

Electronic Supplementary Information

**High-Symmetry Cage-like Molecule $\text{N}_{20}(\text{C}_2\text{B}_2)_{30}$:
Computational Insight into Its Bonding and Reactivity**

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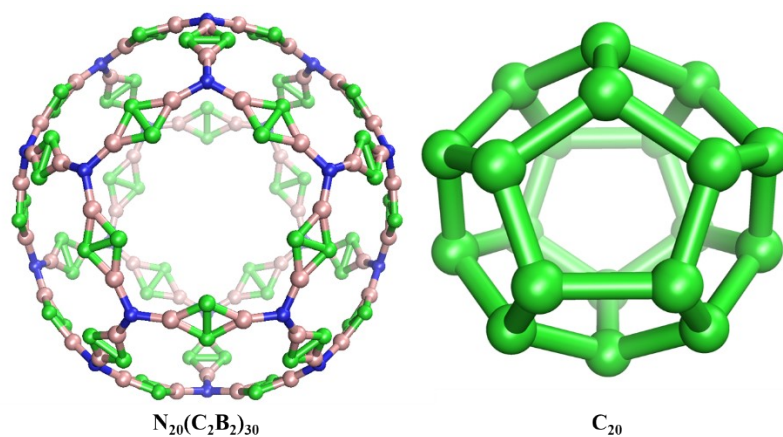


Fig. S1 The optimized structure of $N_{20}(C_2B_2)_{30}$ and C_{20} .

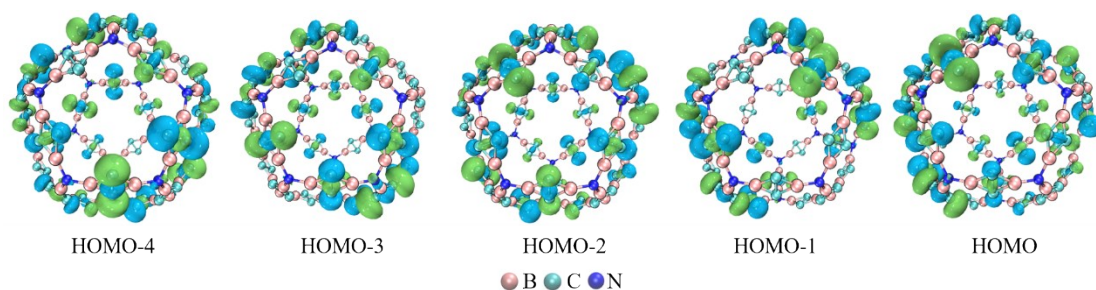


Fig. S2 HOMO-4 to HOMO of $N_{20}(C_2B_2)_{30}$. Color scheme: B atom (in pink), C atom (in cyan), and N atom (in blue).

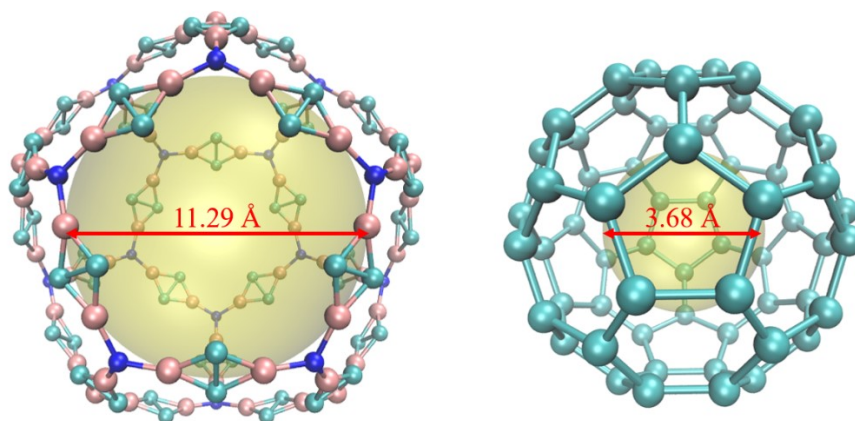


Fig. S3 Diameter of cavity of $N_{20}(C_2B_2)_{30}$ and C_{60} . Color scheme: B atom (in pink), C atom (in cyan), and N atom (in blue).

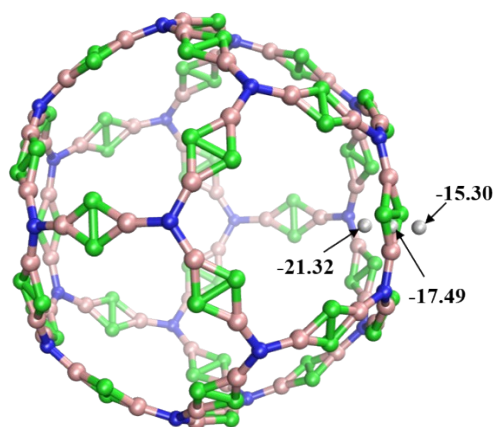


Fig. S4 The NICS(0), NICS(1) (inside cage) and NICS(1) (outside cage) in the center of three-membered cyclic CCB unit of $N_{20}(C_2B_2)_{30}$. Color scheme: B atom (in pink), C atom (in green), N atom (in blue) and Bq (in white).

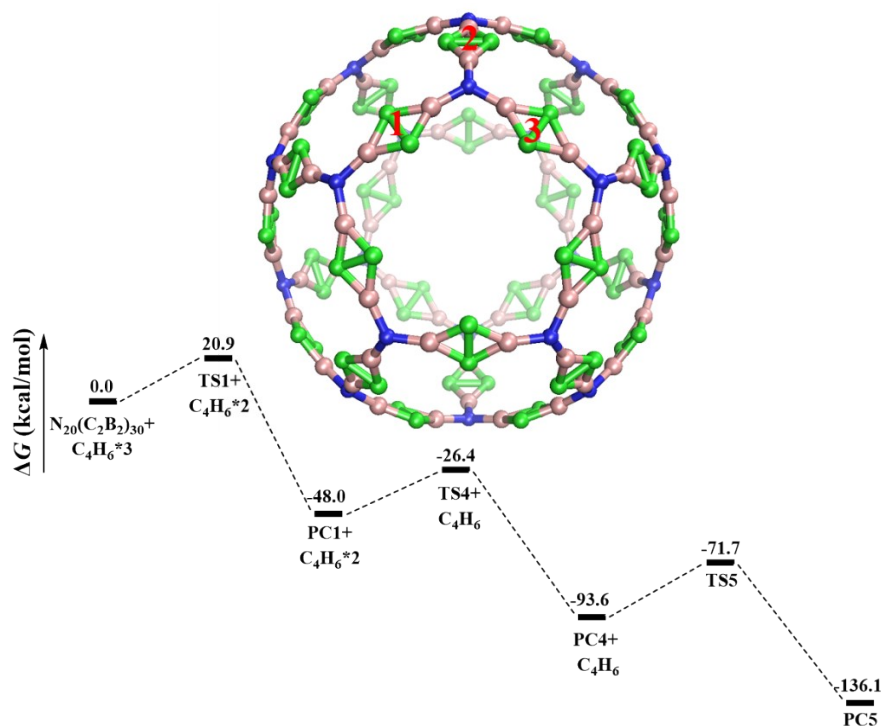


Fig. S5 Predicted relative free energy profiles (in kcal/mol) for the successive addition of $N_{20}(C_2B_2)_{30}$ with butadiene.

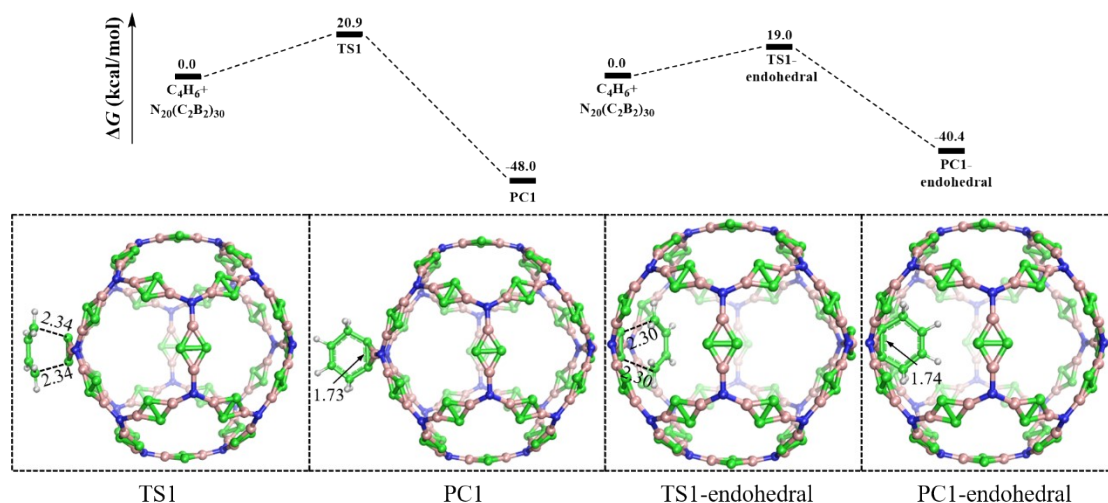


Fig. S6 Predicted relative free energy profiles (in kcal/mol) for the Diels-Alder reactions of exohedral and endohedral $\text{N}_{20}(\text{C}_2\text{B}_2)_{30}$ with butadiene are shown. The interatomic distances are given in Å.

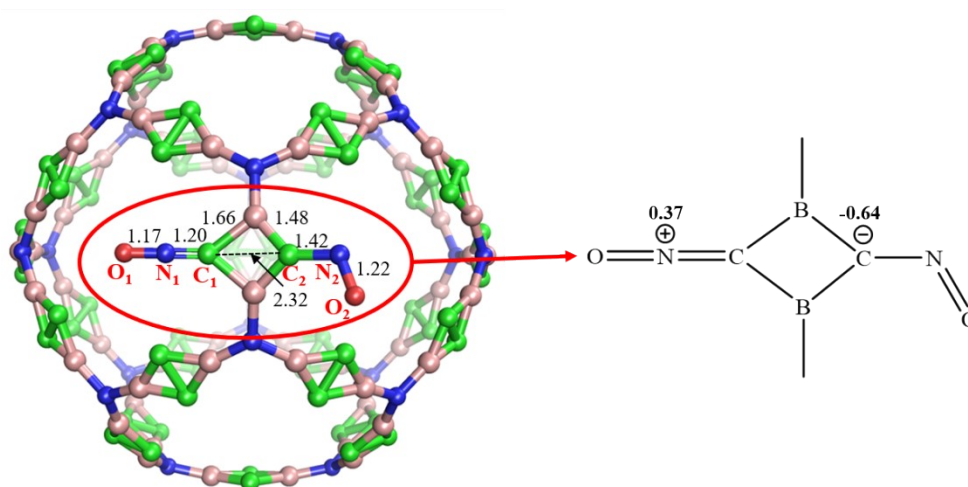


Fig. S7 The structural formula and bonding arrangement of $\text{N}_{20}(\text{C}_2\text{B}_2)_{30}(\text{NO})_2$. Optimized bond lengths (in plain) and calculated NBO charges (in bold) of $\text{N}_{20}(\text{C}_2\text{B}_2)_{30}(\text{NO})_2$. The bond lengths are given in Å.

Table S1 Electron density (ρ) and Laplacian values ($\nabla^2\rho$) of the TM–O and TM–N bonds in $(\text{CO}_2)(\text{TM})\text{N}_{20}(\text{C}_2\text{B}_2)_{30}^+$ and $(\text{N}_2\text{O})(\text{Ag})\text{N}_{20}(\text{C}_2\text{B}_2)_{30}^+$.

