.93205100	-1.22111500	-2.15625400	N	2.92594900	-0.08462700	2.43851300
N	2.94049000	0.27913200	-2.35994000	B	3.64708100	1.14410000	2.13371500
B	3.78633000	-0.87795500	-2.11676400	B	-2.74299200	-2.37582900	1.18473900
B	-3.00587700	1.81321400	-1.01134800	N	-3.42972000	-1.54671700	2.16069900
N	-3.62717500	0.76781400	-1.82136700	N	-1.29665200	-2.44348600	1.24705200
N	-1.68465200	2.10186800	-1.46891700	B	-0.61893600	-1.38552800	1.98250000
B	-0.76777700	1.08097000	-1.89081200	B	1.56521200	-2.24319800	1.18272100
B	1.32510300	2.18654900	-0.99757100	N	0.81830900	-1.40143800	2.10782900
N	0.66897600	1.25086000	-1.88181300	N	3.01465000	-2.26208900	1.24183600
N	2.76358400	2.41122600	-1.08643100	B	3.67592300	-1.27810500	2.08963800
B	3.54192600	1.53498900	-1.94732000	B	-2.74295900	-2.37595400	-1.18474300
B	-2.98652300	1.64573900	1.34510100	N	-3.40948000	-2.89051600	0.00001600
N	-3.61885600	2.31650500	0.21339400	N	-1.29661800	-2.44362700	-1.24701100
N	-1.65910900	1.86543500	1.81798600	B	-0.57655100	-2.67373900	0.00004100
B	1.34461100	2.02223200	1.30199100	B	1.56521600	-2.24334200	-1.18266800
N	0.68151300	2.70167000	0.20014500	N	0.87191800	-2.74297100	0.00005700
N	2.78425800	2.23626900	1.39928200	N	3.01465000	-2.26224000	-1.24179700
B	3.46495300	2.63892100	0.17284000	B	3.73976500	-2.47453200	0.00003400
B	-2.76085700	-0.67782400	2.17798200	B	-2.80590200	-0.24097700	-2.27657900
N	-3.59487000	0.49082500	2.00297600	N	-3.42964300	-1.54692600	-2.16081300
N	-1.31716300	-0.51450800	2.29244100	N	-1.35614300	-0.16888700	-2.28842000
B	-0.73358800	0.80056600	2.07362800	B	-0.61889300	-1.38567900	-1.98247100
B	1.54510500	-0.20273200	2.23105100	B	1.49134400	-0.11734200	-2.22380800
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N	2.98184200	-0.05074200	2.36363300	N	2.92599300	-0.08475900	-2.43834800
B	3.57669500	1.25090500	2.11732300	B	3.67590600	-1.27834900	-2.08973400
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N	-3.27798100	-2.02183400	2.00129300	N	-3.55572500	0.98771200	-2.12275100
N	-1.05473100	-2.69394400	1.09553800	N	-1.49426800	2.10825300	-1.25304500
B	-0.46975100	-1.62645600	1.89232500	B	-0.69389200	1.04379300	-1.82649300
B	1.77671300	-2.24776100	1.03144600	B	1.59361500	1.82501400	-0.87231900
N	0.97011100	-1.51475800	1.99874400	N	0.76254700	1.07881800	-1.79584900
N	3.22400000	-2.16747200	1.08696100	N	2.99589800	2.05250900	-1.21280200
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H	-4.12180400	-3.30665200	-0.16894600	H	-4.62719900	2.22801600	0.00015600
H	-4.60141400	0.56527300	-1.62392100	H	-4.44114200	-1.53092300	2.08529100
H	-4.28447400	-2.08456800	1.89181600	H	-4.55807800	0.87343000	-2.01965800
H	-4.61852600	2.12123300	0.20737900	H	-4.41759600	-2.77558000	-0.00000400
H	-4.56993900	0.311196100	1.78796200	H	-4.44106600	-1.53111500	-2.08540800
H	4.96062100	-0.82149000	-2.30513900	H	4.79137200	1.27596400	2.43862700
H	4.70322400	1.73318200	-2.12152900	H	4.84860300	-1.33697300	2.29122200
H	5.14058900	-2.31687700	-0.18488200	H	4.91553900	2.59661100	0.00031300
H	4.62433000	2.90684300	0.18184500	H	4.92642600	-2.58085100	0.00004300
H	5.00006800	-1.12889400	2.12484900	H	4.79137000	1.27596700	-2.43851100
H	4.74111700	1.42500800	2.29628500	H	4.84863200	-1.33708400	-2.29106200
C	-1.64333600	4.71877100	0.52461000	C	-0.42661000	4.11980500	-0.00081400



O	-1.59575700	5.05380600	-0.55662600	O	0.13642400	5.13057200	-0.00310700
<b>TS-1</b>				<b>TS-2</b>			
B	-2.72962800	-2.33198700	-1.18538600	B	2.78110800	1.88032100	-1.43160300
N	-3.38382800	-2.85948800	0.00000200	N	3.52280600	2.56470000	-0.37557000
N	-1.27962700	-2.38386100	-1.25025400	N	1.32120900	1.98088200	-1.42761900
B	-0.55872500	-2.59551800	-0.00000600	B	0.88470900	2.73065300	-0.24484400
B	1.58595900	-2.16869500	-1.18862500	B	-1.71798400	1.54868500	-1.07804800
N	0.89054400	-2.64817600	-0.00001200	N	-3.13054300	1.69459300	-1.37655700
N	3.03679000	-2.19158300	-1.24073200	B	-3.80637300	2.24430300	-0.20275800
B	3.75808300	-2.42623400	-0.00001700	B	2.76062200	-0.36154800	-2.30854900
B	-2.80501000	-0.21861400	-2.31028400	N	3.42194800	0.92672400	-2.31026800
N	-3.44139900	-1.51253400	-2.15130400	N	1.31206200	-0.37849500	-2.29062600
N	-1.36159800	-0.17928800	-2.42197200	B	0.58151700	0.82768300	-1.93938100
B	-0.60640600	-1.36412200	-2.04281100	B	-1.53673700	-0.50901900	-2.18856700
B	1.50705500	-0.08074700	-2.33795500	N	-0.86741000	0.76919700	-1.93914700
N	0.84032000	-1.35967000	-2.14265100	N	-2.97913700	-0.57155900	-2.33762100
N	2.95146100	-0.01326000	-2.43324200	B	-3.76803200	0.64115800	-2.13311200
B	3.71206300	-1.19359600	-2.05447600	B	2.85189700	-2.35839000	-0.98860700
B	-2.84475400	1.91481100	-1.15849400	N	3.46839500	-1.60424400	-2.06941000
N	-3.50251400	1.03670700	-2.10814600	N	1.41158500	-2.51697200	-1.00187900
N	-1.40222300	1.98767000	-1.18152600	B	0.65390600	-1.59951800	-1.84021200
B	-0.68321000	1.02285700	-1.97390400	B	-1.45472700	-2.47735300	-0.87979100
B	1.40579600	2.02766900	-1.18420500	N	-0.78095000	-1.72477300	-1.93317000
N	0.74611200	1.13632400	-2.10707900	N	-2.89973400	-2.59390300	-0.89489400
N	2.84746800	2.16926100	-1.23288600	B	-3.64374600	-1.75867100	-1.82918900
B	3.60316100	1.22594900	-2.04403400	B	2.91366700	-2.06202300	1.35882600
B	-2.84473000	1.91482000	1.15851500	N	3.57333700	-2.69334400	0.22772700
N	-3.51796000	2.47886900	0.00001800	N	1.47305800	-2.17418200	1.46682700
N	-1.40219300	1.98767000	1.18152100	B	0.73406000	-2.61405400	0.28799500
B	1.40581100	2.02765700	1.18423100	B	-1.39926000	-2.10722800	1.45300900
N	0.67855200	2.49364100	0.00002100	N	-0.70744800	-2.75874100	0.34287800
N	2.84747800	2.16925500	1.23291300	N	-2.84571800	-2.16775000	1.55037100
B	3.55074200	2.47967300	0.00000800	B	-3.58239300	-2.64221300	0.38990800
B	-2.80499000	-0.21860400	2.31030100	B	2.91699200	0.18605800	2.21527100
N	-3.50249200	1.03671400	2.10816900	N	3.59033300	-1.09926300	2.21038500
N	-1.36158300	-0.17930000	2.42197800	N	1.46557800	0.20130200	2.26500000
B	-0.68319100	1.02285800	1.97391900	B	0.76660000	-1.06460900	2.08738700
B	1.50706300	-0.08076900	2.33795400	B	-1.38597100	0.15202600	2.16843700
N	0.74612200	1.13632000	2.10711700	N	-0.66897100	-1.11211500	2.22314700
N	2.95147300	-0.01328500	2.43322900	N	-2.81936800	0.17901300	2.37180100
B	3.60317500	1.22592400	2.04403400	B	-3.53702300	-1.07052400	2.21723100
B	-2.72962400	-2.33198000	1.18539300	B	2.93080400	2.20109500	0.90866900
N	-3.44139100	-1.51253100	2.15131300	N	3.62061700	1.41861800	1.91072200
N	-1.27962100	-2.38387400	1.25024900	N	1.49979200	2.38542600	1.02785800
B	-0.60640300	-1.36412500	2.04279700	B	0.74402000	1.33883600	1.71155600
B	1.58596600	-2.16870800	1.18860200	B	-1.55856500	1.95371900	0.60544500
N	0.84033100	-1.35967500	2.14262100	N	-0.69441200	1.31122700	1.61897800
N	3.03679800	-2.19160400	1.24070300	N	-2.95825600	2.23951100	0.98651900
B	3.71207300	-1.19362000	2.05445600	B	-3.56123200	1.37595200	1.97946300
H	-4.44895600	-1.48818800	-2.03677800	H	4.43354300	0.89642400	-2.24741800
H	-4.39373800	-2.76075500	0.00000800	H	4.52967500	2.45202600	-0.43399200
H	-4.50958700	0.97307700	-2.00907600	H	4.47803600	-1.51979100	-2.01986000
H	-4.44894800	-1.48817400	2.03678400	H	4.62143500	1.31953100	1.78012800
H	-4.52871300	2.39558900	0.00005200	H	4.57522600	-2.53904600	0.18313400
H	-4.50956300	0.97306900	2.00910600	H	4.59817800	-1.05538000	2.10502800
H	4.89274500	-1.22883400	-2.20554300	H	-4.93154400	0.66600100	-2.38712900
H	4.77780400	1.36117700	-2.18633100	H	-4.81562700	-1.90827400	-1.98073400
H	4.94009500	-2.56915700	-0.00002100	H	-4.96908000	2.49652600	-0.18470700
H	4.71057300	2.74408000	0.00000300	H	-4.75741300	-2.82925400	0.44730500
H	4.89275200	-1.22887000	2.20554300	H	-4.70689000	1.49429700	2.28795400
H	4.77782500	1.36113200	2.18629600	H	-4.70935000	-1.12794500	2.42284500
C	-0.77218900	2.60120200	0.00001700	C	-0.33461100	3.67654500	-0.18265700

O	-0.93496000	3.97675300	-0.00006900	O	-0.93490200	4.67349500	-0.27343200
<b>P-1</b>				<b>P-2</b>			
B	-2.72962800	-2.33198700	-1.18538600	B	2.83416600	2.10123900	-1.19118100
N	-3.38382800	-2.85948800	0.00000200	N	3.50506100	2.59419200	-0.00017600
N	-1.27962700	-2.38386100	-1.25025400	N	1.38499200	2.19199200	-1.24003600
B	-0.55872500	-2.59551800	-0.00000600	B	0.69806400	2.53071700	-0.00025400
B	1.58595900	-2.16869500	-1.18862500	B	-1.59584700	1.98266000	-1.17722800
N	0.89054400	-2.64817600	-0.00001200	N	-3.03592800	1.97889000	-1.24202300
N	3.03679000	-2.19158300	-1.24073200	B	-3.74806100	2.28840700	-0.00025400
B	3.75808300	-2.42623400	-0.00001700	B	2.85940000	0.00380800	-2.33872800
B	-2.80501000	-0.21861400	-2.31028400	N	3.51272600	1.28842700	-2.18230700
N	-3.44139900	-1.51253400	-2.15130400	N	1.40702300	-0.03360100	-2.38358200
N	-1.36159800	-0.17928800	-2.42197200	B	0.66704300	1.14197200	-1.95045500
B	-0.60640600	-1.36412200	-2.04281100	B	-1.45735300	-0.17617200	-2.25495500
B	1.50705500	-0.08074700	-2.33795500	N	-0.79373400	1.09198000	-1.97221000
N	0.84032000	-1.35967000	-2.14265100	N	-2.90130400	-0.23393700	-2.36976900
N	2.95146100	-0.01326000	-2.43324200	B	-3.68843500	0.93191000	-2.00187700
B	3.71206300	-1.19359600	-2.05447600	B	2.94478000	-2.09856500	-1.19128100
B	-2.84475400	1.91481100	-1.15849400	N	3.57539500	-1.24945400	-2.18651500
N	-3.50251400	1.03670700	-2.10814600	N	1.50516200	-2.26181800	-1.24798700
N	-1.40222300	1.98767000	-1.18152600	B	0.75056900	-1.28151700	-2.01503300
B	-0.68321000	1.02285700	-1.97390400	B	-1.36142500	-2.29763500	-1.18044800
B	1.40579600	2.02766900	-1.18420500	N	-0.68833500	-1.39850200	-2.10754000
N	0.74611200	1.13632400	-2.10707900	N	-2.80301300	-2.44634300	-1.23979500
N	2.84746800	2.16926100	-1.23288600	B	-3.55542400	-1.49096300	-2.03724800
B	3.60316100	1.22594900	-2.04403400	B	2.94476600	-2.09833000	1.19162100
B	-2.84473000	1.91482000	1.15851500	N	3.64337500	-2.54911200	0.00022200
N	-3.51796000	2.47886900	0.00001800	N	1.50514200	-2.26155600	1.24831700
N	-1.40219300	1.98767000	1.18152100	B	0.80717900	-2.54431000	0.00019100
B	1.40581100	2.02765700	1.18423100	B	-1.36143900	-2.29744700	1.18078300
N	0.67855200	2.49364100	0.00002100	N	-0.62830100	-2.73672900	0.00021000
N	2.84747800	2.16925500	1.23291300	N	-2.80303400	-2.44613900	1.24013000
B	3.55074200	2.47967300	0.00000800	B	-3.50273900	-2.74691700	0.00018600
B	-2.80499000	-0.21860400	2.31030100	B	2.85934500	0.00422800	2.33874300
N	-3.50249200	1.03671400	2.10816900	N	3.57534700	-1.24905200	2.18673000
N	-1.36158300	-0.17930000	2.42197800	N	1.40696500	-0.03317400	2.38353400
B	-0.68319100	1.02285800	1.97391900	B	0.75052300	-1.28117100	2.01521200
B	1.50706300	-0.08076900	2.33795400	B	-1.45740300	-0.17581500	2.25495800
N	0.74612200	1.13632000	2.10711700	N	-0.68837300	-1.39817100	2.10775400
N	2.95147300	-0.01328500	2.43322900	N	-2.90135100	-0.23356700	2.36976900
B	3.60317500	1.22592400	2.04403400	B	-3.55545500	-1.49064800	2.03743000
B	-2.72962400	-2.33198000	1.18539300	B	2.83410400	2.10147900	1.19089800
N	-3.44139100	-1.51253100	2.15131300	N	3.51265100	1.28884100	2.18219600
N	-1.27962100	-2.38387400	1.25024900	N	1.38492800	2.19226300	1.23967700
B	-0.60640300	-1.36412500	2.04279700	B	0.66699200	1.14231800	1.95023000
B	1.58596600	-2.16870800	1.18860200	B	-1.59594000	1.98277100	1.17680500
N	0.84033100	-1.35967500	2.14262100	N	-0.79378700	1.09229200	1.97197800
N	3.03679800	-2.19160400	1.24070300	N	-3.03600900	1.97903300	1.24159100
B	3.71207300	-1.19362000	2.05445600	B	-3.68849700	0.93220200	2.00165000
H	-4.44895600	-1.48818800	-2.03677800	H	4.52227000	1.24678900	-2.09210500
H	-4.39373800	-2.76075500	0.00000800	H	4.51374100	2.48600600	-0.00014300
H	-4.50958700	0.97307700	-2.00907600	H	4.58241600	-1.15857300	-2.10412700
H	-4.44894800	-1.48817400	2.03678400	H	4.52219400	1.24718900	2.09197700
H	-4.52871300	2.39558900	0.00005200	H	4.64272200	-2.37436600	0.00020700
H	-4.50956300	0.97306900	2.00910600	H	4.58237500	-1.15819900	2.10439800
H	4.89274500	-1.22883400	-2.20554300	H	-4.87316000	0.92071200	-2.12877200
H	4.77780400	1.36117700	-2.18633100	H	-4.72482200	-1.62937500	-2.21258400
H	4.94009500	-2.56915700	-0.00002100	H	-4.91646100	2.51039000	-0.00033600
H	4.71057300	2.74408000	0.00000300	H	-4.66681400	-2.99635100	0.00019600
H	4.89275200	-1.22887000	2.20554300	H	-4.87321500	0.92103800	2.12860400
H	4.77782500	1.36113200	2.18629600	H	-4.72486600	-1.62902200	2.21271600
C	-0.77218900	2.60120200	0.00001700	C	-0.86333900	2.81491400	-0.00025600