Bonds	Species	ρ	$\nabla^2\rho$
TM–O	$(\text{CO}_2)(\text{Ag})\text{N}_{20}(\text{C}_2\text{B}_2)_{30}^+$	0.03	0.16
	$(\text{CO}_2)(\text{Cu})\text{N}_{20}(\text{C}_2\text{B}_2)_{30}^+$	0.05	0.33
	$(\text{CO}_2)(\text{Au})\text{N}_{20}(\text{C}_2\text{B}_2)_{30}^+$	0.05	0.29
TM–N	$(\text{N}_2\text{O})(\text{Ag})\text{N}_{20}(\text{C}_2\text{B}_2)_{30}^+$	0.04	0.18
	$(\text{N}_2\text{O})(\text{Cu})\text{N}_{20}(\text{C}_2\text{B}_2)_{30}^+$	0.06	0.37
	$(\text{N}_2\text{O})(\text{Au})\text{N}_{20}(\text{C}_2\text{B}_2)_{30}^+$	0.07	0.36

Cartesian coordinates

$\text{N}_{20}(\text{C}_2\text{B}_2)_{30}$

B	-1.22445100	3.83992600	6.19105000
B	-3.27361000	2.35112400	6.19105000
B	1.22445100	3.83992600	6.19105000
B	3.27361000	2.35112400	6.19105000
B	4.03036200	0.02208000	6.19105000
B	3.24765300	-2.38685100	6.19105000
B	1.26645000	-3.82627900	6.19105000
B	-1.26645000	-3.82627900	6.19105000
B	-4.03036200	0.02208000	6.19105000
B	-3.24765300	-2.38685100	6.19105000
N	4.31292600	1.40135500	5.93623300
N	2.66553500	-3.66879400	5.93623300
N	-2.66553500	-3.66879400	5.93623300
N	-4.31292600	1.40135500	5.93623300
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B	-3.27361000	6.58889800	-0.66581200
B	0.00000000	6.85686200	2.74897300
B	0.00000000	5.52523800	4.90358600
B	-5.25481400	1.70739200	4.90358600
B	-6.52126300	2.11888700	2.74897300
B	-5.25481400	5.14947000	-0.66581200
B	-6.52126300	3.40635100	0.66581200
C	-6.18112800	4.00598300	-0.63470200
C	-5.71999000	4.64068500	0.63470200
C	-1.89984300	7.11651800	-0.63470200
C	-2.64598000	6.87408400	0.63470200
C	0.74613700	6.25678800	3.86690700
C	-0.74613700	6.25678800	3.86690700
C	-6.18112800	1.22383500	3.86690700
C	-5.71999000	2.64307200	3.86690700
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B	-1.22445100	7.25471000	0.66581200
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B	-3.24765300	-4.47001100	4.90358600
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C	-4.28128500	-4.62327900	3.86690700
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N	-4.31292600	-5.93623300	1.40135500
B	3.27361000	-6.58889800	0.66581200
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C	1.89984300	-7.11651800	0.63470200
N	4.31292600	-5.93623300	1.40135500
N	0.00000000	-7.33758800	-1.40135500
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C	-7.35529500	0.39226700	-0.63470200
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B	6.52126300	2.11888700	2.74897300
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B	7.27801600	1.07730700	0.66581200
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C	7.35529500	-0.39226700	0.63470200
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C	-6.66955900	2.64608900	-2.80056900
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C	5.14818200	1.89687700	-4.48986300
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B	-0.03930700	-1.26648400	7.26047500
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C	-7.70837900	-0.74620200	0.32062200
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C	1.78674200	-4.28610600	5.62405600
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C	0.70953200	-0.00000400	7.30410100
C	-2.73224900	-3.07389000	6.28557500
C	-2.00791500	-4.28217700	5.79298900
C	9.89953100	0.71191300	0.52532700
C	9.89953900	-0.71190900	0.52532700
H	10.15612000	1.20087500	1.46231500
H	10.15613700	-1.20086900	1.46231300
C	9.37951100	1.48436100	-0.47535000
H	9.28882700	1.11032400	-1.48944200
H	9.30834500	2.56003100	-0.36667300
C	9.37952800	-1.48436300	-0.47535000
H	9.30837500	-2.56003400	-0.36667400
H	9.28883200	-1.11032600	-1.48944000

PC1

B	-5.16291600	4.03559100	2.91350800
B	-6.45670500	3.24843300	0.88329400
B	-3.87078300	3.27610600	4.84727700
B	-3.01579800	1.21546000	6.05497900
B	-3.01579800	-1.21546000	6.05497900
B	-3.87078300	-3.27610600	4.84727700
B	-5.16291600	-4.03559100	2.91350800
B	-6.45670500	-3.24843300	0.88329400
B	-7.22244100	1.26651400	-0.33401900
B	-7.22244100	-1.26651400	-0.33401900
N	-2.43267400	0.00000000	6.51513000
N	-4.21209000	-4.33100200	3.94047200
N	-6.93012100	-2.66713900	-0.33578400
N	-6.93012100	2.66713900	-0.33578400

N	-4.21209000	4.33100200	3.94047200
B	0.00000000	7.34500800	-1.65219600
B	-1.21679500	6.65399500	2.87120400
B	-3.21641600	5.31804500	3.66246300
B	-6.48874100	3.25316800	-1.56381500
B	-5.24020800	4.04009900	-3.62224200
B	-1.22324500	6.55108000	-3.62156300
B	-3.26736300	5.26881600	-4.39242800
C	-1.89532400	5.73691200	-4.64756600
C	-2.64334600	6.20637100	-3.44456700
C	0.74622500	7.45044700	-0.38759200
C	-0.74622500	7.45044700	-0.38759200
C	-1.85984300	5.83258900	3.90939400
C	-2.62872800	6.27296100	2.70825200
C	-6.15955300	3.08131300	-2.98833400
C	-5.69655500	4.29005900	-2.24547400
N	-4.30451800	4.32247400	-4.66719400
N	0.00000000	7.01954800	-3.04566000
B	0.00000000	7.40075500	0.88060900
N	0.00000000	7.12691400	2.28475300
B	-1.21679500	-6.65399500	2.87120400
B	-3.21641600	-5.31804500	3.66246300
B	-6.48874100	-3.25316800	-1.56381500
B	-5.24020800	-4.04009900	-3.62224200
B	-1.22324500	-6.55108000	-3.62156300
B	-3.26736300	-5.26881600	-4.39242800
C	-1.89532400	-5.73691200	-4.64756600
C	-2.64334600	-6.20637100	-3.44456700
C	-1.85984300	-5.83258900	3.90939400
C	-2.62872800	-6.27296100	2.70825200
C	-6.15955300	-3.08131300	-2.98833400
C	-5.69655500	-4.29005900	-2.24547400
N	-4.30451800	-4.32247400	-4.66719400
B	0.00000000	-7.40075500	0.88060900
B	0.00000000	-7.34500800	-1.65219600
C	0.74622500	-7.45044700	-0.38759200
C	-0.74622500	-7.45044700	-0.38759200
N	0.00000000	-7.12691400	2.28475300
N	0.00000000	-7.01954800	-3.04566000
B	-4.02392500	3.27903700	-5.60490500
B	-3.24614100	-1.22502900	-6.86692900
B	-4.02392500	-3.27903700	-5.60490500
C	-4.27686100	1.90355200	-6.06429300
C	-3.07050400	2.64756000	-6.53163000

C	-3.07050400	-2.64756000	-6.53163000
C	-4.27686100	-1.90355200	-6.06429300
B	-3.24614100	1.22502900	-6.86692900
N	-2.66569300	0.00000000	-7.32482800
B	3.87078300	3.27610600	4.84727700
B	1.08753500	0.00000000	7.04381800
B	-1.08753500	0.00000000	7.04381800
B	3.21641600	5.31804500	3.66246300
B	1.21679500	6.65399500	2.87120400
C	2.62872800	6.27296100	2.70825200
C	1.85984300	5.83258900	3.90939400
C	4.06131100	1.87715900	5.25467600
C	2.89488000	2.65764200	5.76061600
C	0.00000000	-0.86672400	7.60698400
C	0.00000000	0.86672400	7.60698400
N	4.21209000	4.33100200	3.94047200
B	3.01579800	1.21546000	6.05497900
N	2.43267400	0.00000000	6.51513000
B	1.21679500	-6.65399500	2.87120400
B	3.87078300	-3.27610600	4.84727700
B	3.01579800	-1.21546000	6.05497900
C	1.85984300	-5.83258900	3.90939400
C	2.62872800	-6.27296100	2.70825200
C	4.06131100	-1.87715900	5.25467600
C	2.89488000	-2.65764200	5.76061600
B	3.21641600	-5.31804500	3.66246300
N	4.21209000	-4.33100200	3.94047200
C	-5.66216000	-4.29153200	1.55212000
C	-6.08262600	-3.06720400	2.29494000
C	-7.29066600	0.00000000	0.41284600
C	-7.30644500	0.00000000	-1.07965300
C	-6.08262600	3.06720400	2.29494000
C	-5.66216000	4.29153200	1.55212000
C	-4.06131100	1.87715900	5.25467600
C	-2.89488000	2.65764200	5.76061600
C	-4.06131100	-1.87715900	5.25467600
C	-2.89488000	-2.65764200	5.76061600
B	6.48874100	-3.25316800	-1.56381500
B	5.24020800	-4.04009900	-3.62224200
B	7.22244100	-1.26651400	-0.33401900
B	7.22244100	1.26651400	-0.33401900
B	6.48874100	3.25316800	-1.56381500
B	5.24020800	4.04009900	-3.62224200
B	4.02392500	3.27903700	-5.60490500

B	3.24614100	1.22502900	-6.86692900
B	4.02392500	-3.27903700	-5.60490500
B	3.24614100	-1.22502900	-6.86692900
N	6.93012100	2.66713900	-0.33578400
N	4.30451800	4.32247400	-4.66719400
N	2.66569300	0.00000000	-7.32482800
N	4.30451800	-4.32247400	-4.66719400
N	6.93012100	-2.66713900	-0.33578400
B	5.16291600	-4.03559100	2.91350800
B	6.45670500	-3.24843300	0.88329400
B	3.26736300	-5.26881600	-4.39242800
B	1.22324500	-6.55108000	-3.62156300
C	6.08262600	-3.06720400	2.29494000
C	5.66216000	-4.29153200	1.55212000
C	1.89532400	-5.73691200	-4.64756600
C	2.64334600	-6.20637100	-3.44456700
B	1.22324500	6.55108000	-3.62156300
B	3.26736300	5.26881600	-4.39242800
B	1.26643500	0.00000000	-7.62386500
B	-1.26643500	0.00000000	-7.62386500
C	2.64334600	6.20637100	-3.44456700
C	1.89532400	5.73691200	-4.64756600
C	0.00000000	-0.74633200	-7.70103700
C	0.00000000	0.74633200	-7.70103700
B	5.16291600	4.03559100	2.91350800
B	6.45670500	3.24843300	0.88329400
C	5.66216000	4.29153200	1.55212000
C	6.08262600	3.06720400	2.29494000
C	3.07050400	2.64756000	-6.53163000
C	4.27686100	1.90355200	-6.06429300
C	4.27686100	-1.90355200	-6.06429300
C	3.07050400	-2.64756000	-6.53163000
C	6.15955300	-3.08131300	-2.98833400
C	5.69655500	-4.29005900	-2.24547400
C	7.30644500	0.00000000	-1.07965300
C	7.29066600	0.00000000	0.41284600
C	6.15955300	3.08131300	-2.98833400
C	5.69655500	4.29005900	-2.24547400
C	0.00000000	-0.66950700	10.07630900
C	0.00000000	0.66950700	10.07630900
H	0.00000000	-1.15832200	11.04881000
H	0.00000000	1.15832200	11.04881000
C	0.00000000	1.63329900	8.90223600
H	0.87719000	2.28617600	8.97892900

H	-0.87719000	2.28617600	8.97892900
C	0.00000000	-1.63329900	8.90223600
H	-0.87719000	-2.28617600	8.97892900
H	0.87719000	-2.28617600	8.97892900
RC			
B	-2.05579100	-4.78516500	5.04178300
B	0.11345600	-4.08457500	6.14625100
B	-4.18801300	-3.96004600	4.16603600
B	-5.58471900	-1.87776800	3.80504200
B	-5.63560200	0.54772900	4.12022900
B	-4.33737000	2.53225600	5.01083600
B	-2.24270500	3.21017800	6.08155900
B	-0.03665600	2.35632300	6.98673500
B	1.37387800	-2.16656600	7.00173000
B	1.31603800	0.34445300	7.33024100
N	-6.13547300	-0.60883100	3.44442800
N	-3.39615700	3.56675400	5.31394700
N	1.24774300	1.76912600	7.21717000
N	1.37029600	-3.51598100	6.52617100
N	-3.19538600	-4.99056200	4.20168900
B	1.88437400	-7.16729200	-1.08831700
B	-2.46217800	-6.75206400	0.75053300
B	-3.01872400	-5.78300000	3.02371400
B	2.54252600	-3.98650900	5.85432800
B	4.43966700	-4.52245600	4.26380100
B	3.98156200	-6.49116600	-0.02057900
B	4.97850300	-5.45998600	2.06699500
C	5.07032200	-5.73948000	0.62469800
C	3.97555300	-6.33861300	1.44348700
C	0.53810600	-7.20159700	-1.68257500
C	0.72157600	-7.38788900	-0.21318800
C	-3.42477900	-6.08341500	1.64108500
C	-2.12359400	-6.58449000	2.17327100
C	3.90712000	-3.71513900	5.37354400
C	3.13921100	-4.88353500	4.85134100
N	5.36339000	-4.64483200	3.17817700
N	3.26525400	-6.81514500	-1.21600200
B	-0.62861000	-7.26956900	-0.78747000
N	-2.02421200	-7.03008500	-0.58285600
B	-2.77490000	6.18672800	2.43273600
B	-3.26665700	4.64137000	4.37854700
B	2.39240400	2.45008300	6.69488700
B	4.25014000	3.46453500	5.30368200
B	3.66754400	6.43816700	1.66086700

B	4.72661300	4.95606800	3.42097100
C	4.79486600	5.59891700	2.09856000
C	3.67834100	5.91557500	3.03701600
C	-3.69724700	5.26609600	3.11716300
C	-2.41757100	5.67650600	3.76653800
C	3.76451700	2.37558600	6.16691400
C	2.93911600	3.60153300	5.95856300
N	5.15818700	3.90395400	4.28910400
B	-0.97896400	7.16814900	1.08962800
B	1.53418900	7.26587100	0.78865400
C	0.18433400	7.38700900	0.21454300
C	0.36757300	7.19958400	1.68381400
N	-2.36032100	6.81873900	1.21795600
N	2.92951600	7.02376000	0.58403600
B	6.23855000	-3.54248500	2.92185300
B	7.29370700	1.06293900	2.58013800
B	6.08261400	2.94610300	3.76449400
C	6.69939900	-2.19390800	3.29051200
C	7.02575300	-2.76512400	1.95079700
C	6.89942600	2.48012500	2.63215600
C	6.60918300	1.57151900	3.78003900
B	7.35200200	-1.36445400	2.26440200
N	7.70630700	-0.06002400	1.79535200
B	-5.17649900	-2.95224100	-3.76371800
B	-6.95396200	-0.12549400	-0.38632700
B	-6.60549200	-0.44260300	2.09993100
B	-3.82240000	-4.96444700	-3.42084500
B	-2.76307200	-6.44581800	-1.66018200
C	-2.77325800	-5.92315100	-3.03612100
C	-3.89127100	-5.60855200	-2.09879600
C	-5.69356100	-1.57489400	-3.77823900
C	-5.99600200	-2.48485400	-2.63473800
C	-6.84631600	0.45663800	0.96281400
C	-6.85524400	-1.02709900	0.77493100
N	-4.25293900	-3.91227600	-4.28866600
B	-6.37995300	-1.06368000	-2.57880700
N	-6.78760600	0.05996100	-1.79877300
B	-3.07809300	6.49657800	0.02258700
B	-5.33534000	3.54801100	-2.92029700
B	-6.43735000	1.36347000	-2.26341300
C	-4.16880900	5.74823600	-0.62293800
C	-3.07208100	6.34418700	-1.44132700
C	-5.78315600	2.19570900	-3.28818500
C	-6.12674900	2.77001500	-1.95405300

B	-4.07702800	5.46765900	-2.06533400
N	-4.46159500	4.65289300	-3.17634400
C	-0.82867100	3.45471300	6.40968000
C	-1.48464700	2.17157800	6.79816200
C	0.61420800	-0.94953300	7.33098200
C	2.09494100	-0.89208600	7.15311300
C	-1.34275800	-3.92674500	6.00199500
C	-0.62942800	-5.03692600	5.30499600
C	-4.64844100	-2.64607400	4.64275400
C	-5.23779200	-3.25434000	3.41385200
C	-4.73070900	1.11920100	5.13178500
C	-5.35790400	1.99361600	4.09748600
B	0.78943000	4.08348100	-6.14336800
B	2.96028700	4.78325400	-5.04178400
B	-0.47163600	2.16552300	-6.99594900
B	-0.41138700	-0.34566900	-7.32337200
B	0.94396600	-2.35598300	-6.98152700
B	3.15189100	-3.20912900	-6.08015000
B	5.24964100	-2.53338200	-5.01322600
B	6.55278400	-0.54957900	-4.12897600
B	5.09364000	3.95805100	-4.16856300
B	6.49420000	1.87793800	-3.81234700
N	-0.34110300	-1.77026300	-7.21058900
N	4.30609100	-3.56600900	-5.31328700
N	7.04894100	0.60930400	-3.45232200
N	4.10063600	4.98758900	-4.20205800
N	-0.46785500	3.51540400	-6.52162900
B	-3.53632500	4.52817400	-4.26009500
B	-1.63959500	3.98793900	-5.84982400
B	3.92437200	5.77899500	-3.02323300
B	3.36762500	6.74629000	-0.74941800
C	-3.00467700	3.71949900	-5.36952900
C	-2.23467100	4.88651900	-4.84738600
C	4.32972300	6.07667700	-1.63983100
C	3.02996700	6.58091200	-2.17257800
B	3.68075600	-6.18362000	-2.43070700
B	4.17541300	-4.63979500	-4.37693900
B	7.51855500	0.44558600	-2.11084300
B	7.83105000	0.12733200	0.38241600
C	3.32577700	-5.67478400	-3.76561600
C	4.60367000	-5.26254800	-3.11384200
C	7.73345400	1.02924800	-0.77681000
C	7.77029800	-0.45024300	-0.97019700
B	-3.34320400	-3.47130700	-5.30066100

B	-1.48516800	-2.45344500	-6.68916500
C	-2.03068600	-3.60590900	-5.95376000
C	-2.85794000	-2.38143400	-6.16324600
C	6.27110700	-1.99408700	-4.10067100
C	5.64741900	-1.12166300	-5.13881000
C	5.55663600	2.64558500	-4.64798800
C	6.14428400	3.25203500	-3.41726100
C	2.24587300	3.92482000	-6.00067000
C	1.53404400	5.03591800	-5.30353800
C	0.28930300	0.94898700	-7.32434900
C	-1.19138300	0.89026100	-7.14672600
C	2.39225300	-2.17031000	-6.79450900
C	1.73773100	-3.45428300	-6.40639900
C	-9.88645700	0.88258000	-0.85551600
C	-9.94487600	-0.56819500	-1.09049500
H	-9.72721300	1.62695800	-1.62744700
H	-9.83545100	-1.03935200	-2.06068400
C	-10.05690500	1.12478900	0.45751200
H	-10.05683200	2.09184500	0.94348300
C	-10.14941600	-1.19884200	0.08116300
H	-10.23411200	-2.26659900	0.23670500
C	-10.26953400	-0.17704100	1.17474900
H	-9.54225100	-0.33632900	1.98151100
H	-11.26136200	-0.21493100	1.64628500

TS2

B	2.66595400	4.02498700	5.32667100
B	0.58185900	3.24526100	6.53672500
B	4.67594400	3.26735600	4.15041300
B	5.96119000	1.21876400	3.39172400
B	5.96120200	-1.21873700	3.39170400
B	4.67598500	-3.26736000	4.15035900
B	2.66600600	-4.02504100	5.32660500
B	0.58190100	-3.24536300	6.53667200
B	-0.66544900	1.26632000	7.25922200
B	-0.66543300	-1.26645100	7.25920100
N	6.45287200	0.00002000	2.83442300
N	3.73278800	-4.31134200	4.41799800
N	-0.65574400	-2.66569400	6.96113200
N	-0.65577800	2.66556800	6.96117500
N	3.73273100	4.31132000	4.41807000
B	-1.70863800	7.29695300	-0.04040400
B	2.76615800	6.55736100	1.32615900
B	3.48512200	5.26664100	3.38320800
B	-1.86552700	3.24868700	6.46841700

B	-3.87552800	4.03289700	5.14173300
B	-3.72522100	6.52911500	1.11830700
B	-4.57133200	5.25833700	3.13942100
C	-4.77810800	5.72389200	1.75844900
C	-3.59754800	6.18810500	2.54451100
C	-0.41930700	7.38327800	-0.74499400
C	-0.46771300	7.38167600	0.74655100
C	3.77973000	5.75051900	2.02453800
C	2.54870100	6.20153400	2.73753400
C	-3.27659800	3.07603300	6.08622200
C	-2.51640100	4.28320800	5.64805000
N	-4.88586100	4.31576300	4.16880300
N	-3.10551800	6.99016800	-0.08600400
B	0.82295000	7.31293500	0.04182200
N	2.22279300	7.02201600	0.08658300
B	2.76624800	-6.55733900	1.32604500
B	3.48519300	-5.26664700	3.38311900
B	-1.86548400	-3.24882100	6.46836300
B	-3.87547400	-4.03303400	5.14166300
B	-3.72513100	-6.52917900	1.11819300
B	-4.57125900	-5.25844800	3.13932900
C	-4.77802900	-5.72398400	1.75835000
C	-3.59746200	-6.18819100	2.54440300
C	3.77980700	-5.75049400	2.02443800
C	2.54878700	-6.20154400	2.73742700
C	-3.27655800	-3.07617800	6.08617000
C	-2.51634400	-4.28333600	5.64797800
N	-4.88580200	-4.31589700	4.16872800
B	0.82305100	-7.31291800	0.04169400
B	-1.70853700	-7.29696900	-0.04053200
C	-0.41920500	-7.38326200	-0.74512400
C	-0.46761100	-7.38169000	0.74642200
N	2.22289000	-7.02197900	0.08646100
N	-3.10542200	-6.99020200	-0.08612600
B	-5.81636900	3.27499500	3.85612600
B	-7.05552700	-1.22461200	3.03427700
B	-5.81632400	-3.27513600	3.85606800
C	-6.28761800	1.90064500	4.09241400
C	-6.71158200	2.64632300	2.87118800
C	-6.71154300	-2.64645800	2.87114000
C	-6.28759400	-1.90079700	4.09238100
B	-7.05554400	1.22446900	3.03429900
N	-7.49437000	-0.00006900	2.43844200
B	4.93007300	3.27477200	-3.80945000