O	-0.93496000	3.97675300	-0.00006900	O	-1.32126100	4.09198300	0.00018900
<b>IS-3</b>				<b>IS-4</b>			
H	-4.80597200	1.32700100	0.00331500	H	-4.60340400	1.74266200	-0.00141500
H	-4.38740200	0.13971300	2.27004000	H	-4.51357300	0.23605700	1.87194300
H	-4.39529700	0.10498100	-2.25502700	H	-4.51352600	0.23308500	-1.87241300
H	-4.27186800	-2.14440600	1.21202000	H	-4.38440500	-2.04101900	1.20909800
H	-4.27162400	-2.16898000	-1.18828600	H	-4.38434500	-2.04294200	-1.20654100
H	4.80283900	2.34062000	-0.01772200	H	4.92211400	2.15020500	-0.00144000
H	4.82462800	0.82751700	2.10718800	H	4.79899000	0.61198800	2.30505800
H	4.82130200	0.79876500	-2.11950000	H	4.79941800	0.60786300	-2.30515400
H	4.98797700	-1.62243400	1.34227500	H	4.87540800	-1.83475200	1.32042100
H	4.98529000	-1.64634000	-1.33723200	H	4.87498400	-1.83878300	-1.31957300
B	3.63318400	2.12124400	-0.01445900	B	3.75956700	1.89564900	-0.00126600
B	3.66029400	0.72671800	1.87788800	B	3.65865500	0.53246700	1.97081600
B	3.81113300	-1.54829000	1.18018500	B	3.69785700	-1.71243600	1.18715900
B	3.65683100	0.69981900	-1.88980300	B	3.65889900	0.52896100	-1.97138700
B	3.80931100	-1.56685900	-1.17191100	B	3.69767700	-1.71504900	-1.18558300
B	1.57598300	-0.68797300	-1.75009000	B	1.51776500	-0.74411500	-1.79627700
B	1.72332700	-2.15934500	0.00979400	B	1.57354700	-2.19348700	0.00143700
B	1.57855400	-0.66151800	1.75421100	B	1.51776300	-0.74126700	1.79702700
B	1.48421800	1.65106300	-1.09655600	B	1.60355900	1.38964100	-0.87228000
B	1.48698000	1.67074300	1.08069400	B	1.60348000	1.39124200	0.87031200
B	-0.65761000	0.35995900	1.49111700	B	-1.06272800	2.26362900	-0.00182700
B	-0.66144200	0.33086400	-1.48615800	B	-0.66886100	0.46864700	1.69523900
B	-0.45026600	-1.93060500	1.15702300	B	-0.66883900	0.46604600	-1.69607100
B	-0.45183300	-1.95071800	-1.14239600	B	-0.58045200	-1.85359600	1.14722500
B	-2.65882200	-1.04536200	-1.87847200	B	-0.58043600	-1.85545400	-1.14486100
B	-2.57486800	-2.44043500	0.01317500	B	-2.76231600	-0.89459000	-1.82740200
B	-2.65639600	-1.01397700	1.88805200	B	-2.70383200	-2.34240100	0.00154400
B	-2.98031100	1.09474600	-1.09752300	B	-2.76238700	-0.89173300	1.82834100
B	-2.97677000	1.12039000	1.10226700	B	-2.90671500	1.36505200	-1.17040100
N	2.92931200	1.79402500	-1.26206400	B	-2.90674800	1.36692200	1.16814000
N	2.93221500	1.81510100	1.24025700	N	3.00703000	1.59140400	-1.22099900
N	3.01445400	-0.57952200	1.93121400	N	3.00680600	1.59397200	1.21900500
N	3.17066000	-2.14882100	0.00947300	N	2.95458700	-0.75247800	1.99418200
N	3.01120200	-0.60679600	-1.93280500	N	3.02167500	-2.23973700	0.00145100
N	0.76278200	0.52996200	-1.66999300	N	2.95455100	-0.75582100	-1.99370000
N	0.99215300	-1.90893500	1.25395500	N	0.78421000	0.52693400	-1.70865500
N	0.99110800	-1.93213200	-1.23841600	N	0.85704600	-1.93027300	1.25529000
N	0.91436900	2.43258400	-0.01407700	N	0.85704200	-1.93238800	-1.25285500
N	0.76590500	0.55746300	1.67190800	N	0.78415700	0.52962700	1.70790400
N	-1.57642000	1.22263100	-0.74859600	N	-1.47595000	1.59949000	-1.26063100
N	-1.57035100	1.26156000	0.75266500	N	-1.47597400	1.60145600	1.25804800
N	-1.21332200	-0.96127500	-1.89983100	N	-1.31264900	-0.83138600	-1.88906600
N	-1.21100900	-0.93036500	1.89886300	N	-1.31270700	-0.82848200	1.88991300
N	-1.12425500	-2.56024500	0.01365000	N	-1.26135500	-2.46353500	0.00167600
N	-3.25993300	-2.21709300	-1.26048400	N	-3.37253600	-2.09929500	-1.27490000
N	-3.25997700	-2.18930800	1.28241500	N	-3.37259700	-2.09721100	1.27756700
N	-3.38738700	0.19318400	-2.16767200	N	-3.51251200	0.33808900	-2.00515200
N	-3.37940500	0.22740500	2.18116900	N	-3.51254000	0.34121400	2.00445300
N	-3.81565800	1.53182500	-0.00047700	N	-3.60333500	1.92147600	-0.00157500
C	-1.55251400	4.25573600	0.59796800	C	-0.49291400	3.65767300	-0.00174300
O	-1.81717000	4.24226000	-0.50351800	O	-0.05576000	4.72719200	-0.00032700
<b>TS-3</b>				<b>TS-4</b>			
H	-4.47893800	1.99178900	-0.00151700	H	-4.53797500	1.95685400	0.38596100
H	-4.46150700	0.40190600	1.85292200	H	-4.43213300	0.28864700	2.05950600

H	-4.46151800	0.39830700	-1.85305100	H	-4.61306100	0.65148100	-1.70484900
H	-4.41351200	-1.92775900	1.18000400	H	-4.48537200	-1.90613200	1.08600100
H	-4.41337000	-1.93039800	-1.17748200	H	-4.54889800	-1.67034600	-1.31877400
H	4.70124500	2.37979500	-0.00181800	H	4.94463100	2.03081300	0.18389300
H	4.78830100	0.73318700	2.03801800	H	4.88958100	0.01809800	2.20738700
H	4.78853700	0.72903100	-2.03801500	H	4.67915000	0.85513400	-2.21109400
H	4.89068400	-1.77778100	1.30412700	H	4.77406000	-2.29813800	0.96238800
H	4.89045900	-1.78149800	-1.30229800	H	4.72310900	-1.72790500	-1.61420800
B	3.55335700	2.06963400	-0.00153100	B	3.78000200	1.78864400	0.20404000
B	3.61480500	0.62634300	1.86466100	B	3.72980200	0.04637300	1.93901200
B	3.71446400	-1.65345500	1.17053000	B	3.60983700	-2.06411400	0.87540400
B	3.61491600	0.62258200	-1.86518900	B	3.53936800	0.76934900	-1.87341500
B	3.71440600	-1.65615600	-1.16831400	B	3.55061200	-1.60720800	-1.43946900
B	1.52632600	-0.71844500	-1.85221700	B	1.38768100	-0.50041800	-1.82824200
B	1.57788600	-2.13084500	0.00166700	B	1.43345600	-2.22805200	-0.30402700
B	1.52629700	-0.71488200	1.85319100	B	1.50600600	-1.08850400	1.70162000
B	1.42246400	1.54993200	-1.15990700	B	1.53450600	1.51094500	-0.60849300
B	1.42241900	1.55233800	1.15768400	B	1.69185500	1.11868200	1.08196700
B	-0.65550900	0.44112800	1.80470600	B	-0.92198100	2.24579500	0.18501500
B	-0.65549100	0.43766700	-1.80518600	B	-0.60052200	0.27017900	1.76552500
B	-0.58825100	-1.81666800	1.16518200	B	-0.75136300	0.73707700	-1.63922100
B	-0.58820500	-1.81905800	-1.16248600	B	-0.67206300	-1.95288400	0.94092200
B	-2.76896300	-0.83450900	-1.83766800	B	-0.73608200	-1.63398500	-1.33811200
B	-2.72604100	-2.25848000	0.00169800	B	-2.89726900	-0.52219200	-1.85647300
B	-2.76905000	-0.83097700	1.83876000	B	-2.85290300	-2.16303700	-0.19792600
B	-2.80415400	1.44654700	-1.13771200	B	-2.77404900	-0.95042200	1.79775000
B	-2.80412900	1.44888900	1.13574300	B	-2.94413800	1.65307200	-0.94715300
N	2.86135400	1.70286800	-1.23408600	B	-2.79030900	1.36126600	1.36544000
N	2.86125300	1.70565400	1.23178400	N	2.93793100	1.76209300	-0.99647500
N	2.97015900	-0.67815400	1.96162500	N	3.10482900	1.23416400	1.38433400
N	3.02811300	-2.20013400	0.00177900	N	2.94647600	-1.19283500	1.84082800
N	2.97016900	-0.68194600	-1.96089500	N	2.87731000	-2.33451600	-0.36198900
N	0.77211700	0.52727100	-1.95502100	N	2.81870700	-0.50036400	-2.04008800
N	0.85966400	-1.87176500	1.25264500	N	0.68608400	0.75652000	-1.56314500
N	0.85969900	-1.87447600	-1.24990800	N	0.76080600	-2.13502600	0.99862300
N	0.70457700	2.10940200	-0.00170600	N	0.69712400	-1.74230700	-1.47504500
N	0.77207200	0.53096400	1.95450300	N	0.84420500	0.22023500	1.82835400
N	-1.36457600	1.53946000	-1.18839700	N	-1.51938200	1.85956600	-1.09054900
N	-1.36457600	1.54214900	1.18642000	N	-1.33295700	1.48572700	1.38017800
N	-1.32518500	-0.84424500	-1.96620300	N	-1.44712100	-0.50910000	-1.95471300
N	-1.32525400	-0.84055000	1.96716400	N	-1.32656400	-0.99396500	1.83470200
N	-1.27668200	-2.38482800	0.00191900	N	-1.41845900	-2.34736500	-0.25659700
N	-3.40536500	-2.01593800	-1.26897100	N	-3.54191300	-1.75612400	-1.41987000
N	-3.40551600	-2.01312500	1.27172700	N	-3.47792000	-2.02915900	1.11617300
N	-3.45458100	0.44330700	-1.97189200	N	-3.61480900	0.74655400	-1.86334300
N	-3.45455800	0.44703100	1.97164000	N	-3.42057600	0.30662300	2.14303300
N	-3.46760300	2.08181200	-0.00163700	N	-3.53204500	2.08428900	0.32580100
C	-0.74887900	2.17770500	-0.00174400	C	0.25267400	3.24199400	0.11436200
O	-0.96022600	3.54199500	-0.00324000	O	0.83581800	4.24895300	0.16816300
<b>P-3</b>				<b>P-4</b>			
H	-4.47893800	1.99178900	-0.00151700	H	-4.53822400	0.62626100	1.92061100
H	-4.46150700	0.40190600	1.85292200	H	-4.58224200	-1.64466500	1.20501400
H	-4.46151800	0.39830700	-1.85305100	H	-4.52996000	2.06512100	-0.00089500
H	-4.41351200	-1.92775900	1.18000400	H	-4.58237700	-1.64496300	-1.20301200
H	-4.41337000	-1.93039800	-1.17748200	H	-4.53816100	0.62502700	-1.92137500
H	4.70124500	2.37979500	-0.00181800	H	4.82699000	0.31624000	1.94322400

H	4.78830100	0.73318700	2.03801800	H	4.66741200	-2.18866700	1.32893000
H	4.78853700	0.72903100	-2.03801500	H	4.84129300	2.21680100	-0.00057000
H	4.89068400	-1.77778100	1.30412700	H	4.66645200	-2.19255900	-1.32980800
H	4.89045900	-1.78149800	-1.30229800	H	4.82717500	0.31341200	-1.94142900
B	3.55335700	2.06963400	-0.00153100	B	3.64212300	0.35266600	1.81552100
B	3.61480500	0.62634300	1.86466100	B	3.51395300	-1.94450800	1.16816400
B	3.71446400	-1.65345500	1.17053000	B	3.51356700	-1.94664300	-1.16785000
B	3.61491600	0.62258200	-1.86518900	B	3.69475100	1.90504200	-0.00029400
B	3.71440600	-1.65615600	-1.16831400	B	3.64217200	0.35022800	-1.81492200
B	1.52632600	-0.71844500	-1.85221700	B	1.56051100	1.50535800	-1.14996800
B	1.57788600	-2.13084500	0.00166700	B	1.41791500	-0.79201700	-1.79598000
B	1.52629700	-0.71488200	1.85319100	B	1.35484500	-2.25022000	0.00076200
B	1.42246400	1.54993200	-1.15990700	B	1.56045900	1.50698900	1.14946100
B	1.42241900	1.55233800	1.15768400	B	1.41802600	-0.79016400	1.79622200
B	-0.65550900	0.44112800	1.80470600	B	-0.70027200	0.56144100	1.78161000
B	-0.65549100	0.43766700	-1.80518600	B	-0.76750800	-1.73756100	1.15899800
B	-0.58825100	-1.81666800	1.16518200	B	-0.72997200	2.10001600	-0.00081500
B	-0.58820500	-1.81905800	-1.16248600	B	-0.76761900	-1.73864400	-1.15766600
B	-2.76896300	-0.83450900	-1.83766800	B	-0.70027400	0.55992500	-1.78195500
B	-2.72604100	-2.25848000	0.00169800	B	-2.85810500	1.60563400	-1.16508100
B	-2.76905000	-0.83097700	1.83876000	B	-2.88074400	-0.63589600	-1.85699100
B	-2.80415400	1.44654700	-1.13771200	B	-2.92501900	-2.05589500	0.00096700
B	-2.80412900	1.44888900	1.13574300	B	-2.85817500	1.60645200	1.16368100
N	2.86135400	1.70286800	-1.23408600	B	-2.88067800	-0.63457800	1.85760600
N	2.86125300	1.70565400	1.23178400	N	2.99774200	1.52092000	1.24046200
N	2.97015900	-0.67815400	1.96162500	N	2.85967400	-0.87401200	1.91794700
N	3.02811300	-2.20013400	0.00177900	N	2.78920100	-2.44764200	0.00078000
N	2.97016900	-0.68194600	-1.96089500	N	2.85947400	-0.87621000	-1.91812400
N	0.77211700	0.52727100	-1.95502100	N	2.99782700	1.51864300	-1.24039700
N	0.85966400	-1.87176500	1.25264500	N	0.66439300	-1.91821100	-1.25034000
N	0.85969900	-1.87447600	-1.24990800	N	0.75787900	0.51297500	-1.81843500
N	0.70457700	2.10940200	-0.00170600	N	0.75787300	0.51471300	1.81826700
N	0.77207200	0.53096400	1.95450300	N	0.66455000	-1.91681300	1.25156000
N	-1.36457600	1.53946000	-1.18839700	N	-1.41085400	1.71827400	1.23915800
N	-1.36457600	1.54214900	1.18642000	N	-1.43087700	-0.69185900	1.94155200
N	-1.32518500	-0.84424500	-1.96620300	N	-1.41077600	1.71735300	-1.24058400
N	-1.32525400	-0.84055000	1.96716400	N	-1.49111700	-2.26756700	0.00093700
N	-1.27668200	-2.38482800	0.00191900	N	-1.43095300	-0.69344900	-1.94094800
N	-3.40536500	-2.01593800	-1.26897100	N	-3.53013000	0.65425500	-2.04038400
N	-3.40551600	-2.01312500	1.27172700	N	-3.57799000	-1.77690100	-1.27472300
N	-3.45458100	0.44330700	-1.97189200	N	-3.52144000	2.18419500	-0.00091700
N	-3.45455800	0.44703100	1.97164000	N	-3.57781800	-1.77638900	1.27668800
N	-3.46760300	2.08181200	-0.00163700	N	-3.53019800	0.65567800	2.03959300
C	-0.74887900	2.17770500	-0.00174400	C	0.83621800	2.39311200	-0.00082900
O	-0.96022600	3.54199500	-0.00324000	O	1.32741200	3.65069100	-0.00221300
<b>IS-5</b>				<b>IS-6</b>			
B	-4.98599600	0.11049700	-2.36922900	B	5.05151700	2.27749700	0.00008900
N	-5.69137900	-1.15573700	-2.28693100	N	5.71617600	2.04537500	1.27201200
N	-3.53811900	0.08416800	-2.44768600	N	3.61356800	2.46351100	0.00010000
B	-2.85764200	-1.16257200	-2.12531200	B	2.88656000	2.02193000	1.19504100
B	-0.67485300	0.01005700	-2.28230300	N	1.00006200	2.84002200	0.00003600
N	-1.41346400	-1.24302100	-2.20657700	B	1.45033800	2.20734300	1.25565000
N	0.77247500	-0.01314000	-2.33548100	B	-1.61345100	1.89412800	0.87967000
B	1.45022100	-1.27065400	-2.06404700	B	-3.77385700	2.32293200	0.00001400
B	3.63305500	-0.09465400	-2.22582600	N	-3.01002400	2.11046900	1.22477200
N	2.89012000	-1.34133100	-2.15597600	N	-5.21278100	2.37696800	0.00002700
N	5.07764000	-0.12003100	-2.34861300	B	-5.88828600	1.94715700	1.21740600

B	5.75736900	-1.37892900	-2.08521400	B	5.00766300	1.03741600	-2.04190500
B	-4.95712500	2.12277600	-1.05866600	N	5.71614400	2.04529500	-1.27184000
N	-5.63561400	1.38225100	-2.10885700	N	3.56135400	1.11783100	-2.11084000
N	-3.50818600	2.19549900	-1.09099000	B	2.88659200	2.02163200	-1.19470800
B	-2.81306600	1.23644900	-1.93475500	B	0.67142600	1.12583700	-1.83372600
B	-0.66028000	2.11341900	-1.01688100	N	1.45032200	2.20673200	-1.25514800
N	-1.36990200	1.24824200	-1.97534500	N	-0.78301000	1.12990800	-1.79444700
N	0.71393300	2.25918700	-1.37229200	B	-1.61346200	1.89403800	-0.87963400
B	1.50388800	1.16451900	-1.88521200	B	-3.67951900	1.11741100	-2.04544600
B	3.72880600	2.00820200	-1.02689800	N	-3.01003400	2.11038700	-1.22473800
N	2.95011800	1.14813600	-1.88978900	N	-5.12969600	1.14017900	-2.16269100
N	5.18271900	2.03501800	-1.10510500	B	-5.88830400	1.94718200	-1.21735000
B	5.84272400	1.04568800	-1.94132400	B	4.95084600	-1.36099600	-2.05068000
B	-4.99037400	1.95854900	1.31218300	N	5.65049700	-0.17520100	-2.51144900
N	-5.64177000	2.54142000	0.15211800	N	3.50159200	-1.38362600	-2.12686000
N	-3.54424300	2.03025500	1.39592700	B	2.80975000	-0.11185300	-2.29215900
B	-2.80423900	2.35114500	0.17864200	B	0.64762700	-1.30475400	-1.98677400
B	-0.70597200	1.99237300	1.42074200	N	1.36010200	-0.07357000	-2.29892500
N	-1.35420900	2.48580800	0.20942200	N	-0.78949100	-1.35208100	-2.10509100
N	0.64482800	2.12502000	1.84998300	B	-1.49266900	-0.08108200	-2.21942100
B	3.68318200	1.88273100	1.27179100	B	-3.64893700	-1.29209800	-2.04080400
N	3.14196200	2.62444700	0.14686700	N	-2.93055400	-0.07876500	-2.41099400
N	5.13866800	1.90557800	1.38534200	N	-5.09444900	-1.34639700	-2.14896000
B	5.88731900	2.18755400	0.16417500	B	-5.81628200	-0.11500600	-2.42432800
B	-5.04128100	-0.21683600	2.33333800	B	4.94617200	-2.58703500	-0.00001100
N	-5.69141300	1.07726000	2.23009200	N	5.61819100	-2.39193000	-1.27325400
N	-3.59569000	-0.25106800	2.44142500	N	3.50212000	-2.70053100	-0.00003300
B	-2.86753400	0.96746500	2.12429400	B	2.79196900	-2.24584000	-1.18856300
B	-0.72302600	-0.27728600	2.31646600	B	0.63973200	-2.59828900	-0.00003900
N	-1.42944600	0.98745500	2.21841800	N	1.35126500	-2.34744400	-1.25019700
N	0.72715000	-0.29211700	2.35601500	N	-0.80337200	-2.70683900	-0.00001200
B	1.44755000	0.95215200	2.09972700	B	-1.50793600	-2.23022400	-1.18820500
B	3.58387700	-0.33314700	2.23335000	B	-3.66627100	-2.51907700	0.00004900
N	2.89516500	0.93972600	2.03676700	N	-2.94999300	-2.29932100	-1.25006600
N	5.02537600	-0.36989400	2.37884300	N	-5.11280100	-2.59650600	0.00008700
B	5.78831600	0.84036800	2.13160800	B	-5.81565000	-2.18879500	-1.20692400
B	-5.06605500	-2.22291500	1.02648800	B	4.95084400	-1.36096200	2.05062900
N	-5.73777900	-1.46194100	2.06559300	N	5.61816200	-2.39196600	1.27326400
N	-3.62202600	-2.35420300	1.08921500	N	3.50158700	-1.38350600	2.12672600
B	-2.89714800	-1.43248000	1.95427300	B	2.79197200	-2.24575200	1.18846000
B	-0.75387000	-2.32713100	1.05117600	B	0.64766600	-1.30459500	1.98660900
N	-1.45123900	-1.50846600	2.03834400	N	1.35127800	-2.34732600	1.25008300
N	0.68675300	-2.46244500	1.10993000	N	-0.78943300	-1.35194500	2.10497300
B	1.41409600	-1.49596900	1.92090100	B	-1.50789400	-2.23016500	1.18818400
B	3.55864500	-2.41029400	1.06098500	B	-3.64885100	-1.29205300	2.04087200
N	2.85282200	-1.56670900	2.01482100	N	-2.94993900	-2.29929500	1.25013200
N	5.00258700	-2.51883600	1.12953000	N	-5.09435300	-1.34638700	2.14912100
B	5.71810700	-1.58760700	1.98789600	B	-5.81558500	-2.18884600	1.20716000
B	-5.04398400	-2.05808500	-1.35080800	B	5.00766900	1.03749300	2.04205500
N	-5.74020600	-2.60945600	-0.20128400	N	5.65049900	-0.17520200	2.51143500
N	-3.60016800	-2.18842800	-1.40546200	N	3.56137100	1.11799200	2.11107100
B	-2.90720500	-2.53070900	-0.16920200	B	2.80978600	-0.11173300	2.29211000
B	-0.73409500	-2.18603400	-1.32352400	B	0.67148200	1.12611600	1.83381300
N	-1.46783000	-2.69168200	-0.16780700	N	1.36013900	-0.07341000	2.29869800
N	0.70658900	-2.32283800	-1.38280000	N	-0.78295700	1.13007600	1.79450200
B	1.40344400	-2.66590500	-0.14625500	B	-1.49260100	-0.08096300	2.21938300
B	3.57839900	-2.28604300	-1.28769100	B	-3.67948100	1.11746700	2.04548000
N	2.84472300	-2.81856500	-0.14412000	N	-2.93047900	-0.07869300	2.41098700
N	5.02324700	-2.39340300	-1.34462300	N	-5.12965400	1.14018800	2.16275100
B	5.72221700	-2.73866300	-0.11589500	B	-5.81620000	-0.11500500	2.42447000
H	-6.69839500	-1.08199800	-2.18895700	H	6.71950200	1.90727300	1.21242100
H	-6.64484200	1.33642100	-2.01710700	H	6.71947200	1.90721200	-1.21225000

H	-6.65010900	2.43170200	0.12954100	H	6.65834700	-0.19970100	-2.39998400
H	-6.69825400	1.04412800	2.11146100	H	6.62633100	-2.29405900	-1.21496600
H	-6.74250900	-1.37664100	1.95430500	H	6.62630600	-2.29412600	1.21498500
H	-6.74355600	-2.45929700	-0.19955300	H	6.65834800	-0.19969800	2.39996700
H	6.92984500	-1.48207800	-2.26329400	H	-7.07012900	2.04946600	1.31969300
H	7.02257800	1.07635900	-2.09877400	H	-7.07014000	2.04955500	-1.31964000
H	7.07270000	2.28783000	0.19020900	H	-6.98801200	-0.13396900	-2.63426300
H	6.96131800	0.86736800	2.33349500	H	-6.99306100	-2.33780700	-1.30381900
H	6.88862900	-1.70236700	2.17268000	H	-6.99297100	-2.33797000	1.30417000
H	6.89294500	-2.95422600	-0.11675900	H	-6.98792100	-0.13398900	2.63446000
C	1.03569300	4.83177300	0.17125500	C	0.38100400	4.21509900	-0.00045300
O	1.67484900	5.49736000	-0.48526600	O	-0.17929900	5.22691700	-0.00103100
<b>TS-5</b>				<b>TS-6</b>			
B	-4.99670700	-0.02514800	-2.37307800	B	5.04505300	2.32458800	-0.28316800
N	-5.69092900	-1.28777800	-2.19208600	N	5.73983900	2.23152100	0.99027300
N	-3.54925600	-0.04476800	-2.47056300	N	3.60380400	2.49430200	-0.26650600
B	-2.85956600	-1.26060700	-2.05765600	B	2.92739100	2.20597900	0.99747300
B	-0.69236800	-0.09275300	-2.35337600	B	0.92794600	2.77412600	-0.21200300
N	-1.41723700	-1.33870700	-2.14949500	N	1.50139900	2.41475700	1.07607100
N	0.74695700	-0.11088100	-2.45055400	B	-1.55146800	2.03654700	0.57777100
B	1.44926000	-1.32477500	-2.05563400	B	-3.76469200	2.31414500	-0.29869200
B	3.61014400	-0.12318900	-2.34141700	N	-2.96221300	2.31504300	0.92192800
N	2.89367000	-1.37599600	-2.14603000	N	-5.20631500	2.36033500	-0.29020100
N	5.05525200	-0.11196000	-2.42958500	B	-5.85240500	2.11235900	0.99175100
B	5.76846000	-1.32221300	-2.05121500	B	4.96680300	0.87770400	-2.17732000
B	-4.97464600	2.05955600	-1.19366100	N	5.68013200	1.97006400	-1.53985500
N	-5.65783900	1.25430400	-2.19072600	N	3.51513500	0.92594400	-2.21093600
N	-3.52770600	2.14256200	-1.24936900	B	2.84116400	1.89137600	-1.36071800
B	-2.82467900	1.14681300	-2.04713700	B	0.63395300	0.89213600	-1.93792100
B	-0.66554500	2.01928700	-1.17268500	N	1.38512900	2.02362200	-1.38735000
N	-1.37834800	1.17074700	-2.12083800	N	-0.81210200	0.86360700	-1.97042600
N	0.77558800	2.04642900	-1.18484800	B	-1.65763000	1.68184400	-1.13628200
B	1.46525200	1.06550800	-1.98987700	B	-3.71176400	0.79361500	-2.16034700
B	3.58660800	1.98762900	-1.18534600	N	-3.03996100	1.88791500	-1.49170300
N	2.89629300	1.12401000	-2.11303700	N	-5.16145700	0.79287300	-2.24003200
N	5.03165700	2.07501700	-1.23248900	B	-5.90191600	1.72697900	-1.40130700
B	5.75297800	1.10238600	-2.04119200	N	4.95750400	-1.51097400	-1.93885700
B	-4.97463300	2.05963100	1.19371900	N	5.62218900	-0.36595600	-2.53488400
N	-5.64586200	2.54471100	0.00001600	N	3.50959400	-1.56998800	-1.99519000
N	-3.52769700	2.14266100	1.24942200	B	2.79376700	-0.33476400	-2.27498600
B	-2.81822300	2.38991400	0.00001700	B	0.65547400	-1.53663300	-1.84735100
B	-0.66551300	2.01938200	1.17268500	N	1.34759600	-0.32718400	-2.28466000
N	-1.37591000	2.51377600	-0.00000100	N	-0.78082400	-1.63277700	-1.95889800
N	0.77564600	2.04648600	1.18477500	B	-1.50763600	-0.40121300	-2.23378500
B	3.58663300	1.98755200	1.18529300	B	-3.64769400	-1.59519700	-1.86511900
N	2.87378500	2.47482100	-0.00000100	N	-2.94901400	-0.43163200	-2.39694600
N	5.03166800	2.07493900	1.23246700	N	-5.09419800	-1.67565900	-1.94541100
B	5.74613900	2.36115200	-0.00000900	B	-5.83781200	-0.49017600	-2.34274700
B	-4.99669000	-0.02505500	2.37309800	B	4.99447000	-2.51021100	0.23175000
N	-5.65781800	1.25441400	2.19082300	N	5.65086100	-2.43970000	-1.06326100
N	-3.54923700	-0.04469200	2.47057100	N	3.55171900	-2.63903600	0.26379900
B	-2.82465000	1.14689700	2.04717200	B	2.82248000	-2.33701900	-0.96094700
B	-0.69236300	-0.09268100	2.35333500	B	0.68499100	-2.56894200	0.28042500
N	-1.37832300	1.17082700	2.12084000	N	1.38374300	-2.47181500	-0.99930200
N	0.74695600	-0.11084200	2.45050400	N	-0.75682300	-2.69488000	0.30959800
B	1.46527000	1.06551700	1.98983600	B	-1.48167700	-2.39180800	-0.92436900
B	3.61013400	-0.12321500	2.34146100	B	-3.62446000	-2.52666000	0.32037100