B	6.90335600	0.00005500	-0.95789400
B	6.87423800	0.00003200	1.45595500
B	3.69545800	5.27578800	-3.12635500
B	2.84499800	6.56148800	-1.11701700
C	2.71909500	6.20924400	-2.54039300
C	3.90195300	5.75713300	-1.75063300
C	5.38124100	1.89155100	-4.02307300
C	5.81780000	2.65170900	-2.81549500
C	7.20754000	-0.79200700	0.25182400
C	7.20756200	0.79208700	0.25183900
N	4.01065100	4.32117400	-4.14325800
B	6.14410400	1.22095800	-2.95457000
N	6.58020800	0.00006900	-2.35836200
B	2.84508900	-6.56142100	-1.11713200
B	4.93011600	-3.27462900	-3.80951000
B	6.14411800	-1.22081400	-2.95459300
C	3.90203100	-5.75703700	-1.75073200
C	2.71918300	-6.20915800	-2.54050300
C	5.38125800	-1.89139600	-4.02310600
C	5.81784000	-2.65157400	-2.81554900
B	3.69553100	-5.27567600	-3.12644800
N	4.01071000	-4.32104000	-4.14333500
C	1.28104200	-4.27930900	5.75678200
C	2.01080000	-3.06769200	6.23284200
C	0.07792300	-0.00006100	7.35923300
C	-1.41378000	-0.00007100	7.31417400
C	2.01076100	3.06761400	6.23289200
C	1.28098500	4.27922900	5.75685200
C	5.11535700	1.88587200	4.39772400
C	5.63821600	2.64747300	3.22602800
C	5.11537500	-1.88587200	4.39769100
C	5.63825100	-2.64744800	3.22598800
B	-1.44185600	-3.24842300	-6.54701400
B	-3.53348100	-4.03228700	-5.35288500
B	-0.19225200	-1.26638500	-7.25743900
B	-0.19226800	1.26651400	-7.25741600
B	-1.44189900	3.24852300	-6.54695600
B	-3.53353500	4.03233900	-5.35281500
B	-5.55372500	3.27468800	-4.19560100
B	-6.84399200	1.22447900	-3.45572500
B	-5.55368100	-3.27468300	-4.19565800
B	-6.84397500	-1.22450500	-3.45574600
N	-0.20258400	2.66605000	-6.96065500
N	-4.60476300	4.31531600	-4.44741700

N	-7.32068100	-0.00002100	-2.88961800
N	-4.60470400	-4.31529500	-4.44749200
N	-0.20254800	-2.66592600	-6.96070300
B	3.00595000	-4.03322200	-5.11960100
B	1.00481800	-3.24811700	-6.45932700
B	-4.35779600	-5.25815100	-3.40007300
B	-3.64521300	-6.52925100	-1.32832100
C	2.41157100	-3.07325700	-6.06430800
C	1.65121100	-4.28481500	-5.63867300
C	-4.65414700	-5.72388700	-2.03558000
C	-3.42490600	-6.18805600	-2.74311400
B	-3.64530300	6.52923100	-1.32820700
B	-4.35786800	5.25815800	-3.39998200
B	-7.66545100	-0.00003500	-1.50108400
B	-7.74805700	-0.00005800	1.03040400
C	-3.42499100	6.18806400	-2.74300600
C	-4.65422500	5.72386600	-2.03548100
C	-7.78414200	-0.74622200	-0.23786100
C	-7.78415400	0.74612700	-0.23784800
B	3.00589700	4.03335800	-5.11953000
B	1.00477400	3.24824800	-6.45926900
C	1.65115300	4.28494100	-5.63859700
C	2.41153000	3.07340100	-6.06425400
C	-6.51096200	2.64623600	-3.27066600
C	-6.00907700	1.90048200	-4.46190800
C	-6.00905200	-1.90048000	-4.46194100
C	-6.51092500	-2.64626000	-3.27071000
C	-2.87442800	-3.07506100	-6.25602500
C	-2.14479200	-4.28313900	-5.77096800
C	-0.93549400	0.00006000	-7.36006700
C	0.55598600	0.00007000	-7.30902900
C	-2.87446900	3.07513600	-6.25597000
C	-2.14485000	4.28321600	-5.77089300
C	9.72283500	-0.70625400	-1.00658300
C	9.72286000	0.70627200	-1.00657100
H	9.81233400	-1.32861700	-1.88913900
H	9.81238100	1.32864700	-1.88911700
C	9.44394400	-1.16963800	0.27205400
H	9.48300600	-2.20349800	0.58793900
C	9.44398600	1.16964400	0.27207400
H	9.48308400	2.20349700	0.58797700
C	9.65611900	-0.00000900	1.19797400
H	9.10409500	-0.00000800	2.13828500
H	10.72830300	-0.00003000	1.44850200

PC2

B	5.27064100	2.65847600	4.02136200
B	6.49877400	0.58437900	3.24353800
B	4.04636200	4.63938200	3.26353500
B	3.23561900	5.89791600	1.21654900
B	3.23561900	5.89791600	-1.21654900
B	4.04636200	4.63938200	-3.26353500
B	5.27064100	2.65847600	-4.02136200
B	6.49877400	0.58437900	-3.24353800
B	7.22550100	-0.66190400	1.26642400
B	7.22550100	-0.66190400	-1.26642400
N	2.67577400	6.39386000	0.00000000
N	4.35466200	3.71715400	-4.31455100
N	6.93197300	-0.65152800	-2.66670800
N	6.93197300	-0.65152800	2.66670800
N	4.35466200	3.71715400	4.31455100
B	-0.04340900	-1.72453400	7.34143900
B	1.32663400	2.75277500	6.64179800
B	3.35022200	3.47355300	5.30218700
B	6.44725000	-1.86235900	3.25434600
B	5.12748800	-3.87541900	4.04225700
B	1.11091800	-3.73576800	6.54969000
B	3.12806500	-4.57725500	5.26917800
C	1.74727600	-4.78421900	5.73544800
C	2.53674600	-3.60865100	6.20667100
C	-0.74599800	-0.43518800	7.44566100
C	0.74553600	-0.48604700	7.44455300
C	2.00411200	3.76759300	5.81881200
C	2.73131100	2.54022100	6.25793300
C	6.06955400	-3.27487700	3.08419800
C	5.63076900	-2.51482000	4.29125000
N	4.15613700	-4.88757200	4.32383100
N	-0.09170700	-3.11749900	7.01739400
B	0.04282200	0.80677700	7.39321600
N	0.09086700	2.20952900	7.11703400
B	1.32663400	2.75277500	-6.64179800
B	3.35022200	3.47355300	-5.30218700
B	6.44725000	-1.86235900	-3.25434600
B	5.12748800	-3.87541900	-4.04225700
B	1.11091800	-3.73576800	-6.54969000
B	3.12806500	-4.57725500	-5.26917800
C	1.74727600	-4.78421900	-5.73544800
C	2.53674600	-3.60865100	-6.20667100
C	2.00411200	3.76759300	-5.81881200

C	2.73131100	2.54022100	-6.25793300
C	6.06955400	-3.27487700	-3.08419800
C	5.63076900	-2.51482000	-4.29125000
N	4.15613700	-4.88757200	-4.32383100
B	0.04282200	0.80677700	-7.39321600
B	-0.04340900	-1.72453400	-7.34143900
C	-0.74599800	-0.43518800	-7.44566100
C	0.74553600	-0.48604700	-7.44455300
N	0.09086700	2.20952900	-7.11703400
N	-0.09170700	-3.11749900	-7.01739400
B	3.84390000	-5.81445700	3.27969600
B	3.02382800	-7.04841300	-1.22508800
B	3.84390000	-5.81445700	-3.27969600
C	4.08104500	-6.28138600	1.90393500
C	2.85961200	-6.70805000	2.64774800
C	2.85961200	-6.70805000	-2.64774800
C	4.08104500	-6.28138600	-1.90393500
B	3.02382800	-7.04841300	1.22508800
N	2.42804700	-7.48582700	0.00000000
B	-3.68769100	4.90449600	3.26608900
B	-0.84988400	7.06498800	0.00000000
B	1.36643700	6.99120000	0.00000000
B	-3.07556400	3.69602600	5.30658600
B	-1.10520000	2.83727500	6.64402200
C	-2.52170200	2.72260200	6.26255300
C	-1.71162200	3.89639500	5.82183600
C	-3.85911500	5.32154000	1.86712500
C	-2.68243500	5.78992900	2.65567900
C	0.27584300	7.61317400	-0.84430500
C	0.27584300	7.61317400	0.84430500
N	-4.06060400	4.00746800	4.31886100
B	-2.78689100	6.09599600	1.21614000
N	-2.19148900	6.54367900	0.00000000
B	-1.10520000	2.83727500	-6.64402200
B	-3.68769100	4.90449600	-3.26608900
B	-2.78689100	6.09599600	-1.21614000
C	-1.71162200	3.89639500	-5.82183600
C	-2.52170200	2.72260200	-6.26255300
C	-3.85911500	5.32154000	-1.86712500
C	-2.68243500	5.78992900	-2.65567900
B	-3.07556400	3.69602600	-5.30658600
N	-4.06060400	4.00746800	-4.31886100
C	5.72410100	1.28228200	-4.28249100
C	6.17133300	2.00697400	-3.05670500

C	7.32134200	0.08186200	0.00000000
C	7.28310000	-1.41021800	0.00000000
C	6.17133300	2.00697400	3.05670500
C	5.72410100	1.28228200	4.28249100
C	4.24946000	5.04855100	1.86605300
C	3.10573600	5.59410500	2.65375500
C	4.24946000	5.04855100	-1.86605300
C	3.10573600	5.59410500	-2.65375500
B	-6.52861200	-1.41716100	-3.25310400
B	-5.34978400	-3.51658900	-4.03910900
B	-7.22175600	-0.16428700	-1.26642400
B	-7.22175600	-0.16428700	1.26642400
B	-6.52861200	-1.41716100	3.25310400
B	-5.34978400	-3.51658900	4.03910900
B	-4.20038100	-5.53941300	3.27853200
B	-3.46490200	-6.82738600	1.22505100
B	-4.20038100	-5.53941300	-3.27853200
B	-3.46490200	-6.82738600	-1.22505100
N	-6.92814200	-0.17517500	2.66664100
N	-4.44954700	-4.59228100	4.32142200
N	-2.90014500	-7.30470200	0.00000000
N	-4.44954700	-4.59228100	-4.32142200
N	-6.92814200	-0.17517500	-2.66664100
B	-5.04598800	3.01331700	-4.02491600
B	-6.41118600	1.02757700	-3.24481300
B	-3.40364800	-4.35202400	-5.26751900
B	-1.33422600	-3.65068800	-6.54911400
C	-5.98868100	2.42500800	-3.05980700
C	-5.59118700	1.67032800	-4.28456300
C	-2.04111900	-4.65375200	-5.73582000
C	-2.74723100	-3.42502000	-6.20381300
B	-1.33422600	-3.65068800	6.54911400
B	-3.40364800	-4.35202400	5.26751900
B	-1.51198100	-7.65138700	0.00000000
B	1.01955600	-7.73764100	0.00000000
C	-2.74723100	-3.42502000	6.20381300
C	-2.04111900	-4.65375200	5.73582000
C	-0.24879600	-7.77173700	-0.74628700
C	-0.24879600	-7.77173700	0.74628700
B	-5.04598800	3.01331700	4.02491600
B	-6.41118600	1.02757700	3.24481300
C	-5.59118700	1.67032800	4.28456300
C	-5.98868100	2.42500800	3.05980700
C	-3.27839800	-6.49774800	2.64751900