N	2.89629600	1.12397300	2.11299500	N	-2.92436000	-2.48418600	-0.96022500
N	5.05524300	-0.11198500	2.42963500	N	-5.07042900	-2.60995900	0.35573900
B	5.75297600	1.10234600	2.04121300	B	-5.79307200	-2.39026700	-0.88759300
B	-5.03015300	-2.10940900	1.19335600	B	5.01277400	-1.06994100	2.13814100
N	-5.69092000	-1.28766700	2.19204200	N	5.67834900	-2.17464500	1.46861900
N	-3.58569600	-2.23036800	1.24939000	N	3.56333200	-1.08713100	2.22760600
B	-2.85955900	-1.26052800	2.05763700	B	2.84900900	-2.04947700	1.39641500
B	-0.71509800	-2.19254000	1.19582900	B	0.70473600	-1.03385600	2.09964700
N	-1.41723600	-1.33863600	2.14946500	N	1.40900300	-2.14576000	1.47746400
N	0.72923800	-2.30723800	1.25206600	N	-0.73130300	-1.06700700	2.21157600
B	1.44924300	-1.32476100	2.05563400	B	-1.45379600	-2.06007000	1.42778500
B	3.60437400	-2.21270400	1.18891000	B	-3.58725900	-1.00456300	2.15106500
N	2.89365400	-1.37600700	2.14607000	N	-2.89398600	-2.11984300	1.51320900
N	5.05246800	-2.29391100	1.24011500	N	-5.02909900	-1.04226800	2.28558700
B	5.76845400	-1.32224800	2.05127900	B	-5.76049400	-2.01424700	1.49093200
B	-5.03015700	-2.10947200	-1.19335900	B	5.05908500	1.31272700	1.88853900
N	-5.71454400	-2.57588900	0.00001200	N	5.71572600	0.15730800	2.46702900
N	-3.58570000	-2.23044100	-1.24939800	N	3.61569300	1.40216500	1.98974400
B	-2.87702000	-2.47782100	0.00000300	B	2.86563400	0.19129000	2.28855100
B	-0.71509300	-2.19256900	-1.19582400	B	0.71495700	1.37301400	1.73692700
N	-1.43427900	-2.61973200	0.00000500	N	1.41463500	0.22323600	2.30247000
N	0.72924900	-2.30723200	-1.25204300	N	-0.72118300	1.35766500	1.60223100
B	1.44118800	-2.54851200	0.00001300	B	-1.43341900	0.20795200	2.15150600
B	3.60437800	-2.21268400	-1.18886400	B	-3.61138000	1.40674800	1.85166100
N	2.88694300	-2.65984300	0.00001600	N	-2.86692100	0.24611300	2.33380700
N	5.05247500	-2.29385900	-1.24004400	N	-5.06216400	1.43346100	2.00763100
B	5.76407700	-2.56072200	0.00003400	B	-5.74125500	0.21842600	2.42666900
H	-6.69735500	-1.21215300	-2.08919800	H	6.74304900	2.09639700	0.92227000
H	-6.66565500	1.20450100	-2.08623200	H	6.68611500	1.84768500	-1.49217200
H	-6.65367300	2.42891800	0.00002600	H	6.63263200	-0.35884500	-2.44667500
H	-6.66563300	1.20460200	2.08631300	H	6.65811600	-2.32401900	-1.02832500
H	-6.69734800	-1.21204900	2.08917800	H	6.68510000	-2.07701400	1.38957500
H	-6.71862100	-2.43110000	0.00001100	H	6.72178400	0.12238000	2.34291900
H	6.94710000	-1.40238600	-2.19904600	H	-7.02970800	2.23889900	1.11548800
H	6.93202000	1.19273800	-2.18005800	H	-7.08866600	1.79005300	-1.48108800
H	6.91435600	2.58453900	-0.00001100	H	-7.01331900	-0.54451200	-2.52332800
H	6.93203700	1.19263800	2.17995700	H	-6.96810900	-2.57177600	-0.94994600
H	6.94707100	-1.40249100	2.19924700	H	-6.93775600	-2.14066100	1.61916100
H	6.93812500	-2.75710600	0.00003200	H	-6.90851900	0.22627000	2.66203500
C	1.42785000	2.63335500	-0.00003000	C	-0.29149600	3.72537400	-0.15859600
O	1.31080700	4.01258500	-0.00023400	O	-0.86215200	4.74021200	-0.25973000
<b>P-5</b>				<b>P-6</b>			
B	-4.99670700	-0.02514800	-2.37307800	B	5.04554000	2.34637600	0.00015100
N	-5.69092900	-1.28777800	-2.19208600	N	5.71417700	2.13905300	1.27261500
N	-3.54925600	-0.04476800	-2.47056300	N	3.60239100	2.48823000	0.00014800
B	-2.85956600	-1.26060700	-2.05765600	B	2.88301300	2.05807500	1.19236400
B	-0.69236800	-0.09275300	-2.35337600	B	0.76389700	2.55187500	0.00012700
N	-1.41723700	-1.33870700	-2.14949500	N	1.44070400	2.19365900	1.24168000
N	0.74695700	-0.11088100	-2.45055400	B	-1.54237600	2.08741500	1.18911600
B	1.44926000	-1.32477500	-2.05563400	B	-3.69416600	2.36296700	0.00036400
B	3.61014400	-0.12318900	-2.34141700	N	-2.97800400	2.12499900	1.25670200
N	2.89367000	-1.37599600	-2.14603000	N	-5.13948100	2.40470500	0.00027500
N	5.05525200	-0.11196000	-2.42958500	B	-5.83875600	1.96051100	1.19835100
B	5.76846000	-1.32221300	-2.05121500	B	5.02245800	1.13758900	-2.06459300
B	-4.97464600	2.05955600	-1.19366100	N	5.71419600	2.13926700	-1.27233900
N	-5.65783900	1.25430400	-2.19072600	N	3.57471600	1.20184200	-2.14374300



N	-3.52770600	2.14256200	-1.24936900	B	2.88301800	2.05830300	-1.19215800
B	-2.82467900	1.14681300	-2.04713700	B	0.69124000	1.16894100	-1.95942600
B	-0.66554500	2.01928700	-1.17268500	N	1.44070100	2.19397100	-1.24153200
N	-1.37834800	1.17074700	-2.12083800	N	-0.76906300	1.16797000	-1.98647900
N	0.77558800	2.04642900	-1.18484800	B	-1.54234200	2.08709100	-1.18853900
B	1.46525200	1.06550800	-1.98987700	B	-3.65797100	1.09676400	-2.02767900
B	3.58660800	1.98762900	-1.18534600	N	-2.97793000	2.12464400	-1.25586700
N	2.89629300	1.12401000	-2.11303700	N	-5.10581600	1.10702700	-2.11978400
N	5.03165700	2.07501700	-1.23248900	B	-5.83873100	1.96037100	-1.19774900
B	5.75297800	1.10238600	-2.04119200	B	5.00483700	-1.25413700	-2.06592400
B	-4.97463300	2.05963100	1.19371900	N	5.68482600	-0.06285100	-2.54129700
N	-5.64586200	2.54471100	0.00001600	N	3.55612900	-1.29952100	-2.14588400
N	-3.52769700	2.14266100	1.24942200	B	2.84683700	-0.04212200	-2.34078300
B	-2.81822300	2.38991400	0.00001700	B	0.69556100	-1.25770600	-2.02358200
B	-0.66551300	2.01938200	1.17268500	N	1.39589500	-0.03143300	-2.39187900
N	-1.37591000	2.51377600	-0.00000100	N	-0.74467700	-1.32734800	-2.12008200
N	0.77564600	2.04648600	1.18477500	B	-1.47027300	-0.07889300	-2.28717300
B	3.58663300	1.98755200	1.18529300	B	-3.61129900	-1.30887500	-2.03755100
N	2.87378500	2.47482100	-0.00000100	N	-2.90963200	-0.08921700	-2.42247100
N	5.03166800	2.07493900	1.23246700	N	-5.05627600	-1.37704900	-2.13087100
B	5.74613900	2.36115200	-0.00000900	B	-5.79286400	-0.14683000	-2.37269100
B	-4.99669000	-0.02505500	2.37309800	B	5.01340200	-2.46191000	-0.00007300
N	-5.65781800	1.25441400	2.19082300	N	5.68414100	-2.26450200	-1.27306200
N	-3.54923700	-0.04469200	2.47057100	N	3.56932700	-2.58624900	-0.00010200
B	-2.82465000	1.14689700	2.04717200	B	2.85512000	-2.15045300	-1.19273700
B	-0.69236300	-0.09268100	2.35333500	B	0.70616500	-2.51904700	-0.00013700
N	-1.37832300	1.17082700	2.12084000	N	1.41422300	-2.26206400	-1.25041100
N	0.74695600	-0.11084200	2.45050400	N	-0.73403800	-2.65561900	-0.00017400
B	1.46527000	1.06551700	1.98983600	B	-1.44859100	-2.20406400	-1.19045700
B	3.61013400	-0.12321500	2.34146100	B	-3.60087400	-2.54011200	-0.00022600
N	2.89629600	1.12397300	2.11299500	N	-2.88938100	-2.30219900	-1.25054300
N	5.05524300	-0.11198500	2.42963500	N	-5.04477000	-2.65394700	-0.00024800
B	5.75297600	1.10234600	2.04121300	B	-5.75878100	-2.24907500	-1.20164100
B	-5.03015300	-2.10940900	1.19335600	B	5.00478100	-1.25440300	2.06591200
N	-5.69092000	-1.28766700	2.19204200	N	5.68410400	-2.26468900	1.27296200
N	-3.58569600	-2.23036800	1.24939000	N	3.55607200	-1.29979400	2.14584000
B	-2.85955900	-1.26052800	2.05763700	B	2.85508000	-2.15060400	1.19257200
B	-0.71509800	-2.19254000	1.19582900	B	0.69549700	-1.25792200	2.02345100
N	-1.41723600	-1.33863600	2.14946500	N	1.41417900	-2.26220800	1.25018500
N	0.72923800	-2.30723800	1.25206600	N	-0.74475000	-1.32752000	2.11984800
B	1.44924300	-1.32476100	2.05563400	B	-1.44863500	-2.20411600	1.19011000
B	3.60437400	-2.21270400	1.18891000	B	-3.61137200	-1.30896000	2.03719600
N	2.89365400	-1.37600700	2.14607000	N	-2.88943100	-2.30220100	1.25010300
N	5.05246800	-2.29391100	1.24011500	N	-5.05635700	-1.37713600	2.13043000
B	5.76845400	-1.32224800	2.05127900	B	-5.75882600	-2.24909700	1.20112700
B	-5.03015700	-2.10947200	-1.19335900	B	5.02242500	1.13731200	2.06477600
N	-5.71454400	-2.57588900	0.00001200	N	5.68477500	-0.06316600	2.54140700
N	-3.58570000	-2.23044100	-1.24939800	N	3.57468500	1.20155600	2.14389500
B	-2.87702000	-2.47782100	0.00000300	B	2.84677100	-0.04240900	2.34084400
B	-0.71509300	-2.19256900	-1.19582400	B	0.69115900	1.16869900	1.95957500
N	-1.43427900	-2.61973200	0.00000500	N	1.39583500	-0.03172000	2.39194500
N	0.72924900	-2.30723200	-1.25204300	N	-0.76912500	1.16782500	1.98669600
B	1.44118800	-2.54851200	0.00001300	B	-1.47032500	-0.07905900	2.28711400
B	3.60437800	-2.21268400	-1.18886400	B	-3.65800900	1.09677100	2.02811700
N	2.88694300	-2.65984300	0.00001600	N	-2.90970100	-0.08940000	2.42237000
N	5.05247500	-2.29385900	-1.24004400	N	-5.10586900	1.10697400	2.12023000

B	5.76407700	-2.56072200	0.00003400	B	-5.79294300	-0.14697900	2.37257400
H	-6.69735500	-1.21215300	-2.08919800	H	6.72007700	2.02038900	1.21566200
H	-6.66565500	1.20450100	-2.08623200	H	6.72009600	2.02060100	-1.21539100
H	-6.65367300	2.42891800	0.00002600	H	6.69261700	-0.07039600	-2.42598600
H	-6.66563300	1.20460200	2.08631300	H	6.69132100	-2.15707400	-1.21604500
H	-6.69734800	-1.21204900	2.08917800	H	6.69128700	-2.15725400	1.21598700
H	-6.71862100	-2.43110000	0.00001100	H	6.69256800	-0.07071300	2.42611600
H	6.94710000	-1.40238600	-2.19904600	H	-7.01846900	2.08644600	1.29535800
H	6.93202000	1.19273800	-2.18005800	H	-7.01844500	2.08631100	-1.29479300
H	6.91435600	2.58453900	-0.00001100	H	-6.96993800	-0.16978600	-2.55050400
H	6.93203700	1.19263800	2.17995700	H	-6.93199500	-2.42520500	-1.30087500
H	6.94707100	-1.40249100	2.19924700	H	-6.93205600	-2.42517600	1.30027600
H	6.93812500	-2.75710600	0.00003200	H	-6.97002200	-0.16999300	2.55036700
C	1.42785000	2.63335500	-0.00003000	C	-0.78739100	2.88360800	0.00040000
O	1.31080700	4.01258500	-0.00023400	O	-1.19105700	4.18069300	-0.00126300
<b>IS-7</b>				<b>IS-8</b>			
B	1.78867100	-2.90232800	1.67176100	B	-2.75123500	1.56924800	1.83968300
N	2.12381100	-3.87618800	0.64731900	N	-3.33904900	2.49286300	0.88368700
N	0.40910600	-2.46227200	1.77703700	N	-1.30202100	1.51436700	1.92587700
B	-0.47151300	-2.72610800	0.64459700	B	-0.54804300	2.19296500	0.88092000
B	-2.23997000	-1.34834900	1.72744300	B	1.65628200	1.09336400	1.82497200
N	-1.85750200	-2.30261200	0.69334800	N	3.08910400	0.94587100	1.88947900
N	-3.61213000	-0.88333700	1.81599900	B	3.86445200	1.58387300	0.82395100
B	-4.50127000	-1.16811400	0.70089500	B	-2.97472500	-0.78332300	2.22348300
B	2.63069500	-0.72851600	2.21279200	N	-3.52410000	0.53111500	2.49315800
N	2.81230000	-2.15707900	2.38541400	N	-1.53183100	-0.95317100	2.26509800
N	1.28975500	-0.19303800	2.33474200	B	-0.68988100	0.23301400	2.25244000
B	0.16961600	-1.12216300	2.29235900	B	1.31679100	-1.28271100	2.12108600
B	-1.39608700	0.81266700	2.29479400	N	0.76121900	0.05801900	2.26979900
N	-1.18394100	-0.62237400	2.42042100	N	2.74730000	-1.49474000	2.22113600
N	-2.73083900	1.36461000	2.40195500	B	3.63365600	-0.34342700	2.26450200
B	-3.85480100	0.44366600	2.35870500	B	-3.17837300	-2.37823500	0.44742000
B	3.21320900	0.89409500	0.51845700	N	-3.77783100	-1.85415200	1.66233500
N	3.65803500	0.14134400	1.67534100	N	-1.75785700	-2.66877200	0.45712900
N	1.86950000	1.45304900	0.55473000	B	-0.95857800	-2.06132400	1.51149900
B	0.97108800	1.02032200	1.60777100	B	1.09853600	-2.91308000	0.40155900
B	-0.78359900	2.39927700	0.59953600	N	0.46317700	-2.31983100	1.57045800
N	-0.32475800	1.62484800	1.73491200	N	2.52179700	-3.19089300	0.41842500
N	-2.09676800	3.01466000	0.64828100	B	3.31501700	-2.62272200	1.49749700
B	-3.00611000	2.61373900	1.71032300	B	-3.09773900	-1.57960500	-1.79400900
B	2.94507100	0.33373200	-1.73980400	N	-3.86825200	-2.34753500	-0.83111800
N	3.88820800	0.83426500	-0.76099500	N	-1.67348800	-1.83199600	-1.89322400
N	1.60470000	0.89316100	-1.75300700	B	-1.04095800	-2.57370800	-0.80900400
B	-1.04591400	1.81250100	-1.67148200	B	1.17931700	-2.12289800	-1.82236100
N	-0.08794500	2.26934400	-0.67413600	N	0.37568600	-2.87126000	-0.86366500
N	-2.37142500	2.40247900	-1.72298000	N	2.60759600	-2.35886700	-1.91689800
B	-2.80677200	3.21547200	-0.60218800	B	3.24012100	-3.11200300	-0.84469100
B	2.12183000	-1.86545800	-2.29388000	B	-2.81532000	0.77345400	-2.17109300
N	3.18322800	-0.89550300	-2.47812900	N	-3.62930400	-0.39606200	-2.44667000
N	0.75889600	-1.38445900	-2.36265200	N	-1.37005400	0.63116200	-2.21292900
B	0.53629500	0.04458500	-2.24536500	B	-0.82145300	-0.71766600	-2.28092600
B	-1.91183900	-0.34889500	-2.24559200	B	1.46829000	0.21945300	-2.12340400
N	-0.79375600	0.57292900	-2.37235300	N	0.60612500	-0.91570300	-2.39970200
N	-3.26757700	0.15737500	-2.31761300	N	2.90697900	0.08725200	-2.24462900
B	-3.46063700	1.59713000	-2.25146500	B	3.45529600	-1.25671600	-2.34453000
B	1.53471800	-3.47957300	-0.62015100	B	-2.66738400	2.37207400	-0.39975200

N	2.34873300	-3.20769400	-1.79259100	N	-3.37214900	1.98821500	-1.60841300
N	0.13996700	-3.07549800	-0.63233900	N	-1.21400400	2.35814300	-0.40599300
B	-0.27488600	-2.12645600	-1.65630500	B	-0.55583200	1.53653300	-1.41613700
B	-2.49962300	-1.93687500	-0.56369700	B	1.73455000	1.89394700	-0.39819100
N	-1.65251500	-1.68161600	-1.72027500	N	0.89310400	1.37047300	-1.44065400
N	-3.88432600	-1.50178600	-0.57288700	N	3.17206000	1.78875300	-0.44875000
B	-4.30611200	-0.57552100	-1.61197700	B	3.76636700	1.00384100	-1.51241800
H	3.76037000	-2.49119900	2.24952100	H	-4.53035800	0.60689900	2.39005900
H	3.10846500	-4.11639600	0.59930400	H	-4.35242700	2.47410100	0.83917800
H	4.57996000	-0.27091600	1.58292400	H	-4.77071900	-1.65471500	1.60391000
H	3.32213700	-3.48201100	-1.71484000	H	-4.38433500	2.00503300	-1.54321700
H	4.79092200	0.37269200	-0.75108200	H	-4.85054300	-2.09920600	-0.77807300
H	4.12568800	-1.26012700	-2.39159200	H	-4.62914300	-0.25608800	-2.34828900
H	-4.96557000	0.83204900	2.54192800	H	4.80897100	-0.49501000	2.38902900
H	-4.05256900	3.16517100	1.84788600	H	4.46170900	-2.91397200	1.63005800
H	-5.66150900	-0.90863900	0.76572900	H	5.04872100	1.66816000	0.89666700
H	-3.82601000	3.82849700	-0.64305100	H	4.38347300	-3.43635300	-0.91708900
H	-5.44962600	-0.25954700	-1.71611600	H	4.94994700	0.94418000	-1.63644400
H	-4.54221100	2.07031400	-2.40666200	H	4.61605700	-1.42433900	-2.54957000
C	1.32750800	1.91655900	-0.73506200	C	1.02862200	2.32584100	0.99659600
O	2.08033500	3.05080400	-0.96859000	O	1.57565400	3.49885800	1.40445900
C	4.36172400	3.60617400	0.83231700	C	1.16510200	4.74723800	-1.05188200
O	4.46403700	4.66135900	0.43835100	O	0.85573000	5.82343500	-0.89377500
<b>TS-7</b>				<b>TS-8</b>			
B	-2.38203100	-3.01595600	-0.79472500	B	-2.50473600	2.18299600	1.55319800
N	-3.00233600	-3.39615300	0.46268800	N	-2.99679400	3.00825000	0.46310900
N	-0.93400400	-2.92006000	-0.84629300	N	-1.07293900	1.95266200	1.63676500
B	-0.21979100	-2.83739500	0.42352500	B	-0.26851100	2.33313700	0.48346100
B	1.89012600	-2.38623000	-0.81818700	B	1.79498000	1.14884300	1.59157600
N	1.22607500	-2.72903600	0.43368000	N	3.19989100	0.81673000	1.66022800
N	3.33569500	-2.26103200	-0.86430000	B	4.01304700	1.13664200	0.48621900
B	4.05328100	-2.20209000	0.39980600	B	-3.02277900	-0.02757700	2.29890200
B	-2.65914400	-1.15389200	-2.27889800	N	-3.38684900	1.37409900	2.37230800
N	-3.15563000	-2.46032300	-1.89263800	N	-1.61400600	-0.38109000	2.35535000
N	-1.22693800	-0.97094500	-2.38128700	B	-0.62459200	0.66788800	2.15989700
B	-0.35738800	-1.98296300	-1.80045900	B	1.16236400	-1.09972600	2.23768400
B	1.60929200	-0.54915900	-2.31867200	N	0.79173800	0.31002400	2.19626900
N	1.08088800	-1.83834300	-1.89793500	N	2.55541000	-1.48345000	2.35412900
N	3.04005500	-0.34441300	-2.41793300	B	3.58256700	-0.46311500	2.22632000
B	3.91519900	-1.34973100	-1.83850800	B	-3.48341500	-1.82700100	0.78402900
B	-2.96480700	1.11044600	-1.49728600	N	-3.97403700	-1.05242300	1.91026500
N	-3.49186300	0.03280100	-2.31520600	N	-2.11266100	-2.29718000	0.82479600
N	-1.53430800	1.35855400	-1.53983400	B	-1.21082800	-1.65169200	1.76644800
B	-0.68889200	0.35888700	-2.16237400	B	0.68575900	-2.92563600	0.78204000
B	1.26053900	1.68886100	-1.52473300	N	0.16705500	-2.08306900	1.84992100
N	0.71811400	0.60168500	-2.31236700	N	2.06153700	-3.38215900	0.82803300
N	2.68108900	1.97853200	-1.59838100	B	2.95469600	-2.76633900	1.79550700
B	3.54829400	1.00637900	-2.24393300	B	-3.36909100	-1.41378200	-1.56060100
B	-3.00163700	1.50508400	0.79953400	N	-4.20196500	-1.90398800	-0.47604500
N	-3.73147100	1.72365400	-0.43350200	N	-1.99377900	-1.86749800	-1.63157300
N	-1.57435200	1.76058300	0.80494200	B	-1.42901400	-2.50225900	-0.44672600
B	1.21309700	2.08659300	0.80107500	B	0.79678900	-2.52284900	-1.54407600
N	0.46454500	2.24192700	-0.43876500	N	-0.06541700	-2.99017600	-0.46559600
N	2.63114600	2.39797300	0.83048900	N	2.17802500	-2.95985600	-1.61359000
B	3.32349000	2.56342100	-0.43516600	B	2.74184400	-3.60736100	-0.43875200
B	-2.74967700	-0.36407600	2.30856800	B	-2.79450800	0.78857400	-2.30475000

N	-3.57203100	0.76144300	1.91063300	N	-3.76205800	-0.28982200	-2.39300600
N	-1.32218100	-0.14941300	2.40325100	N	-1.38191600	0.45087400	-2.34422600
B	-0.76967100	1.02855500	1.75907100	B	-1.01635400	-0.95318800	-2.20385800
B	1.51653100	0.24633800	2.31066800	B	1.38077800	-0.31844200	-2.21989000
N	0.63332800	1.31884700	1.88084500	N	0.36899700	-1.35707800	-2.30642000
N	2.94387500	0.48359300	2.39271500	N	2.78595600	-0.65847000	-2.32917700
B	3.46606000	1.70234400	1.79709300	B	3.14913100	-2.06306700	-2.22053000
B	-2.42974400	-2.61286800	1.54452800	B	-2.38613700	2.59523500	-0.78921300
N	-3.24215900	-1.72777300	2.36191400	N	-3.17182000	2.13419800	-1.91759700
N	-0.98425300	-2.49623900	1.61814500	N	-0.94944400	2.37802400	-0.80518300
B	-0.43836600	-1.29153700	2.22810500	B	-0.43512100	1.34372700	-1.69484600
B	1.84305200	-1.98389200	1.52476400	B	1.90001900	1.53633600	-0.75277100
N	0.99638400	-1.11377900	2.32885600	N	0.97992800	0.98768100	-1.71264300
N	3.28640200	-1.83972600	1.58158800	N	3.31275100	1.22792400	-0.79583700
B	3.83412200	-0.65213600	2.21681700	B	3.77532600	0.22867200	-1.73843100
H	-4.16221400	-2.52711000	-1.78697600	H	-4.37685000	1.56517300	2.26151000
H	-4.01673900	-3.40993900	0.44444700	H	-4.00458300	3.12033000	0.43130400
H	-4.48772700	-0.12788800	-2.21076700	H	-4.93478100	-0.73627200	1.83294300
H	-4.24435700	-1.83110600	2.24438100	H	-4.17073400	2.29443200	-1.84352000
H	-4.71248200	1.46863000	-0.40592900	H	-5.14232000	-1.52385900	-0.45438600
H	-4.56369100	0.56831500	1.82259500	H	-4.73080400	-0.00240200	-2.30366400
H	5.09580100	-1.28206900	-1.97941300	H	4.73052800	-0.74756400	2.37124000
H	4.70227300	1.24638400	-2.41450200	H	4.06147100	-3.17609900	1.95121500
H	5.24362300	-2.21437600	0.42565900	H	5.19971900	1.05976500	0.52650000
H	4.45173000	2.93978600	-0.47649800	H	3.83062000	-4.08846800	-0.46921500
H	5.00879900	-0.53345200	2.37326900	H	4.93766300	-0.00626500	-1.85586700
H	4.61414200	1.99423800	1.92141100	H	4.27058800	-2.41604800	-2.40782700
C	-0.99321000	2.21658700	-0.46752600	C	1.31250400	2.26205200	0.54862700
O	-1.47533100	3.47504900	-0.82741500	O	2.00201900	3.45338500	0.79966700
C	-0.94126700	4.75496700	0.54833700	C	2.27587400	4.46367300	-0.69377100
O	-1.30522400	5.82718300	0.45932200	O	2.72484500	5.50453800	-0.55535600
<b>P-7</b>				<b>P-8</b>			
B	2.21998500	-3.23234300	0.31986400	B	3.20730500	0.86792200	-0.76231500
N	2.87455300	-3.37649200	-0.96941800	N	3.91874200	0.89712300	0.51064400
N	0.77540700	-3.08372100	0.34308600	N	1.90314200	1.50218100	-0.81131600
B	0.11644600	-2.70876100	-0.90362300	B	1.27349200	1.82056300	0.47363900
B	-2.02553500	-2.43315800	0.33412300	B	-0.92074200	2.43679900	-0.84299200
N	-1.32298400	-2.53746400	-0.93991100	N	-2.27936700	2.94825800	-0.88052000
N	-3.46574000	-2.25392800	0.35745500	B	-2.95726600	3.18912800	0.39145500
B	-4.12780900	-1.90321800	-0.88939100	B	2.55809100	-0.85262300	-2.28489000
B	2.50703700	-1.72740500	2.16396400	N	3.62500300	0.03870500	-1.87176400
N	2.97098900	-2.94714600	1.53080800	N	1.20750000	-0.32326600	-2.36884200
N	1.07630100	-1.51833000	2.26453600	B	0.91849400	0.96551800	-1.75256100
B	0.19292500	-2.34530600	1.45433200	B	-1.50202000	0.62200300	-2.32099000
B	-1.73940600	-0.95354800	2.18198400	N	-0.43828400	1.50355200	-1.85267200
N	-1.24271600	-2.15789200	1.53112100	N	-2.85938000	1.12039900	-2.45436000
N	-3.16287800	-0.69893000	2.27066200	B	-3.19466800	2.40814500	-1.87042800
B	-4.05129700	-1.52804000	1.47305200	B	1.77295400	-2.97573100	-1.51777500
B	2.91550700	0.64379900	1.88158400	N	2.74406200	-2.29103100	-2.35291000
N	3.37662300	-0.60576000	2.46471900	N	0.38751200	-2.56044900	-1.60478400
N	1.49839000	0.92795900	1.92389500	B	0.10815900	-1.26678600	-2.21264500
B	0.59913400	-0.15133800	2.30594800	B	-2.27672900	-1.50729700	-1.55898100
B	-1.26835800	1.38405000	1.88208000	N	-1.25872000	-0.81224900	-2.33458000
N	-0.80167700	0.12858400	2.43790700	N	-3.66237800	-1.08878500	-1.64632000
N	-2.67456300	1.72894500	1.97730800	B	-3.95290900	0.17119900	-2.31004600
B	-3.60726500	0.68350900	2.36587200	B	1.60501200	-3.36377500	0.83325100