C	-4.46835000	-5.99052700	1.90312800
C	-4.46835000	-5.99052700	-1.90312800
C	-3.27839800	-6.49774800	-2.64751900
C	-6.24806100	-2.85201100	-3.08118400
C	-5.75929600	-2.12518100	-4.28959600
C	-7.33213700	-0.90661500	0.00000000
C	-7.26482400	0.58443800	0.00000000
C	-6.24806100	-2.85201100	3.08118400
C	-5.75929600	-2.12518100	4.28959600
C	-1.04161800	9.70166700	-0.67127000
C	-1.04161800	9.70166700	0.67127000
H	-1.88130200	9.93449100	-1.31657200
H	-1.88130200	9.93449100	1.31657200
C	0.29323300	9.15106900	-1.15693800
H	0.59645800	9.41785200	-2.16811100
C	0.29323300	9.15106900	1.15693800
H	0.59645800	9.41785200	2.16811100
C	1.18869800	9.66943300	0.00000000
H	2.19941400	9.24528500	0.00000000
H	1.24375100	10.76081600	0.00000000

TS3

B	3.47226400	-3.61500300	5.23968900
B	3.01853000	-1.47097200	6.50882300
B	2.39592000	-5.42750800	4.00563000
B	0.15026200	-6.29380200	3.20858600
B	-2.27075300	-5.96086900	3.20347600
B	-4.10270500	-4.40109800	3.99836200
B	-4.52214600	-2.33079400	5.23395100
B	-3.40635500	-0.43968600	6.49741700
B	1.25094000	0.04841100	7.25919700
B	-1.25037700	0.44883200	7.25218400
N	-1.11941800	-6.57446800	2.62615400
N	-4.97885600	-3.30728600	4.29388200
N	-2.63133300	0.67343100	6.95453400
N	2.63458600	-0.17150700	6.96715900
N	3.58653000	-4.68927300	4.30054900
B	7.39656900	0.33384600	0.00000000
B	5.95463600	-4.00824600	1.22406700
B	4.56977100	-4.57132600	3.26925900
B	3.40489900	0.94603900	6.51512700
B	4.50859600	2.84437300	5.25312200
B	6.96096700	2.41084400	1.22407400
B	5.83886900	3.39149200	3.27234100
C	6.33792900	3.56162200	1.89789300

C	6.59749100	2.29633500	2.64588300
C	7.27916700	-0.92991400	-0.74622300
C	7.27916700	-0.92991400	0.74622300
C	4.99733600	-4.90091400	1.89873800
C	5.64120200	-3.77963500	2.64351400
C	3.46143800	2.37726900	6.17602600
C	4.53637500	1.44827200	5.71867200
N	4.95646300	3.82462700	4.31186400
N	7.31920600	1.76213900	0.00000000
B	7.00994200	-2.16967700	0.00000000
N	6.50020900	-3.50714300	0.00000000
B	-7.00218400	-1.88638800	1.22300900
B	-5.86883000	-2.87103100	3.26266700
B	-3.00911700	1.97733600	6.50308400
B	-3.45321200	4.13173600	5.24734300
B	-5.92432300	4.51841900	1.22404500
B	-4.54292000	5.08161100	3.27117200
C	-4.96302500	5.40627400	1.89831600
C	-5.61459900	4.29053100	2.64502000
C	-6.37889700	-3.03941600	1.89219000
C	-6.63011600	-1.77380700	2.64271900
C	-2.60855500	3.35385600	6.16832400
C	-3.92202500	2.81478300	5.70817800
N	-3.56603500	5.20650400	4.30931300
B	-7.42270400	0.19305100	0.00000000
B	-7.00072800	2.69063300	0.00000000
C	-7.28807900	1.45506600	-0.74626100
C	-7.28807900	1.45506600	0.74626100
N	-7.36086900	-1.23579800	0.00000000
N	-6.47292900	4.02070500	0.00000000
B	4.08063000	4.92013500	4.02804200
B	-0.16019600	6.88730400	3.24692100
B	-2.38773400	5.96704800	4.02632000
C	2.79889800	5.59844100	4.28050800
C	3.60729900	5.93384400	3.07158900
C	-1.61778600	6.78098600	3.07144100
C	-0.95676800	6.20359400	4.27864200
B	2.25813700	6.49622900	3.24690800
N	1.12215900	7.14310900	2.66572300
B	2.39592000	-5.42750800	-4.00563000
B	-1.13983800	-6.91429300	-1.22669000
B	-1.13983800	-6.91429300	1.22669000
B	4.56977100	-4.57132600	-3.26925900
B	5.95463600	-4.00824600	-1.22406700

C	5.64120200	-3.77963500	-2.64351400
C	4.99733600	-4.90091400	-1.89873800
C	0.95433900	-5.60309700	-4.22903400
C	1.62119000	-6.25420900	-3.06348300
C	-1.84499500	-7.28092000	0.00000000
C	-0.29773700	-6.98920900	0.00000000
N	3.58653000	-4.68927300	-4.30054900
B	0.15026200	-6.29380200	-3.20858600
N	-1.11941800	-6.57446800	-2.62615400
B	-7.00218400	-1.88638800	-1.22300900
B	-4.10270500	-4.40109800	-3.99836200
B	-2.27075300	-5.96086900	-3.20347600
C	-6.37889700	-3.03941600	-1.89219000
C	-6.63011600	-1.77380700	-2.64271900
C	-2.81868700	-5.07452400	-4.24574100
C	-3.62444500	-5.40398400	-3.03392700
B	-5.86883000	-2.87103100	-3.26266700
N	-4.97885600	-3.30728600	-4.29388200
C	-4.54178900	-0.93499400	5.70293800
C	-3.46907300	-1.86935000	6.15399400
C	-0.11771200	-0.48844500	7.32981700
C	0.11830200	0.98525600	7.33376600
C	2.62330100	-2.84614700	6.16366100
C	3.93690500	-2.30049400	5.71119900
C	0.95433900	-5.60309700	4.22903400
C	1.62119000	-6.25420900	3.06348300
C	-2.81868700	-5.07452400	4.24574100
C	-3.62444500	-5.40398400	3.03392700
B	-3.00911700	1.97733600	-6.50308400
B	-3.45321200	4.13173600	-5.24734300
B	-1.25037700	0.44883200	-7.25218400
B	1.25094000	0.04841100	-7.25919700
B	3.40489900	0.94603900	-6.51512700
B	4.50859600	2.84437300	-5.25312200
B	4.08063000	4.92013500	-4.02804200
B	2.25813700	6.49622900	-3.24690800
B	-2.38773400	5.96704800	-4.02632000
B	-0.16019600	6.88730400	-3.24692100
N	2.63458600	-0.17150700	-6.96715900
N	4.95646300	3.82462700	-4.31186400
N	1.12215900	7.14310900	-2.66572300
N	-3.56603500	5.20650400	-4.30931300
N	-2.63133300	0.67343100	-6.95453400
B	-4.52214600	-2.33079400	-5.23395100

B	-3.40635500	-0.43968600	-6.49741700
B	-4.54292000	5.08161100	-3.27117200
B	-5.92432300	4.51841900	-1.22404500
C	-3.46907300	-1.86935000	-6.15399400
C	-4.54178900	-0.93499400	-5.70293800
C	-4.96302500	5.40627400	-1.89831600
C	-5.61459900	4.29053100	-2.64502000
B	6.96096700	2.41084400	-1.22407400
B	5.83886900	3.39149200	-3.27234100
B	1.16990800	7.43755300	-1.26644600
B	1.16990800	7.43755300	1.26644600
C	6.59749100	2.29633500	-2.64588300
C	6.33792900	3.56162200	-1.89789300
C	0.44567100	7.63359600	0.00000000
C	1.91885100	7.39341700	0.00000000
B	3.47226400	-3.61500300	-5.23968900
B	3.01853000	-1.47097200	-6.50882300
C	3.93690500	-2.30049400	-5.71119900
C	2.62330100	-2.84614700	-6.16366100
C	3.60729900	5.93384400	-3.07158900
C	2.79889800	5.59844100	-4.28050800
C	-0.95676800	6.20359400	-4.27864200
C	-1.61778600	6.78098600	-3.07144100
C	-2.60855500	3.35385600	-6.16832400
C	-3.92202500	2.81478300	-5.70817800
C	0.11830200	0.98525600	-7.33376600
C	-0.11771200	-0.48844500	-7.32981700
C	3.46143800	2.37726900	-6.17602600
C	4.53637500	1.44827200	-5.71867200
C	0.92213300	-8.79325200	0.00000000
H	1.45873300	-8.71654900	-0.93718900
H	1.45873300	-8.71654900	0.93718900
N	-1.18481300	-9.99216400	0.00000000
N	-0.11587700	-9.60626500	0.00000000

IM

B	3.98801700	-3.05273200	5.17539200
B	3.23145800	-1.01069900	6.46848200
B	3.20641100	-4.98499200	3.89183100
B	1.14243800	-6.19000500	3.04652200
B	-1.29718600	-6.17206200	3.04343900
B	-3.32932400	-4.91473200	3.88750300
B	-4.06217200	-2.96413400	5.17377900
B	-3.25774200	-0.93988200	6.46629100
B	1.26700200	0.23148700	7.23492200

B	-1.26572900	0.25855200	7.23335800
N	-0.07939600	-6.64967500	2.46286300
N	-4.36600700	-3.98721600	4.22101900
N	-2.66556500	0.27413100	6.93838900
N	2.66738500	0.21607900	6.94100400
N	4.26722500	-4.08496300	4.22426600
B	7.34733400	1.46761200	0.00000000
B	6.59066600	-3.04577800	1.21746900
B	5.25294600	-3.81901600	3.22291400
B	3.26812900	1.43628200	6.49694000
B	4.07830600	3.48299500	5.24412800
B	6.58328100	3.44814700	1.22354700
B	5.31355900	4.23620000	3.26889900
C	5.78336600	4.48475600	1.89622400
C	6.23766800	3.27575500	2.64393700
C	7.43310000	0.20131600	-0.74620700
C	7.43310000	0.20131600	0.74620700
C	5.75732600	-4.07273200	1.86401800
C	6.21663400	-2.87730500	2.63078900
C	3.11337500	2.86206100	6.16595500
C	4.31197800	2.10360200	5.70186000
N	4.37194000	4.52329300	4.30696800
N	7.04283700	2.86549100	0.00000000
B	7.36419200	-1.06564900	0.00000000
N	7.06896400	-2.46590300	0.00000000
B	-6.66606100	-2.88862500	1.21703400
B	-5.34498200	-3.69521400	3.21999200
B	-3.23815500	1.50780000	6.49417500
B	-4.00099200	3.57338900	5.24245700
B	-6.50995400	3.60184600	1.22355200
B	-5.22021800	4.35720300	3.26869700
C	-5.68483400	4.61843400	1.89664600
C	-6.16759800	3.42001400	2.64363200
C	-5.85483000	-3.93419900	1.86095600
C	-6.28767400	-2.73060900	2.63055400
C	-3.05012800	2.92973600	6.16341200
C	-4.26636500	2.19962600	5.69968600
N	-4.27096300	4.62091900	4.30619600
B	-7.39622700	-0.89152700	0.00000000
B	-7.32164900	1.64062900	0.00000000
C	-7.43659000	0.37688200	-0.74622200
C	-7.43659000	0.37688200	0.74622200
N	-7.13177500	-2.29744200	0.00000000
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B	3.33945100	5.47322500	4.02613400
B	-1.14956000	6.78584600	3.24683700
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C	1.96939900	5.94857300	4.27854300
C	2.71882000	6.40612500	3.07179700
C	-2.57574700	6.46647100	3.07173600
C	-1.83663000	5.99104600	4.27796800
B	1.30020300	6.75799400	3.24691500
N	0.08060400	7.22914300	2.66585400
B	3.20641100	-4.98499200	-3.89183100
B	-0.07336900	-7.15794800	-1.12486700
B	-0.07336900	-7.15794800	1.12486700
B	5.25294600	-3.81901600	-3.22291400
B	6.59066600	-3.04577800	-1.21746900
C	6.21663400	-2.87730500	-2.63078900
C	5.75732600	-4.07273200	-1.86401800
C	1.80520500	-5.38843500	-4.08714700
C	2.58154300	-5.89938600	-2.91970500
C	-0.89655000	-7.72640600	0.00000000
C	0.77911400	-7.69787500	0.00000000
N	4.26722500	-4.08496300	-4.22426600
B	1.14243800	-6.19000500	-3.04652200
N	-0.07939600	-6.64967500	-2.46286300
B	-6.66606100	-2.88862500	-1.21703400
B	-3.32932400	-4.91473200	-3.88750300
B	-1.29718600	-6.17206200	-3.04343900
C	-5.85483000	-3.93419900	-1.86095600
C	-6.28767400	-2.73060900	-2.63055400
C	-1.94324000	-5.36527900	-4.09075800
C	-2.72302200	-5.83193300	-2.90707000
B	-5.34498200	-3.69521400	-3.21999200
N	-4.36600700	-3.98721600	-4.22101900
C	-4.30498700	-1.59950800	5.66948900
C	-3.08964600	-2.35419800	6.09475200
C	-0.00729100	-0.50182000	7.30368100
C	0.00869600	0.99062800	7.31764800
C	3.03063300	-2.42085500	6.09686400
C	4.26293900	-1.69442900	5.67083300
C	1.80520500	-5.38843500	4.08714700
C	2.58154300	-5.89938600	2.91970500
C	-1.94324000	-5.36527900	4.09075800
C	-2.72302200	-5.83193300	2.90707000
B	-3.23815500	1.50780000	-6.49417500
B	-4.00099200	3.57338900	-5.24245700

B	-1.26572900	0.25855200	-7.23335800
B	1.26700200	0.23148700	-7.23492200
B	3.26812900	1.43628200	-6.49694000
B	4.07830600	3.48299500	-5.24412800
B	3.33945100	5.47322500	-4.02613400
B	1.30020300	6.75799400	-3.24691500
B	-3.21728000	5.54709300	-4.02555800
B	-1.14956000	6.78584600	-3.24683700
N	2.66738500	0.21607900	-6.94100400
N	4.37194000	4.52329300	-4.30696800
N	0.08060400	7.22914300	-2.66585400
N	-4.27096300	4.62091900	-4.30619600
N	-2.66556500	0.27413100	-6.93838900
B	-4.06217200	-2.96413400	-5.17377900
B	-3.25774200	-0.93988200	-6.46629100
B	-5.22021800	4.35720300	-3.26869700
B	-6.50995400	3.60184600	-1.22355200
C	-3.08964600	-2.35419800	-6.09475200
C	-4.30498700	-1.59950800	-5.66948900
C	-5.68483400	4.61843400	-1.89664600
C	-6.16759800	3.42001400	-2.64363200
B	6.58328100	3.44814700	-1.22354700
B	5.31355900	4.23620000	-3.26889900
B	0.08406200	7.52782600	-1.26652300
B	0.08406200	7.52782600	1.26652300
C	6.23766800	3.27575500	-2.64393700
C	5.78336600	4.48475600	-1.89622400
C	-0.66120500	7.61350000	0.00000000
C	0.83117800	7.59601900	0.00000000
B	3.98801700	-3.05273200	-5.17539200
B	3.23145800	-1.01069900	-6.46848200
C	4.26293900	-1.69442900	-5.67083300
C	3.03063300	-2.42085500	-6.09686400
C	2.71882000	6.40612500	-3.07179700
C	1.96939900	5.94857300	-4.27854300
C	-1.83663000	5.99104600	-4.27796800
C	-2.57574700	6.46647100	-3.07173600
C	-3.05012800	2.92973600	-6.16341200
C	-4.26636500	2.19962600	-5.69968600
C	0.00869600	0.99062800	-7.31764800
C	-0.00729100	-0.50182000	-7.30368100
C	3.11337500	2.86206100	-6.16595500
C	4.31197800	2.10360200	-5.70186000
C	1.10790600	-9.18201700	0.00000000

H	1.64292900	-9.53583600	-0.88529200
H	1.64292900	-9.53583600	0.88529200
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N	-0.24407700	-9.88316900	0.00000000

PC3

B	3.16648800	4.00584300	5.12204900
B	1.14255700	3.23645100	6.43573500
B	5.09021200	3.25261500	3.80388700
B	6.32559800	1.21934500	2.92822900
B	6.32550200	-1.21968400	2.92848500
B	5.09001200	-3.25271700	3.80456000
B	3.16616000	-4.00557800	5.12274800
B	1.14224800	-3.23581000	6.43624000
B	-0.07822500	1.26650300	7.21781100
B	-0.07835500	-1.26563000	7.21799200
N	6.81636700	-0.00023800	2.35787800
N	4.18676500	-4.30201200	4.16492500
N	-0.07691500	-2.66502100	6.92080500
N	-0.07665100	2.66584500	6.92041600
N	4.18711600	4.30206300	4.16419100
B	-1.40424300	7.36628000	-0.00046500
B	3.11858300	6.67867400	1.21272100
B	3.91120800	5.30941000	3.18768400
B	-1.30432500	3.25548300	6.48270900
B	-3.36356900	4.04416800	5.23702400
B	-3.36912200	6.56049200	1.22272100
B	-4.13610900	5.27382700	3.26546300
C	-4.39209800	5.74193100	1.89368400
C	-3.19109100	6.21503800	2.64249900
C	-0.14031000	7.47849100	-0.74662800
C	-0.14028900	7.47861600	0.74564500
C	4.15562800	5.84401600	1.83957900
C	2.95977000	6.27892500	2.62010200
C	-2.73002500	3.08657200	6.15794200
C	-1.98509800	4.29194100	5.68963700
N	-4.40920100	4.32618200	4.30203800
N	-2.79536300	7.03177200	-0.00041600
B	1.12793400	7.43357600	-0.00050700
N	2.53209500	7.16044500	-0.00049100
B	3.11790300	-6.67863200	1.21354900
B	3.91067200	-5.30932900	3.18843600
B	-1.30464100	-3.25458400	6.48314200
B	-3.36396700	-4.04318900	5.23754600
B	-3.36980600	-6.55999600	1.22354200

B	-4.13664300	-5.27300000	3.26613300
C	-4.39268700	-5.74123900	1.89441000
C	-3.19172300	-6.21438000	2.64327300
C	4.15505700	-5.84407300	1.84037300
C	2.95907800	-6.27869200	2.62087200
C	-2.73032100	-3.08555600	6.15835600
C	-1.98552600	-4.29106200	5.69019500
N	-4.40962900	-4.32520300	4.30259600
B	1.12717500	-7.43349900	0.00041400
B	-1.40499600	-7.36608100	0.00045000
C	-0.14106900	-7.47847700	-0.74570000
C	-0.14104600	-7.47840600	0.74657300
N	2.53135700	-7.16045800	0.00039100
N	-2.79609600	-7.03148200	0.00045900
B	-5.34598600	3.28167900	4.02159700
B	-6.60589400	-1.22490200	3.24503200
B	-5.34630200	-3.28063300	4.02202300
C	-5.80281700	1.90539000	4.27455000
C	-6.27279400	2.64899500	3.06906100
C	-6.27303800	-2.64798000	3.06939900
C	-5.80298800	-1.90426300	4.27479100
B	-6.60577900	1.22597000	3.24487600
N	-7.06304700	0.00051700	2.66502600
B	5.09023000	3.25206900	-3.80445500
B	7.51116600	-0.00073400	-1.11375800
B	7.51020500	-0.00058400	1.11293800
B	3.91121600	5.30893400	-3.18839500
B	3.11858300	6.67847700	-1.21362300
C	2.95975600	6.27850300	-2.62093900
C	4.15561700	5.84371200	-1.84035800
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C	6.01636900	2.65431200	-2.82652700
C	8.11897600	-0.86407300	-0.00010100
C	8.11829000	0.86339900	-0.00020500
N	4.18706400	4.30144800	-4.16477700
B	6.32584500	1.21895700	-2.92875000
N	6.81673800	-0.00056500	-2.35836200
B	3.11790000	-6.67875900	-1.21281700
B	5.08998600	-3.25315700	-3.80433400
B	6.32569700	-1.22007000	-2.92869100
C	4.15504000	-5.84425800	-1.83973900
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C	5.49644800	-1.84884900	-3.96933300
C	6.01602300	-2.65535500	-2.82635700

B	3.91066900	-5.30969400	-3.18787300
N	4.18670100	-4.30248700	-4.16449100
C	1.81302700	-4.27354400	5.63655300
C	2.54769200	-3.04019500	6.04511900
C	0.66872900	0.00040300	7.28560200
C	-0.82375600	0.00048000	7.30614700
C	2.54795200	3.04061100	6.04454300
C	1.81341700	4.27401500	5.63590500
C	5.49670100	1.84834700	3.96898400
C	6.01591100	2.65463400	2.82568100
C	5.49667300	-1.84846000	3.96946100
C	6.01569200	-2.65495000	2.82622200
B	-1.30483200	-3.25541400	-6.48269200
B	-3.36414400	-4.04386400	-5.23697000
B	-0.07856400	-1.26655100	-7.21781800
B	-0.07842600	1.26557900	-7.21793500
B	-1.30450300	3.25465400	-6.48304200
B	-3.36373500	4.04350800	-5.23744300
B	-5.34613000	3.28117600	-4.02188800
B	-6.60589600	1.22555900	-3.24488100
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B	-6.60601100	-1.22531400	-3.24473100
N	-0.07683700	2.66495300	-6.92068800
N	-4.40935200	4.32564500	-4.30247800
N	-7.06314400	0.00017800	-2.66486300
N	-4.40978800	-4.32575600	-4.30196500
N	-0.07711300	-2.66590400	-6.92044600
B	3.16601500	-4.00616200	-5.12226600
B	1.14206100	-3.23661200	-6.43581800
B	-4.13677200	-5.27342100	-3.26538700
B	-3.36985700	-6.56015200	-1.22265800
C	2.54751600	-3.04092500	-6.04476800
C	1.81287700	-4.27422400	-5.63600200
C	-4.39276200	-5.74147800	-1.89359200
C	-3.19183100	-6.21472400	-2.64244300
B	-3.36916900	6.56033300	-1.22347100
B	-4.13623000	5.27341500	-3.26602600
B	-7.36457000	0.00027900	-1.26625300
B	-7.36452200	0.00044000	1.26642600
C	-3.19118700	6.21470000	-2.64321100
C	-4.39216500	5.74168200	-1.89429300
C	-7.44231500	-0.74582300	0.00013500
C	-7.44224200	0.74655000	0.00004000
B	3.16634800	4.00508900	-5.12250200