B	3.07545000	1.50656200	-0.27955100	N	2.16666400	-3.84033200	-0.41882000
N	3.73774900	1.46586500	1.01119100	N	0.21106000	-2.96787200	0.85507500
N	1.65942600	1.80727300	-0.29356100	B	-0.44827700	-2.74563500	-0.42507000
B	-1.10447700	2.27223900	-0.29648500	B	-2.44718300	-1.89733600	0.77810600
N	-0.38948000	2.11476700	0.97282000	N	-1.84334700	-2.36346300	-0.46271000
N	-2.50388300	2.65215400	-0.30463900	N	-3.84072700	-1.49603000	0.79772800
B	-3.24430700	2.57477600	0.94251300	B	-4.50646400	-1.28586600	-0.47807100
B	2.81867500	-0.01317400	-2.14815100	B	2.21846800	-1.62722800	2.36297000
N	3.66323200	0.97202400	-1.49723400	N	2.43366700	-3.00917200	1.97134900
N	1.40254200	0.27595700	-2.25789500	N	0.85476300	-1.13046300	2.42857500
B	0.86625900	1.32451000	-1.41538700	B	-0.18561400	-1.94155600	1.80905500
B	-1.42417400	0.77425900	-2.15658500	B	-1.84265300	-0.15517200	2.29970600
N	-0.51593300	1.69382800	-1.49170600	N	-1.56769600	-1.51925300	1.87457900
N	-2.83588200	1.09162100	-2.22310100	N	-3.21705900	0.30357000	2.39636200
B	-3.32833400	2.19541400	-1.41157900	B	-4.25442600	-0.51590100	1.78817800
B	2.37908600	-2.35620400	-1.87762000	B	3.03228200	0.48189900	1.59234500
N	3.26135100	-1.35835000	-2.45876100	N	3.30998500	-0.67216500	2.42404000
N	0.94314000	-2.16162000	-1.97398300	N	1.71417000	1.07805800	1.64905400
B	0.46694500	-0.83639000	-2.34396100	B	0.62319400	0.29500900	2.22412300
B	-1.86630100	-1.55205600	-1.86824300	B	-1.09962700	2.02613600	1.59071200
N	-0.95489000	-0.57453600	-2.44483000	N	-0.74553200	0.80497800	2.30127200
N	-3.29960200	-1.33277900	-1.93970000	N	-2.46286200	2.52806600	1.59640800
B	-3.77640200	-0.01199500	-2.31860000	B	-3.49600500	1.71918900	2.21946300
H	3.97790800	-3.03344300	1.44331000	H	4.53827000	-0.39194300	-1.77580800
H	3.88605800	-3.44242500	-0.92165300	H	4.82482800	0.44008700	0.49998800
H	4.37108600	-0.77973900	2.37055800	H	3.70327700	-2.60078500	-2.23876500
H	4.25206900	-1.53075800	-2.32644700	H	4.23578200	-1.07237700	2.31614600
H	4.72097000	1.21816400	0.98369300	H	3.15408000	-4.07076300	-0.38625500
H	4.64571500	0.73118800	-1.42618700	H	3.40730400	-3.28406000	1.89715500
H	-5.23330500	-1.43619700	1.58545400	H	-4.27628100	2.88041000	-2.03057400
H	-4.75845000	0.93678700	2.53673700	H	-5.07701100	0.50515500	-2.51653700
H	-5.31570900	-1.86375400	-0.95858300	H	-4.02971500	3.70941600	0.40003800
H	-4.35891600	2.98366100	1.02488900	H	-5.67314600	-1.05074400	-0.52345800
H	-4.93918600	0.19168200	-2.47652200	H	-4.59958300	2.14086000	2.37108400
H	-4.46035300	2.55289800	-1.50808800	H	-5.40432900	-0.23705700	1.92317300
C	0.99726300	1.88028600	0.97988700	C	-0.12063300	2.47664400	0.48001600
O	2.75075400	4.68709800	0.05665000	O	3.00397900	3.94845000	0.81908000
C	1.62599400	4.64158700	-0.23243300	C	3.75710500	3.77669600	-0.05198500
O	0.50141000	4.63109700	-0.53514700	O	4.50938600	3.62857500	-0.92582600
<b>IS-9</b>				<b>IS-10</b>			
H	4.58187100	0.28571200	-0.49760500	H	-4.60718200	-0.26412000	2.03717900
H	4.02249000	-1.43139800	-2.07355900	H	-4.74210700	-1.99707300	0.40844200
H	4.31401200	-0.57899500	1.70130600	H	-4.46763800	1.84017400	0.88511000
H	3.45022700	-3.42854100	-0.83145600	H	-4.66680600	-0.95239200	-1.77309400
H	3.63898200	-2.90737200	1.47543800	H	-4.48058700	1.40186600	-1.46819000
H	-4.17704500	3.23951700	-0.46449600	H	4.72140800	-1.11895200	2.02639700
H	-4.81177100	1.31323100	-2.12565300	H	4.46647900	-3.06516800	0.34725900
H	-4.50263400	2.18163200	1.91463400	H	4.91420400	1.35470700	0.98931100
H	-5.49100900	-0.85801600	-0.81237100	H	4.54598000	-1.93609000	-2.05537900
H	-5.29549200	-0.31187000	1.73436300	H	4.84565000	0.58768800	-1.57614100
B	-3.14016000	2.65792900	-0.41806200	B	3.54788900	-0.95903900	1.89309200
B	-3.69715800	0.93966300	-1.93598400	B	3.32899100	-2.71822800	0.30583900
B	-4.31449100	-1.02149100	-0.73438200	B	3.40176200	-1.71378600	-1.81651500
B	-3.41616900	1.72760300	1.73768900	B	3.74241000	1.19103100	0.87167800
B	-4.13886100	-0.53079100	1.55714200	B	3.66204800	0.62297500	-1.43930900
B	-1.74031400	-0.08431700	1.98988600	B	1.62116200	1.49887900	-0.34956600

B	-2.28478800	-1.77697600	0.47797500	B	1.38561000	-0.28618000	-1.91723200
B	-2.02115100	-0.86674400	-1.66201000	B	1.19465200	-2.35791700	-0.89632200
B	-1.12651200	1.85117900	0.78771500	B	1.55009000	0.49566400	1.75460500
B	-1.29667700	1.37376300	-1.47272900	B	1.27205900	-1.84264100	1.36431800
B	0.37094700	-0.35164200	-1.92911400	B	-0.77248800	-0.49388800	1.91213900
B	0.65110900	0.42745500	1.64696400	B	-0.93617500	-2.27868300	0.35357700
B	-0.20826500	-2.30580100	-0.76613600	B	-0.66994200	1.65300800	0.93308700
B	-0.03065200	-1.81283900	1.50854500	B	-0.86280000	-1.28125200	-1.74684500
B	2.37045100	-1.31560900	1.93135400	B	-0.65763800	1.05322600	-1.34358000
B	1.83681400	-3.02641000	0.42867700	B	-2.78094600	1.84928700	-0.34569400
B	2.08385400	-2.12108700	-1.70759900	B	-2.89357500	0.13469800	-1.93149700
B	2.93459600	0.64546800	0.73381100	B	-3.07033900	-1.93436300	-0.84419600
B	2.76789200	0.13130400	-1.50952300	B	-2.85760900	0.84120200	1.76372300
N	-2.46951800	2.39634000	0.85088600	B	-3.01276600	-1.47304200	1.44686400
N	-2.65165400	1.88513400	-1.55494900	N	2.98378200	0.37986900	1.83675300
N	-3.41366800	-0.48001300	-1.74794600	N	2.70170900	-2.06441800	1.45294900
N	-3.69953100	-1.45781400	0.51665900	N	2.61873700	-2.61076500	-0.96768500
N	-3.11669200	0.34928400	2.11588600	N	2.82312300	-0.39450100	-2.06415600
N	-0.68961600	0.91444600	1.80822300	N	3.06101300	1.44910800	-0.40535300
N	-1.62191100	-1.98933000	-0.81095700	N	0.55986000	-1.49093400	-1.89290500
N	-1.43470800	-1.47056800	1.63051700	N	0.79379200	0.94306100	-1.39273000
N	-0.38056400	1.91492900	-0.46870800	N	0.67934400	-0.63994400	1.95165300
N	-0.98756600	0.08338400	-2.07343600	N	0.48175000	-2.56116100	0.36707600
N	1.57085900	1.14193100	0.76979200	N	-1.40959300	0.82302500	1.88410500
N	1.39878500	0.61722700	-1.56287700	N	-1.57177200	-1.65069300	1.51414300
N	0.98363400	-0.92397700	2.07487400	N	-1.32779300	1.89866100	-0.35228300
N	0.68116400	-1.76797500	-1.79559900	N	-1.64843000	-2.20064800	-0.92303100
N	0.40819000	-2.76132700	0.48199300	N	-1.44755200	0.03254900	-2.02851200
N	2.65110000	-2.70617500	1.59711100	N	-3.46901700	1.41956400	-1.55611500
N	2.44975500	-3.25982600	-0.87661500	N	-3.66801400	-1.10007800	-1.88182300
N	3.35811200	-0.25292800	1.80488300	N	-3.45539700	1.89244300	0.94733400
N	3.05513500	-1.13786600	-2.16827300	N	-3.74777100	-2.20333300	0.42006800
N	3.66276700	0.71526500	-0.52819600	N	-3.60233700	-0.34685800	2.15871300
C	1.04730900	1.61567000	-0.52540800	C	0.90537200	1.81546400	1.08069800
O	1.72997400	2.73643500	-0.94896000	O	1.44095300	2.95368300	1.57658200
C	4.00315400	3.45338900	0.86772200	O	1.04190900	4.28074300	-0.91363700
O	4.23087300	4.35200000	0.21915300	O	0.72615800	5.36416000	-0.84427000
<b>TS-9</b>				<b>TS-10</b>			
H	-4.57520500	1.18012400	-0.34157900	H	-4.58400700	0.66495200	1.99345000
H	-4.43905600	0.16911800	1.81038400	H	-4.94207400	-1.37710200	0.82666000
H	-4.39521000	-0.54143300	-1.99593500	H	-4.27374900	2.44040000	0.41105700
H	-4.23510100	-2.22889100	1.49426700	H	-4.84344300	-0.87300300	-1.52853900
H	-4.20377800	-2.66052100	-0.83721500	H	-4.42169000	1.45775800	-1.76786200
H	4.60007800	2.32969300	-0.43193100	H	4.60636000	-1.11543900	2.11482600
H	4.74330700	1.17253300	1.91450400	H	4.11753100	-3.34667000	0.90968700
H	4.79798500	0.41802400	-2.21664400	H	5.00774300	0.94392200	0.49170600
H	5.03526200	-1.41875700	1.59076000	H	4.22524800	-2.81264300	-1.67948000
H	5.07048900	-1.87583700	-0.97390900	H	4.77158000	-0.28339200	-1.85122600
B	3.46496400	1.97599400	-0.38313500	B	3.45228200	-0.86929900	1.94953400
B	3.58918700	0.93827500	1.73817400	B	3.01554000	-2.91036200	0.80340200
B	3.85430400	-1.40289400	1.44089100	B	3.11214200	-2.43501700	-1.49357800
B	3.63867200	0.25986400	-1.99567500	B	3.81959500	0.92145400	0.44004000
B	3.88540900	-1.82021000	-0.87534800	B	3.60333800	-0.11292000	-1.68994600
B	1.64751000	-1.19467700	-1.73553200	B	1.68917900	1.18494500	-0.78742000
B	1.77141500	-2.21887000	0.36486900	B	1.23693700	-0.87685300	-1.90832700
B	1.59794600	-0.52121100	1.96136700	B	0.88512000	-2.62545300	-0.42714400

B	1.38147300	1.13044100	-1.43593500	B	1.59933600	0.72022300	1.50276000
B	1.35145900	1.54285700	0.84657800	B	1.08765500	-1.61349300	1.65247800
B	-0.65308100	0.45738500	1.70240800	B	-0.79706000	0.02293800	1.90024200
B	-0.60290900	-0.20768700	-1.91127600	B	-1.18509200	-2.04713400	0.79590100
B	-0.42464900	-1.86336100	1.45776800	B	-0.51573500	1.85536500	0.45267800
B	-0.39430800	-2.28259300	-0.83873800	B	-1.09023200	-1.57386600	-1.47806600
B	-2.62414100	-1.61508900	-1.70761700	B	-0.64760800	0.75727600	-1.63028200
B	-2.51532800	-2.64387200	0.38690200	B	-2.64352400	1.97606900	-0.80855600
B	-2.67097900	-0.93446200	1.97147600	B	-2.98210200	-0.03824300	-1.95541500
B	-2.84414300	0.71932400	-1.40701500	B	-3.31683200	-1.77760800	-0.42448000
B	-2.86389600	1.13932400	0.85213200	B	-2.74309900	1.49729200	1.47280100
N	2.80960700	1.37087900	-1.53606500	B	-3.13586700	-0.80329800	1.69357400
N	2.77761500	1.80881500	0.89219000	N	3.02045600	0.47383000	1.58913900
N	3.03452400	-0.37163000	2.07060300	N	2.49092800	-1.95189700	1.77448600
N	3.22181600	-2.17578000	0.37542800	N	2.27582500	-3.03034700	-0.45171800
N	3.08644400	-1.08444700	-1.85053900	N	2.65116900	-1.16174100	-2.04235300
N	0.81205100	-0.04393800	-2.07996400	N	3.11847000	0.97300000	-0.85090100
N	1.02121800	-1.80314300	1.55112500	N	0.30081200	-1.95269000	-1.59052700
N	1.05340800	-2.24795500	-0.91069100	N	0.78559100	0.49446500	-1.67756600
N	0.61174200	1.79780800	-0.38837900	N	0.63419900	-0.25596200	1.95483700
N	0.75981100	0.67158800	1.84798200	N	0.19969600	-2.45775400	0.85764700
N	-1.40871600	0.92573600	-1.47569100	N	-1.30068500	1.35971300	1.58380900
N	-1.43248100	1.36632000	0.87325800	N	-1.71700300	-1.10541600	1.78430000
N	-1.18209600	-1.54214100	-1.82374900	N	-1.19448800	1.86533600	-0.84521300
N	-1.23284200	-0.82276200	2.09286000	N	-1.93054700	-2.19884200	-0.45481300
N	-1.06183500	-2.66075000	0.40793300	N	-1.55717700	-0.30719800	-2.04690700
N	-3.19112700	-2.69198300	-0.90645600	N	-3.41729600	1.34936600	-1.87207800
N	-3.22451200	-2.22850400	1.59353000	N	-3.86928500	-1.14544400	-1.61833800
N	-3.39063200	-0.44102300	-2.10412600	N	-3.25973800	2.39639900	0.44602800
N	-3.43694000	0.30295600	1.90476800	N	-3.97234000	-1.67470900	0.87592300
N	-3.59003800	1.42162100	-0.37685800	N	-3.58964400	0.51031600	2.12903300
C	-0.84752800	1.79751100	-0.41397300	C	1.07042100	1.87654300	0.52296600
O	-1.30799200	3.05201200	-0.79633800	O	1.70698900	3.07730700	0.83530900
C	-0.70994000	4.38531700	0.50642800	C	1.93450400	4.17978400	-0.60161100
O	-0.97420900	5.47356400	0.31771100	O	2.34357400	5.22771800	-0.40567100
<b>P-9</b>				<b>P-10</b>			
H	4.55162500	0.99564600	0.98732400	H	4.33115200	-0.68306900	-1.73004300
H	4.50290900	0.60045200	-1.42787900	H	3.62859800	-2.93923200	-1.45923500
H	4.30847600	-1.20930500	2.03052100	H	4.62999200	0.34948700	0.42331100
H	4.26062700	-1.79790600	-1.80878300	H	3.48629700	-3.36422600	0.90429400
H	4.14118800	-2.88571400	0.27195900	H	4.09670700	-1.36120300	2.03245000
H	-4.58136300	2.18654000	1.09077200	H	-4.63845600	1.98899700	-2.01687400
H	-4.66174200	1.77947300	-1.47415000	H	-5.30984900	-0.49564700	-1.68881700
H	-4.87058400	-0.14579100	2.21716200	H	-4.39386000	3.04294700	0.35621500
H	-5.00399300	-0.78088400	-1.94622400	H	-5.47274600	-0.96702900	0.90979100
H	-5.13481700	-1.98424600	0.36026900	H	-4.89659600	1.23429900	2.16216500
B	-3.44898000	1.84042500	0.97282000	B	-3.53296700	1.60004200	-1.80472900
B	-3.51599400	1.48197800	-1.34625900	B	-4.14536600	-0.66427200	-1.50650100
B	-3.82893400	-0.83854100	-1.76397200	B	-4.29136900	-1.08568000	0.82277200
B	-3.70620000	-0.26287700	1.99801400	B	-3.29934400	2.57158300	0.33713500
B	-3.94680900	-1.92384500	0.31489000	B	-3.76625200	0.91817100	1.96070600
B	-1.73208800	-1.64049000	1.38246800	B	-1.38421600	1.47707500	1.48969400
B	-1.79484100	-1.99053200	-0.92380700	B	-1.99200500	-0.81356800	1.71236100
B	-1.54371000	0.09558300	-1.94304800	B	-2.25255000	-1.80341700	-0.38728000
B	-1.42196700	0.65275900	1.78679000	B	-1.23749300	1.91108300	-0.88753100
B	-1.30282200	1.74431800	-0.27765000	B	-1.76252100	-0.14557600	-1.96165800