B	1.14237800	3.23558900	-6.43606500
C	1.81326000	4.27321400	-5.63633300
C	2.54777500	3.03976600	-6.04487300
C	-6.27291400	2.64860800	-3.06925100
C	-5.80296300	1.90485400	-4.27465900
C	-5.80313700	-1.90480800	-4.27442800
C	-6.27315600	-2.64837100	-3.06892900
C	-2.73050900	-3.08634700	-6.15791000
C	-1.98570500	-4.29179000	-5.68959900
C	-0.82396200	-0.00045100	-7.30612200
C	0.66852400	-0.00053000	-7.28560700
C	-2.73020200	3.08579300	-6.15824600
C	-1.98526000	4.29120900	-5.69008400
C	9.38506100	0.00026900	0.00094600
H	9.98856400	0.00021600	-0.90277500
H	9.98701900	0.00031700	0.90571900

N₂₀(C₂B₂)₃₀(H₂)₂

B	-2.82634500	1.20919700	-6.33331100
B	-3.74439300	3.24873900	-5.13067400
B	-0.98835000	0.00000000	-7.55256400
B	0.98835000	0.00000000	-7.55256400
B	2.82634500	1.20919700	-6.33331100
B	3.74439300	3.24873900	-5.13067400
B	3.16950900	5.32687600	-3.96989500
B	1.21089300	6.71917900	-3.17705300
B	-3.16950900	5.32687600	-3.96989500
B	-1.21089300	6.71917900	-3.17705300
N	2.24124100	0.00000000	-6.81442500
N	4.13020900	4.30510800	-4.24376300
N	0.00000000	7.20629400	-2.58952100
N	-4.13020900	4.30510800	-4.24376300
N	-2.24124100	0.00000000	-6.81442500
B	-6.41659900	-3.23639900	-1.21152000
B	-3.74439300	-3.24873900	-5.13067400
B	-2.82634500	-1.20919700	-6.33331100
B	-5.09225000	4.00568900	-3.22868100
B	-6.41659900	3.23639900	-1.21152000
B	-7.20095200	-1.26620700	0.00729400
B	-7.20095200	1.26620700	0.00729400
C	-7.29115800	0.00000000	0.75264100
C	-7.26556500	0.00000000	-0.73992000
C	-5.61918800	-4.27690500	-1.88081200
C	-6.01279300	-3.03692500	-2.61260600
C	-2.74930400	-2.65532700	-6.04067300

C	-3.88202300	-1.83816800	-5.51801200
C	-5.61918800	4.27690500	-1.88081200
C	-6.01279300	3.03692500	-2.61260600
N	-6.90704200	2.66638900	0.00605300
N	-6.90704200	-2.66638900	0.00605300
B	-5.09225000	-4.00568900	-3.22868100
N	-4.13020900	-4.30510800	-4.24376300
B	6.41659900	3.23639900	-1.21152000
B	5.09225000	4.00568900	-3.22868100
B	0.00000000	7.47090300	-1.18370800
B	0.00000000	7.38574500	1.34835300
B	3.26434100	5.27802000	4.07313700
B	1.22279600	6.56914400	3.30984500
C	1.89297800	5.74680200	4.33059800
C	2.64216900	6.22237400	3.13075400
C	6.01279300	3.03692500	-2.61260600
C	5.61918800	4.27690500	-1.88081200
C	-0.74618100	7.50680200	0.08503500
C	0.74618100	7.50680200	0.08503500
N	0.00000000	7.04384000	2.73785400
B	6.47475800	3.25791400	1.23459900
B	5.23406700	4.04808000	3.29638100
C	6.15304600	3.08983200	2.66121700
C	5.68444300	4.29567700	1.91716600
N	6.90704200	2.66638900	0.00605300
N	4.30054600	4.32932200	4.34356100
B	-6.47475800	3.25791400	1.23459900
B	-3.26434100	5.27802000	4.07313700
B	-1.22279600	6.56914400	3.30984500
C	-5.68444300	4.29567700	1.91716600
C	-6.15304600	3.08983200	2.66121700
C	-1.89297800	5.74680200	4.33059800
C	-2.64216900	6.22237400	3.13075400
B	-5.23406700	4.04808000	3.29638100
N	-4.30054600	4.32932200	4.34356100
B	1.21089300	-6.71917900	-3.17705300
B	3.74439300	-3.24873900	-5.13067400
B	2.82634500	-1.20919700	-6.33331100
B	-1.21089300	-6.71917900	-3.17705300
B	-3.16950900	-5.32687600	-3.96989500
C	-2.61465000	-6.30678200	-3.02126500
C	-1.82734600	-5.87733100	-4.21469400
C	2.61465000	-6.30678200	-3.02126500
C	1.82734600	-5.87733100	-4.21469400

C	3.88202300	-1.83816800	-5.51801200
C	2.74930400	-2.65532700	-6.04067300
N	0.00000000	-7.20629400	-2.58952100
B	3.16950900	-5.32687600	-3.96989500
N	4.13020900	-4.30510800	-4.24376300
B	7.20095200	1.26620700	0.00729400
B	6.41659900	-3.23639900	-1.21152000
B	5.09225000	-4.00568900	-3.22868100
C	7.26556500	0.00000000	-0.73992000
C	7.29115800	0.00000000	0.75264100
C	5.61918800	-4.27690500	-1.88081200
C	6.01279300	-3.03692500	-2.61260600
B	7.20095200	-1.26620700	0.00729400
N	6.90704200	-2.66638900	0.00605300
C	2.61465000	6.30678200	-3.02126500
C	1.82734600	5.87733100	-4.21469400
C	-1.82734600	5.87733100	-4.21469400
C	-2.61465000	6.30678200	-3.02126500
C	-2.74930400	2.65532700	-6.04067300
C	-3.88202300	1.83816800	-5.51801200
C	2.74930400	2.65532700	-6.04067300
C	3.88202300	1.83816800	-5.51801200
B	4.02089500	-3.28326800	5.27871500
B	3.24538100	-1.22560500	6.53637700
B	3.26434100	-5.27802000	4.07313700
B	1.22279600	-6.56914400	3.30984500
B	-1.22279600	-6.56914400	3.30984500
B	-3.26434100	-5.27802000	4.07313700
B	-4.02089500	-3.28326800	5.27871500
B	-3.24538100	-1.22560500	6.53637700
B	1.26646200	0.00000000	7.29360300
B	-1.26646200	0.00000000	7.29360300
N	0.00000000	-7.04384000	2.73785400
N	-4.30054600	-4.32932200	4.34356100
N	-2.66547500	0.00000000	6.99344300
N	2.66547500	0.00000000	6.99344300
N	4.30054600	-4.32932200	4.34356100
B	6.47475800	-3.25791400	1.23459900
B	5.23406700	-4.04808000	3.29638100
B	3.24538100	1.22560500	6.53637700
B	4.02089500	3.28326800	5.27871500
C	5.68444300	-4.29567700	1.91716600
C	6.15304600	-3.08983200	2.66121700
C	3.06896400	2.64900100	6.20504700

C	4.27457700	1.90637500	5.73366800
B	-6.47475800	-3.25791400	1.23459900
B	-5.23406700	-4.04808000	3.29638100
B	-3.24538100	1.22560500	6.53637700
B	-4.02089500	3.28326800	5.27871500
C	-5.68444300	-4.29567700	1.91716600
C	-6.15304600	-3.08983200	2.66121700
C	-3.06896400	2.64900100	6.20504700
C	-4.27457700	1.90637500	5.73366800
B	0.00000000	-7.47090300	-1.18370800
B	0.00000000	-7.38574500	1.34835300
C	-0.74618100	-7.50680200	0.08503500
C	0.74618100	-7.50680200	0.08503500
C	-4.27457700	-1.90637500	5.73366800
C	-3.06896400	-2.64900100	6.20504700
C	0.00000000	-0.74624500	7.37091000
C	0.00000000	0.74624500	7.37091000
C	3.06896400	-2.64900100	6.20504700
C	4.27457700	-1.90637500	5.73366800
C	1.89297800	-5.74680200	4.33059800
C	2.64216900	-6.22237400	3.13075400
C	-1.89297800	-5.74680200	4.33059800
C	-2.64216900	-6.22237400	3.13075400
C	0.00000000	1.18403900	-7.89207900
H	0.00000000	1.28223000	-8.98731900
H	0.00000000	2.16446000	-7.42100600
C	0.00000000	-1.18403900	-7.89207900
H	0.00000000	-1.28223000	-8.98731900
H	0.00000000	-2.16446000	-7.42100600
N₂₀(C₂B₂)₃₀(CO)₂			
B	6.15917900	1.21139400	-3.03937200
B	4.97031200	3.27734500	-3.91125500
B	6.95674100	0.00047900	-1.01563100
B	6.95672500	0.00052600	1.01569600
B	6.15913100	1.21152900	3.03938300
B	4.97025100	3.27749500	3.91121100
B	3.78405800	5.30392800	3.23695400
B	2.99924100	6.61483300	1.21878800
B	3.78411100	5.30380600	-3.23708100
B	2.99926200	6.61478800	-1.21897800
N	6.58690200	0.00053400	2.42687200
N	4.06494800	4.33245800	4.24866000
N	2.41501000	7.08419400	-0.00010900
N	4.06500900	4.33229700	-4.24874700

N	6.58694200	0.00042000	-2.42681300
B	1.00475400	-3.25167600	-6.48657800
B	4.97085500	-3.27678700	-3.91120200
B	6.15941200	-1.21064300	-3.03936500
B	3.03898200	4.04330800	-5.20278500
B	1.00427600	3.25160500	-6.48669800
B	-0.21467800	-1.26679000	-7.24300100
B	-0.21486300	1.26651200	-7.24305000
C	-0.96049900	-0.00019500	-7.32348800
C	0.53195400	-0.00008600	-7.31387300
C	1.67540900	-4.29574000	-5.69451700
C	2.41959400	-3.07454900	-6.12136500
C	5.84900600	-2.64946600	-2.90906400
C	5.40611100	-1.88617500	-4.10943800
C	1.67478200	4.29580400	-5.69468900
C	2.41914300	3.07470100	-6.12147900
N	-0.21639100	2.66732600	-6.95123000
N	-0.21600100	-2.66759400	-6.95113200
B	3.03958800	-4.04304400	-5.20265700
N	4.06568100	-4.33186800	-4.24863900
B	1.00419300	3.25184500	6.48661800
B	3.03891100	4.04350300	5.20269800
B	1.01303200	7.36893800	-0.00012600
B	-1.51991800	7.32828000	-0.00013900
B	-4.26352600	5.26428500	3.26964000
B	-3.49155500	6.54276100	1.22355300
C	-4.51853300	5.73105400	1.89711600
C	-3.31425300	6.19918800	2.64391500
C	2.41906300	3.07493000	6.12142200
C	1.67470700	4.29601800	5.69458200
C	-0.25475400	7.42632000	-0.74633800
C	-0.25476200	7.42634200	0.74607200
N	-2.91474900	7.00894200	-0.00014500
B	-1.44315300	3.25224000	6.50317300
B	-3.49700600	4.03742400	5.24583400
C	-2.86584500	3.07910700	6.16770200
C	-2.12191000	4.28816400	5.70731900
N	-0.21648400	2.66758200	6.95114500
N	-4.53969700	4.31920700	4.30765500
B	-1.44307100	3.25199800	-6.50330400
B	-4.26347800	5.26416100	-3.26988400
B	-3.49153400	6.54271500	-1.22383600
C	-2.12184600	4.28795600	-5.70750900
C	-2.86576800	3.07887700	-6.16785400