B	0.70920100	0.90358200	-1.39478700	B	0.65217400	0.44771000	-1.68975200
B	0.52324100	-0.82852600	1.92951700	B	-0.01816900	-1.81819700	-1.43971700
B	0.44583200	-1.38697400	-1.80186400	B	1.00934300	1.48914400	0.40884100
B	0.32906300	-2.46769500	0.26866400	B	-0.16108700	-2.23822600	0.85278200
B	2.54087000	-2.12177300	1.36520100	B	0.42386800	-0.21856900	1.94716100
B	2.49221800	-2.48585900	-0.93881100	B	2.82793000	0.20321900	1.47802400
B	2.72884800	-0.38947700	-1.94657100	B	2.13646000	-2.01732900	1.75117700
B	2.78694600	0.19923600	1.77383800	B	1.85878500	-3.00322600	-0.35261700
B	2.90494600	1.27185900	-0.26627400	B	2.97314400	0.61599500	-0.82244500
N	-2.84067500	0.91091000	1.91968700	B	2.36360700	-1.35192900	-1.92899400
N	-2.71572300	2.05806900	-0.26878500	N	-2.62226800	2.34633800	-0.94371500
N	-2.97093000	0.31082200	-2.03288600	N	-3.15697800	0.22413900	-2.11353500
N	-3.24403600	-1.91233300	-0.96480600	N	-3.67331200	-1.52520100	-0.42521900
N	-3.17016500	-1.52351700	1.48449800	N	-3.40213000	-0.48712200	1.81541400
N	-0.88737800	-0.67249500	2.08641700	N	-2.77476700	1.89594400	1.52658800
N	-0.99472000	-1.26248400	-1.91036600	N	-1.57750100	-1.95864500	0.90149400
N	-1.12003700	-2.41751400	0.30353300	N	-0.97715300	0.18649900	2.04639800
N	-0.57358900	1.55501400	0.99172100	N	-0.73682600	0.88797800	-1.80672000
N	-0.68615100	1.18774700	-1.47964900	N	-1.42359400	-1.50898500	-1.55686500
N	1.35462900	0.39127400	1.85267000	N	1.64013400	1.18504300	-0.88919300
N	1.47547800	1.51480400	-0.28475700	N	0.97766500	-0.93427700	-2.04722900
N	1.09492900	-2.07562800	1.45316900	N	1.47994200	0.72440600	1.56798900
N	1.29526400	-0.22940200	-2.08621900	N	0.43725500	-2.73029900	-0.38933100
N	1.04016800	-2.46825700	-1.01187800	N	0.73553800	-1.64592900	1.84569600
N	3.12690400	-2.92398600	0.30157600	N	3.14074200	-1.04389400	2.16060900
N	3.25523300	-1.74574900	-1.94114700	N	2.48755600	-3.18627700	0.95100800
N	3.30034000	-1.12424900	2.11447900	N	3.70114500	0.76048300	0.44130100
N	3.50374300	0.76606700	-1.49783000	N	2.63846900	-2.73576400	-1.55694800
N	3.55657400	1.19170500	1.03397700	N	3.39030500	-0.32172400	-1.85235500
C	0.78652400	1.32399700	0.94710800	C	-0.42275400	2.06373400	0.42336800
O	0.02925200	4.20850600	-0.43284500	O	2.50085100	3.65109800	0.82166000
C	1.14175300	4.32086700	-0.10611600	C	3.32401900	3.60372200	-0.00167000
O	2.24886000	4.46539500	0.21577600	O	4.14061900	3.58524900	-0.82769600
<b>IS-11</b>				<b>IS-12</b>			
B	-5.11136800	-0.84210100	-2.20408800	B	-5.04430200	2.06895100	0.80107500
N	-5.84300400	-1.93495800	-1.58855300	N	-5.70901900	2.30798800	-0.46787900
N	-3.66727500	-0.94694300	-2.29439200	N	-3.60042500	2.19384400	0.85059200
B	-3.00984200	-1.96800200	-1.48929600	B	-2.87995000	2.18748300	-0.41653300
B	-0.81183400	-1.05676400	-2.18465000	B	-0.76215900	2.23731500	0.87339900
N	-1.57276800	-2.12651800	-1.55646400	N	-1.43687300	2.32950200	-0.41771100
N	0.62410300	-1.15936000	-2.27440700	B	1.54228700	2.19929100	-0.40084300
B	1.29381100	-2.18685100	-1.48898300	B	3.69315300	2.03753400	0.81510500
B	3.48747100	-1.23953900	-2.18494400	N	2.97913100	2.24587400	-0.44750900
N	2.73375100	-2.31966200	-1.56409400	N	5.13917800	2.06860000	0.83081400
N	4.93069100	-1.31156800	-2.27565100	B	5.83849300	2.05086100	-0.44670900
B	5.60983300	-2.34378600	-1.50917200	B	-5.03309700	0.23953200	2.34654000
B	-5.00006700	1.52444000	-1.84098200	N	-5.71876000	1.44986100	1.92789000
N	-5.72672200	0.44290200	-2.48207200	N	-3.58514500	0.26667100	2.44515300
N	-3.55218100	1.52896300	-1.92973100	B	-2.88700200	1.38531300	1.82990000
B	-2.89647500	0.28945400	-2.32326200	B	-0.70023400	0.27844700	2.26078300
B	-0.69458700	1.33591800	-1.82790000	N	-1.44390200	1.48627600	1.92029800
N	-1.45178900	0.23236700	-2.40664000	N	0.75939600	0.26158000	2.28921700
N	0.74618200	1.30288800	-1.85400100	B	1.53907900	1.39112000	1.84562200
B	1.38951500	0.07542900	-2.26149400	B	3.64837100	0.16585400	2.30486500
B	3.55239700	1.14451700	-1.84912200	N	2.97465200	1.39542700	1.91895900
N	2.81880500	0.03318800	-2.40491400	N	5.09594000	0.13741200	2.39617700



N	4.99898700	1.15633900	-1.92904600	B	5.83434300	1.24508600	1.80931300
B	5.67506000	-0.06496300	-2.34090600	B	-5.02658700	-2.01865700	1.55814900
B	-4.95615300	2.37279400	0.38819200	N	-5.70247700	-1.04735500	2.39887000
N	-5.63311000	2.42862100	-0.89635600	N	-3.57820500	-2.09496000	1.61949200
N	-3.50632800	2.42191600	0.40363000	B	-2.86353500	-0.97649500	2.21878400
B	-2.81245900	2.18176800	-0.85636000	B	-0.71734500	-2.03222900	1.51971300
B	-0.65098000	2.17774000	0.35913700	N	-1.41266200	-0.99258300	2.27135400
N	-1.36668300	2.24687900	-0.90955100	N	0.72253400	-2.13690400	1.58828400
N	0.79168200	2.16835300	0.35578000	B	1.45332300	-1.01765400	2.15905100
B	3.59448100	2.01753900	0.36168500	B	3.58908100	-2.10801500	1.51964200
N	2.87803100	2.05626200	-0.92242100	N	2.89250700	-1.07941800	2.28312600
N	5.04225000	2.06115400	0.36703300	N	5.03367300	-2.21129700	1.58716000
B	5.74232700	1.84738700	-0.88859100	B	5.77592000	-1.13344500	2.22039700
B	-5.02392500	0.83255900	2.22082700	B	-5.03641500	-2.46743500	-0.79002100
N	-5.64747200	1.99070900	1.60743600	N	-5.70779300	-2.70772500	0.47530500
N	-3.57624600	0.79473800	2.30667300	N	-3.59309100	-2.59199700	-0.83177700
B	-2.82142700	1.73876600	1.49338600	B	-2.87892400	-2.58591700	0.43809200
B	-0.72503000	0.60483800	2.19809100	B	-0.72915400	-2.54649000	-0.80732100
N	-1.37375000	1.73457700	1.54695700	N	-1.43892100	-2.72041500	0.45643300
N	0.71424900	0.56651800	2.28010800	N	0.71047300	-2.68348200	-0.85239800
B	1.46325600	1.48692800	1.44316000	B	1.42476100	-2.66014800	0.42082900
B	3.57243900	0.41183400	2.16629200	B	3.57823400	-2.58754300	-0.81033800
N	2.89494100	1.52628900	1.52778200	N	2.86496400	-2.78204000	0.44671100
N	5.01905900	0.40133600	2.23121400	N	5.02188400	-2.70032800	-0.84735300
B	5.74565800	1.38901600	1.45157900	B	5.73401500	-2.72902100	0.42107200
B	-5.14604000	-1.53403600	1.85922800	B	-5.01678500	-0.63921200	-2.33650300
N	-5.76108200	-0.38656100	2.50277300	N	-5.70446700	-1.85026900	-1.92184900
N	-3.70552600	-1.67956000	1.94591500	N	-3.56809700	-0.66457600	-2.42742800
B	-2.93360700	-0.51237100	2.34913900	B	-2.87386000	-1.78780000	-1.80958600
B	-0.83697400	-1.76888700	1.86427700	B	-0.70719400	-0.68236300	-2.29480200
N	-1.49310400	-0.60516900	2.45364300	N	-1.43340400	-1.88203700	-1.89935600
N	0.60320600	-1.91025000	1.94974000	N	0.73254800	-0.72477400	-2.40865400
B	1.37035400	-0.73278600	2.34200900	B	1.43008900	-1.86353200	-1.82196600
B	3.47875000	-1.95068300	1.83873500	B	3.59900900	-0.74582600	-2.31938300
N	2.81335000	-0.80185900	2.43637900	N	2.87092700	-1.94156900	-1.90878400
N	4.92441300	-2.06045800	1.90656000	N	5.04391500	-0.78599600	-2.43025500
B	5.68717800	-0.88798700	2.30435500	B	5.74097400	-1.91952500	-1.84127400
B	-5.19024300	-2.38110200	-0.36977600	B	-5.02149500	1.61870400	-1.54615400
N	-5.86716800	-2.37053100	0.91567000	N	-5.68940300	0.64623200	-2.39134800
N	-3.75194600	-2.56889600	-0.38903100	N	-3.57306600	1.69678900	-1.59870500
B	-3.02885700	-2.38261500	0.86304100	B	-2.85143400	0.58218600	-2.19304500
B	-0.88118900	-2.62008000	-0.36833200	B	-0.68997000	1.58804600	-1.43166800
N	-1.59183000	-2.56849400	0.90547400	N	-1.40066300	0.60075100	-2.23438100
N	0.55701600	-2.80290200	-0.38943600	N	0.76732400	1.58175900	-1.44946100
B	1.28366700	-2.61003000	0.86319900	B	1.46348300	0.50439700	-2.14516500
B	3.43388900	-2.79825700	-0.37930600	B	3.65470000	1.52389000	-1.51482100
N	2.72459400	-2.76885700	0.89539100	N	2.90329200	0.53492400	-2.27601800
N	4.87681700	-2.94954600	-0.40808300	N	5.10316400	1.55598200	-1.60003100
B	5.60216400	-2.78439300	0.84233500	B	5.78516500	0.45245000	-2.25206600
H	-6.84379300	-1.78899100	-1.51020200	H	-6.71625700	2.18789100	-0.45551600
H	-6.73404300	0.47198500	-2.36652200	H	-6.72441000	1.35911500	1.83016200
H	-6.64380500	2.35450400	-0.84846700	H	-6.70981100	-1.01050200	2.28504300
H	-6.65776100	1.94134900	1.53002500	H	-6.71492800	-2.58731700	0.45766500
H	-6.76683300	-0.31637000	2.39044500	H	-6.71064600	-1.75925000	-1.82980500
H	-6.86534100	-2.19537000	0.86885300	H	-6.69728200	0.60637100	-2.28344000
H	6.78216200	-2.51526200	-1.62725200	H	7.01820400	2.20230400	-0.49684600

H	6.85422500	-0.07303900	-2.50632500	H	7.01487500	1.32350300	1.94132800
H	6.91824500	2.00561000	-0.97446600	H	6.95304600	-1.21936100	2.37790700
H	6.92958900	1.47624200	1.54397600	H	6.90459600	-2.94232200	0.45802500
H	6.86595900	-0.95212800	2.45978700	H	6.91470000	-2.05391600	-1.98890100
H	6.76779900	-3.01700800	0.90720300	H	6.96261800	0.48445200	-2.42673200
C	1.43941800	2.25466600	-0.96816600	C	0.78981200	2.54012600	0.99623600
O	1.36611900	3.54428800	-1.47129200	O	1.19234900	3.77009900	1.40993300
C	2.67539600	4.72456600	0.86611900	C	0.61686000	4.95920900	-1.02762800
O	2.16134800	5.72462000	0.98310200	O	0.15842100	5.98053200	-0.86815300
<b>TS-11</b>				<b>TS-12</b>			
B	-5.06786300	-0.46016600	-2.34020200	B	-5.03068200	2.25067300	0.43957300
N	-5.79416600	-1.65401300	-1.94267300	N	-5.69622800	2.29810100	-0.85061500
N	-3.62198000	-0.53506200	-2.43953600	N	-3.58431000	2.35601900	0.46961100
B	-2.96118000	-1.67869100	-1.82308000	B	-2.86753700	2.13184500	-0.77966700
B	-0.76542400	-0.63613200	-2.32118200	B	-0.74278800	2.33678000	0.48627100
N	-1.52162700	-1.80806900	-1.90260600	N	-1.42167600	2.23882500	-0.80191300
N	0.67297500	-0.70912900	-2.41477100	B	1.54161000	2.05977700	-0.76725400
B	1.34404800	-1.85757200	-1.81739300	B	3.69678200	2.05597100	0.46196200
B	3.53574800	-0.79008500	-2.31862100	N	2.98321900	2.07383900	-0.81846200
N	2.78453600	-1.96664900	-1.90148000	N	5.14378300	2.06655400	0.47141900
N	4.98005200	-0.84070800	-2.40752100	B	5.84146600	1.83441600	-0.78537000
B	5.66008500	-1.98605700	-1.82372300	B	-5.04992500	0.67587600	2.24193600
B	-4.98340000	1.78978400	-1.52524300	N	-5.71372700	1.82263200	1.64828600
N	-5.69518500	0.84882300	-2.37180900	N	-3.60181500	0.69140500	2.33643000
N	-3.53551200	1.82113700	-1.59812500	B	-2.88419200	1.69240800	1.56287900
B	-2.86365800	0.69079100	-2.22251500	B	-0.71868800	0.62545500	2.16358600
B	-0.67770500	1.64129200	-1.51420600	N	-1.43943700	1.78079500	1.63995200
N	-1.41660600	0.66674500	-2.30871000	N	0.74014300	0.59000600	2.19811100
N	0.77025000	1.63142100	-1.54397400	B	1.53109000	1.63547200	1.59347600
B	1.43320200	0.50651300	-2.17810100	B	3.62427600	0.44848600	2.22450900
B	3.58058800	1.47419500	-1.51917300	N	2.97034300	1.61823900	1.65829300
N	2.86060700	0.50031800	-2.31352400	N	5.07115300	0.40928100	2.32218700
N	5.02972200	1.50991900	-1.58660900	B	5.82712500	1.39841600	1.57075200
B	5.71662100	0.40022000	-2.22751400	B	-5.08576300	-1.67624800	1.80593600
B	-4.96453800	2.19698200	0.82956300	N	-5.74133400	-0.57586800	2.48960500
N	-5.63181800	2.48699600	-0.42786500	N	-3.63888900	-1.76755600	1.87774800
N	-3.51576100	2.24975500	0.86630100	B	-2.90311600	-0.58444900	2.30413900
B	-2.81016200	2.25340000	-0.40919500	B	-0.77713500	-1.76887100	1.77157700
B	-0.65311700	2.03753700	0.80035700	N	-1.45302300	-0.61764700	2.36135000
N	-1.36771500	2.32578300	-0.43383100	N	0.66079100	-1.88483400	1.85439600
N	0.79297100	2.03613300	0.80554000	B	1.41167800	-0.70591700	2.25560600
B	3.59562400	1.87165500	0.80735900	B	3.52745300	-1.91619800	1.78398900
N	2.88772700	2.15566800	-0.43405700	N	2.84968500	-0.77396100	2.38739700
N	5.04506900	1.93147000	0.84165200	N	4.97020800	-2.03175200	1.86685500
B	5.76016500	1.97815300	-0.42178500	B	5.72955500	-0.88510800	2.34015000
B	-5.03104900	0.34979200	2.34900000	B	-5.10845500	-2.48506200	-0.44450500
N	-5.66107800	1.59683400	1.95350300	N	-5.78228800	-2.51060200	0.84226100
N	-3.58379900	0.30843300	2.44500600	N	-3.66736300	-2.64093500	-0.46672000
B	-2.83040700	1.39048300	1.82167800	B	-2.95061800	-2.44450500	0.78634900
B	-0.73034400	0.16404300	2.32814000	B	-0.80277300	-2.63804900	-0.44960700
N	-1.38228000	1.39012800	1.88735400	N	-1.51278600	-2.59666500	0.82561600
N	0.70792700	0.12216400	2.42110800	N	0.63442300	-2.80479400	-0.47270700
B	1.45829800	1.18385300	1.76928200	B	1.35130800	-2.59097000	0.78110800
B	3.56802900	0.00714700	2.31895600	B	3.50374200	-2.75181000	-0.44549400
N	2.88875300	1.22020300	1.88769600	N	2.78944900	-2.73018700	0.82579600
N	5.01387700	-0.01201900	2.39977800	N	4.94555900	-2.89254700	-0.46318300

B	5.74348500	1.09811900	1.80717000	B	5.66079800	-2.72893200	0.79299300
B	-5.12917800	-1.90094700	1.53400500	B	-5.06226700	-0.91134400	-2.24792200
N	-5.76049800	-0.90608500	2.38264100	N	-5.76915700	-2.03421300	-1.65731500
N	-3.68804400	-2.04839300	1.60453100	N	-3.61487300	-0.97633700	-2.33429100
B	-2.93088300	-0.97730400	2.23652500	B	-2.93748100	-2.00554900	-1.55692800
B	-0.81971600	-2.09955500	1.53976400	B	-0.75386900	-1.02469700	-2.20570600
N	-1.49108200	-1.07798600	2.33644600	N	-1.49874900	-2.13694500	-1.63166000
N	0.62044500	-2.24346900	1.61074700	N	0.68494800	-1.10878400	-2.31240000
B	1.37275400	-1.16063200	2.23449700	B	1.36488500	-2.15600400	-1.55907300
B	3.49497000	-2.24504100	1.52786700	B	3.55098200	-1.16671300	-2.22068000
N	2.81467900	-1.23990800	2.33167900	N	2.80416600	-2.27210800	-1.63230800
N	4.94025500	-2.35969700	1.58797600	N	4.99451200	-1.24832100	-2.32437500
B	5.68964400	-1.28697900	2.22127400	B	5.67416600	-2.28919400	-1.56965800
B	-5.14675600	-2.30735700	-0.81910600	B	-5.02337000	1.44041500	-1.81020100
N	-5.83342300	-2.54489600	0.43865700	N	-5.71046100	0.36297300	-2.49897300
N	-3.70639700	-2.47474300	-0.85823700	N	-3.57404800	1.48241200	-1.87307100
B	-2.99584500	-2.52593600	0.41365300	B	-2.87503700	0.27810400	-2.29655300
B	-0.83653600	-2.50435200	-0.81788800	B	-0.69439500	1.34774300	-1.70057400
N	-1.55771400	-2.70347300	0.43439100	N	-1.42488800	0.26354000	-2.34521100
N	0.60282500	-2.66672900	-0.85721500	N	0.76268200	1.31737700	-1.72727800
B	1.31641400	-2.71560400	0.41648300	B	1.43866400	0.13325100	-2.24856900
B	3.47794800	-2.64752600	-0.81672100	B	3.64758300	1.19452400	-1.76765000
N	2.75760700	-2.86679000	0.43241200	N	2.87857900	0.11719200	-2.37725500
N	4.92178900	-2.78148000	-0.85674500	N	5.09612300	1.18923800	-1.85361500
B	5.63338500	-2.85864200	0.40998400	B	5.75739700	-0.01022100	-2.33780200
H	-6.79674700	-1.53202700	-1.84748700	H	-6.70446500	2.19117000	-0.81718000
H	-6.70266500	0.84325100	-2.25410900	H	-6.72109500	1.73663600	1.56456600
H	-6.64260100	2.40380700	-0.40484300	H	-6.74903600	-0.53922200	2.37892400
H	-6.67018400	1.55415800	1.85882400	H	-6.78600200	-2.36865700	0.80326800
H	-6.76490100	-0.82035100	2.26872600	H	-6.77326300	-1.91258900	-1.57919300
H	-6.83416200	-2.37986500	0.41705500	H	-6.71948300	0.35965400	-2.39475800
H	6.83552800	-2.12443500	-1.95430000	H	7.02466600	1.94672800	-0.85333200
H	6.89623800	0.43239400	-2.38699100	H	7.00856200	1.48001900	1.69145700
H	6.93537700	2.16047800	-0.46039600	H	6.90422700	-0.96626200	2.51717100
H	6.92490900	1.17988700	1.93132600	H	6.82989000	-2.94376800	0.86059600
H	6.86749700	-1.37525900	2.37226100	H	6.84427300	-2.46836000	-1.69690900
H	6.79958700	-3.09484000	0.44125300	H	6.93387300	-0.02464200	-2.52050300
C	1.44813600	2.38376500	-0.46706700	C	0.81500700	2.61580800	0.54773500
O	1.18629100	3.70335300	-0.83043700	C	1.21766000	3.92946600	0.81615700
C	1.92628700	4.88174200	0.54120300	O	1.25413200	4.99785000	-0.66393500
O	1.77592000	6.00219900	0.43636500	O	1.46829700	6.10902200	-0.51147100
<b>P-11</b>				<b>P-12</b>			
B	-5.01170100	0.72082300	-2.23426600	B	5.02543000	1.80539600	0.47506200
N	-5.73395500	-0.51243700	-2.49336000	N	5.66648400	1.31802300	1.68452500
N	-3.56395600	0.70076100	-2.32510100	N	3.59068900	2.02749200	0.50035300
B	-2.90571700	-0.59880200	-2.33993200	B	2.83412200	1.41676700	1.59339200
B	-0.71148800	0.54903000	-2.22018900	B	0.76262100	2.22023000	0.50197300
N	-1.46401400	-0.67600900	-2.44502300	N	1.40510100	1.61576400	1.66485200
N	0.72929800	0.52554400	-2.31541500	B	-1.55701200	1.73813200	1.64252900
B	1.40270100	-0.76731700	-2.34077800	B	-3.67587100	2.32757700	0.46015500
B	3.59077800	0.41016900	-2.18779500	N	-3.00118800	1.84034600	1.66600900
N	2.84646900	-0.81907100	-2.43189600	N	-5.12049500	2.46548000	0.46704800
N	5.03645300	0.41756300	-2.24926000	B	-5.86635700	1.87562600	1.56903000
B	5.72089100	-0.86398600	-2.29417600	B	4.96611700	1.02346400	-1.78647500
B	-4.95997900	2.28808900	-0.42465900	N	5.70063700	1.80830300	-0.80992400
N	-5.64871600	1.88007500	-1.63734700	N	3.52788300	1.19123000	-1.86085100

N	-3.51127800	2.35152400	-0.44271500	B	2.86983300	1.87321800	-0.76233900
B	-2.81924800	1.66703100	-1.52729200	B	0.64197000	1.33472700	-1.74321700
B	-0.65635000	2.14256200	-0.39836200	N	1.44239200	2.11292200	-0.79303600
N	-1.37158600	1.68362400	-1.58715300	N	-0.81069200	1.46831100	-1.82769300
N	0.78796300	2.14598200	-0.40045900	B	-1.52360300	2.21892100	-0.79854000
B	1.46929400	1.46977200	-1.50196600	B	-3.70379200	1.54789000	-1.80102500
B	3.59227500	2.01693000	-0.39144700	N	-2.96632200	2.33143600	-0.82184900
N	2.89692500	1.52872300	-1.56963500	N	-5.14667100	1.67206400	-1.88750700
N	5.03940900	2.09488500	-0.40058300	B	-5.83403400	2.33915600	-0.79417000
B	5.75036900	1.42640000	-1.48070300	B	4.79671800	-1.31711900	-2.24952600
B	-4.99199700	1.48406600	1.82368100	N	5.56062300	-0.10385000	-2.48171000
N	-5.63693300	2.35812700	0.85915000	N	3.35018400	-1.25224500	-2.34751400
N	-3.54468400	1.50684600	1.91100700	B	2.72523700	0.06378800	-2.31002400
B	-2.81278500	2.14014900	0.82020600	B	0.49442200	-1.03134800	-2.23172300
B	-0.68597500	1.34726900	1.81691500	N	1.28146700	0.18753700	-2.38221600
N	-1.36958500	2.21516900	0.86848300	N	-0.94566600	-0.98114600	-2.34045800
N	0.75641700	1.33618500	1.85417800	B	-1.58514700	0.32805200	-2.31332400
B	3.56206700	1.20125600	1.82283400	B	-3.80532900	-0.79693200	-2.26156500
N	2.85437300	2.05752600	0.87440400	N	-3.02586900	0.42417200	-2.43593700
N	5.00871200	1.24421700	1.91521000	N	-5.25144700	-0.76015100	-2.36903300
B	5.74581900	1.91054100	0.85505200	B	-5.90598700	0.53825100	-2.38691300
B	-5.07596400	-0.87333300	2.23240200	B	4.69362500	-2.89455100	-0.45345100
N	-5.70586400	0.40872900	2.49046300	N	5.39578300	-2.50372300	-1.66385100
N	-3.63096500	-0.96087500	2.32615000	N	3.24448900	-2.91217600	-0.47681800
B	-2.87374500	0.28531200	2.33622900	B	2.57844800	-2.21056800	-1.56707600
B	-0.77585700	-1.03800800	2.22182700	B	0.39523900	-2.63800900	-0.46281700
N	-1.42864300	0.24770900	2.42939800	N	1.13457700	-2.20142700	-1.64282900
N	0.66227600	-1.12902600	2.31754800	N	-1.04912300	-2.66493500	-0.48878400
B	1.41391300	0.11106200	2.29933200	B	-1.71529600	-1.95686400	-1.57706100
B	3.52750300	-1.16992000	2.21913900	B	-3.89991200	-2.37650200	-0.47321800
N	2.84070400	0.09636100	2.42633800	N	-3.15809200	-1.95188300	-1.65444400
N	4.97118600	-1.21866400	2.30766700	N	-5.34855500	-2.39376500	-0.49757300
B	5.69876600	0.04115500	2.35384300	B	-6.01907700	-1.73109300	-1.60551900
B	-5.13678000	-2.44140000	0.42103600	B	4.74023600	-2.11476100	1.80883800
N	-5.79497900	-1.98306600	1.63207900	N	5.36139800	-2.99341100	0.83290000
N	-3.69609300	-2.61038300	0.44290800	N	3.29150000	-2.08246000	1.88415600
B	-2.96188100	-1.98366200	1.53423900	B	2.54600800	-2.66934200	0.77876600
B	-0.82457700	-2.62380300	0.42190900	B	0.43831900	-1.82500300	1.78795800
N	-1.52249400	-2.12232300	1.60271600	N	1.10052800	-2.68421400	0.81357000
N	0.61579600	-2.78735400	0.44477800	N	-1.00518800	-1.81073700	1.86501000
B	1.34576100	-2.15434700	1.53873700	B	-1.74842200	-2.41746500	0.76737800
B	3.49317200	-2.75044100	0.43284500	B	-3.86358000	-1.59614700	1.78367500
N	2.78720500	-2.26766900	1.61284500	N	-3.19310800	-2.43559200	0.80030500
N	4.93776000	-2.88245100	0.46205400	N	-5.31272800	-1.59293400	1.85517700
B	5.66374600	-2.25029200	1.55346700	B	-6.05379700	-2.19488400	0.75859800
B	-5.10438200	-1.63793800	-1.82537900	B	4.90848900	0.22550600	2.27057900
N	-5.81436000	-2.46318800	-0.86390600	N	5.49084600	-1.08339500	2.50381600
N	-3.66199800	-1.76652800	-1.90918200	N	3.46836800	0.36261100	2.36818400
B	-2.97574300	-2.43712100	-0.81235000	B	2.65993600	-0.84860400	2.33578300
B	-0.79219200	-1.81703400	-1.82916200	B	0.58515200	0.54654900	2.23468800
N	-1.53623700	-2.60380500	-0.85177900	N	1.21406600	-0.75965300	2.41456800
N	0.64984300	-1.94138200	-1.91204500	N	-0.86986100	0.64757800	2.32706500
B	1.33996500	-2.60778400	-0.81111100	B	-1.65154700	-0.58649500	2.32153000
B	3.52642800	-1.94421200	-1.80451600	B	-3.76053900	0.74677400	2.25266100
N	2.78234300	-2.74821800	-0.84118300	N	-3.09561800	-0.53723800	2.43133900
N	4.97302700	-2.03757300	-1.86994000	N	-5.20556800	0.83775200	2.34233000

B	5.66053600	-2.72930700	-0.79113900	B	-5.97374400	-0.39551400	2.34987400
H	-6.74024600	-0.45182700	-2.38014300	H	6.66278600	1.14655900	1.59978600
H	-6.65818400	1.81958300	-1.55717900	H	6.69605000	1.61664500	-0.77084100
H	-6.64663700	2.27076500	0.81376200	H	6.56407400	-0.19998100	-2.36770200
H	-6.71349600	0.42351300	2.37460700	H	6.40657700	-2.47506300	-1.58237200
H	-6.79718300	-1.84902400	1.55053400	H	6.37360200	-2.93801200	0.79456700
H	-6.81473400	-2.30029500	-0.82010200	H	6.49761700	-1.13362900	2.39002200
H	6.90034300	-0.91723200	-2.44870900	H	-7.03677900	2.06576800	1.67952600
H	6.93230800	1.53150100	-1.57902200	H	-7.00231600	2.56178700	-0.85605000
H	6.92111800	2.07846000	0.93356700	H	-7.07743500	0.62580000	-2.58167400
H	6.87692200	0.05024700	2.52654200	H	-7.20086900	-1.80450900	-1.73085900
H	6.83873000	-2.40334300	1.67073500	H	-7.23849500	-2.30113500	0.81326100
H	6.82961800	-2.94542600	-0.85154900	H	-7.15053300	-0.38001500	2.53081100
C	1.44995900	2.11623100	0.87476000	C	-0.75838100	2.45565500	0.52627000
C	1.47339900	4.92149100	-0.20203500	C	2.65753200	4.78601200	-0.05036800
O	0.42790700	5.18825100	0.22915400	O	3.39695800	4.82210100	-0.94644800
O	2.52389900	4.68244100	-0.64558800	O	1.91188000	4.76278100	0.84387600