C	-4.51850600	5.73098800	-1.89738400
C	-3.31420600	6.19907900	-2.64417900
B	-3.49694400	4.03722200	-5.24602500
N	-4.53964100	4.31904100	-4.30786400
B	3.00027700	-6.61432900	1.21901800
B	4.97079000	-3.27662200	3.91135100
B	6.15935500	-1.21050900	3.03944900
B	3.00029800	-6.61437800	-1.21875700
B	3.78493700	-5.30337300	-3.23692800
C	2.83701300	-6.25564000	-2.63677700
C	4.03087100	-5.78996500	-1.87029500
C	2.83696600	-6.25552900	2.63701700
C	4.03084300	-5.78989400	1.87054000
C	5.40605200	-1.88600700	4.10954200
C	5.84893700	-2.64933500	2.90918700
N	2.41611700	-7.08381000	0.00013400
B	3.78488100	-5.30324200	3.23714800
N	4.06561800	-4.33169600	4.24882200
B	-0.21496200	1.26677800	7.24301100
B	1.00468900	-3.25143400	6.48672200
B	3.03952700	-4.04284300	5.20283300
C	0.53186000	0.00018500	7.31389500
C	-0.96059300	0.00007000	7.32346100
C	1.67535200	-4.29553200	5.69471000
C	2.41953000	-3.07431900	6.12150600
B	-0.21476600	-1.26652500	7.24305300
N	-0.21607500	-2.66733900	6.95123700
C	2.83600500	6.25607100	2.63680800
C	4.02992400	5.79055900	1.87032400
C	4.02995300	5.79048300	-1.87046300
C	2.83604900	6.25597200	-2.63698600
C	5.84847700	2.65015600	-2.90904200
C	5.40575400	1.88679000	-4.10943500
C	5.84843300	2.65028600	2.90902700
C	5.40568800	1.88694100	4.10942500
B	-5.47783800	-3.27738200	4.02656200
B	-6.74150800	-1.22516900	3.24699600
B	-4.26270900	-5.26480600	3.26982900
B	-3.49053500	-6.54323900	1.22379200
B	-3.49052300	-6.54327900	-1.22359700
B	-4.26268200	-5.26492100	-3.26968600
B	-5.47780800	-3.27752800	-4.02650800
B	-6.74148400	-1.22528600	-3.24703000
B	-7.49788200	-0.00054000	1.26648500

B	-7.49787100	-0.00058700	-1.26656700
N	-2.91365700	-7.00937000	0.00010800
N	-4.53899500	-4.31988300	-4.30770000
N	-7.19934600	-0.00059000	-2.66592000
N	-7.19936800	-0.00049500	2.66584000
N	-4.53903000	-4.31972900	4.30780400
B	-1.44265500	-3.25219800	6.50328500
B	-3.49638600	-4.03774700	5.24597400
B	-6.74169300	1.22426700	3.24695700
B	-5.47834000	3.27670100	4.02645500
C	-2.12125200	-4.28825800	5.70747100
C	-2.86537000	-3.07929300	6.16779900
C	-6.40477900	2.64645900	3.07202800
C	-5.93939200	1.90170000	4.27869700
B	-1.44259000	-3.25243200	-6.50317800
B	-3.49633900	-4.03793200	-5.24586700
B	-6.74166200	1.22415100	-3.24707400
B	-5.47829300	3.27655200	-4.02663300
C	-2.12119900	-4.28846200	-5.70733500
C	-2.86531000	-3.07951500	-6.16772100
C	-6.40473800	2.64634600	-3.07218800
C	-5.93935400	1.90154600	-4.27883400
B	1.01418000	-7.36876000	0.00012700
B	-1.51877600	-7.32848700	0.00012000
C	-0.25359800	-7.42634600	-0.74608000
C	-0.25360300	-7.42632400	0.74633100
C	-5.93907400	-1.90260000	-4.27876400
C	-6.40435200	-2.64742500	-3.07209200
C	-7.57478300	-0.74681400	-0.00002800
C	-7.57488900	0.74567600	-0.00005500
C	-6.40437000	-2.64731400	3.07211100
C	-5.93910800	-1.90244600	4.27876200
C	-4.51764600	-5.73167500	1.89732500
C	-3.31328900	-6.19958400	2.64414100
C	-4.51763000	-5.73174200	-1.89716900
C	-3.31326000	-6.19966800	-2.64395400
C	7.07316600	1.15654800	0.00000700
C	7.07339800	-1.15551800	0.00006200
C	7.02344100	-2.47380000	0.00010400
C	7.02289700	2.47485500	-0.00003700
O	7.02951000	-3.62678200	0.00019600
O	7.02878900	3.62784000	-0.00010800
N₂₀(C₂B₂)₃₀(NO)₂			
B	5.99552100	1.21975700	-3.25060000

B	4.75027800	3.28224600	-4.05573100
B	7.01965700	-0.01717400	-1.31501900
B	7.13061200	-0.01506300	0.76493000
B	6.25355700	1.18072700	2.79456200
B	5.06285500	3.22386600	3.72261400
B	3.84965800	5.25625300	3.11956200
B	2.98860100	6.59535300	1.15149200
B	3.59632900	5.30889800	-3.33178700
B	2.89357200	6.61587800	-1.28114500
N	6.71021300	0.00124600	2.15062500
N	4.17016900	4.27203900	4.10623600
N	2.35922600	7.07941700	-0.03825500
N	3.83719500	4.33957100	-4.35552800
N	6.49760300	0.02555900	-2.66778100
B	0.73576400	-3.19090200	-6.52995000
B	4.80352500	-3.24274400	-4.08784700
B	6.05464400	-1.20322000	-3.25390800
B	2.77992500	4.06391300	-5.28053600
B	0.70100900	3.29465800	-6.50431500
B	-0.52470700	-1.21423200	-7.23917600
B	-0.54126100	1.31825700	-7.23239100
C	-1.28127500	0.04784400	-7.28973900
C	0.21048300	0.05753700	-7.33567900
C	1.44073200	-4.23742400	-5.77316200
C	2.15971600	-3.00405100	-6.20765700
C	5.71975400	-2.62848600	-3.11252900
C	5.25038400	-1.85628600	-4.29997300
C	1.40289600	4.32842900	-5.72512200
C	2.12679800	3.10776900	-6.18743000
N	-0.53563900	2.71742700	-6.93053600
N	-0.50535100	-2.61447800	-6.94949600
B	2.81904600	-3.97974800	-5.32371700
N	3.87544400	-4.28348200	-4.40898000
B	1.20580600	3.18685000	6.46865500
B	3.18619600	3.97853700	5.10365900
B	0.95829800	7.36727300	0.01834400
B	-1.57215200	7.32109200	0.11509700
B	-4.18024100	5.21965700	3.47064200
B	-3.49150500	6.51737600	1.40714600
C	-4.48884800	5.69686200	2.11272100
C	-3.25813800	6.16272500	2.81649100
C	2.60341600	3.00682200	6.04151600
C	1.84645900	4.23379600	5.65517600
C	-0.33644400	7.42933700	-0.67820900

C	-0.27918900	7.41654100	0.81298200
N	-2.96380100	6.99557500	0.16579100
B	-1.23855800	3.18795400	6.58272200
B	-3.33827000	3.97863600	5.40750100
C	-2.67241300	3.01552600	6.29945100
C	-1.94714400	4.22813600	5.81923900
N	0.00507600	2.60171900	6.97881500
N	-4.41502300	4.26548500	4.51025000
B	-1.74450500	3.29668300	-6.42994400
B	-4.43333500	5.27558500	-3.06509100
B	-3.58593200	6.53821300	-1.03914000
C	-2.39031400	4.32402600	-5.59672200
C	-3.15223000	3.11955700	-6.03923900
C	-4.63570000	5.72969600	-1.67956600
C	-3.46222800	6.20732600	-2.46809900
B	-3.74563900	4.06771000	-5.08234700
N	-4.74910300	4.33928600	-4.09954600
B	2.99012000	-6.64942500	1.02365200
B	5.09258900	-3.29035600	3.60564500
B	6.30603800	-1.24486700	2.73045800
B	2.90067200	-6.63827400	-1.40451600
B	3.62420600	-5.27980000	-3.41325700
C	2.69000200	-6.24250200	-2.80672300
C	3.91397400	-5.80623400	-2.07157200
C	2.88374800	-6.27192000	2.44233600
C	4.04592800	-5.81872600	1.62194700
C	5.60506800	-1.92927800	3.83005300
C	5.89639200	-2.64681300	2.55404900
N	2.36075100	-7.12335900	-0.17136600
B	3.85747200	-5.31242100	2.98937000
N	4.18873700	-4.33541300	3.98002900
B	0.02171500	1.19775700	7.25722900
B	1.23767200	-3.29486700	6.37691400
B	3.21588800	-4.05436300	4.98868900
C	0.77807300	-0.06409100	7.28058700
C	-0.71275900	-0.07374200	7.35066700
C	1.87960700	-4.32490500	5.54557200
C	2.63008300	-3.09785400	5.94295200
B	0.03660100	-1.33442100	7.21982700
N	0.03321800	-2.72924300	6.90483900
C	2.88303400	6.21941200	2.57005600
C	4.04183900	5.75797600	1.74927200
C	3.89562100	5.78783500	-1.97282200
C	2.67766400	6.26392300	-2.69350300

C	5.66958700	2.65400700	-3.08873000
C	5.18851300	1.89627400	-4.27653300
C	5.91036200	2.61616500	2.68019800
C	5.52214900	1.83734100	3.88814500
B	-5.34267400	-3.33183200	4.19701100
B	-6.64062200	-1.27631100	3.48567200
B	-4.16200100	-5.31431900	3.37649400
B	-3.48406100	-6.58352300	1.29186400
B	-3.58201900	-6.56360900	-1.15375100
B	-4.42115700	-5.25971100	-3.15661600
B	-5.65905300	-3.26287200	-3.84830000
B	-6.89479100	-1.22005100	-3.00228000
B	-7.47904900	-0.03698700	1.54752700
B	-7.57812400	-0.01501800	-0.98323100
N	-2.96131100	-7.04389800	0.04229500
N	-4.73116600	-4.30197800	-4.17363700
N	-7.33211400	-0.00158200	-2.39262800
N	-7.12389700	-0.04784900	2.93341600
N	-4.39197000	-4.37485400	4.43105700
B	-1.20763300	-3.31697900	6.50258000
B	-3.31044600	-4.09813800	5.32602000
B	-6.64759400	1.17323100	3.50646500
B	-5.36149200	3.22275400	4.25537700
C	-1.91535300	-4.34649600	5.72412100
C	-2.64450000	-3.14725000	6.23102900
C	-6.32150700	2.59806300	3.33116500
C	-5.80864000	1.84442600	4.51274700
B	-1.71266500	-3.20896000	-6.46339000
B	-3.72104100	-4.00983000	-5.14383300
B	-6.90045100	1.22946000	-2.97947700
B	-5.67417500	3.29213800	-3.79001700
C	-2.36079000	-4.25181700	-5.65173100
C	-3.12415900	-3.04315900	-6.07988300
C	-6.56030900	2.65113600	-2.80524800
C	-6.14126100	1.91833700	-4.03596600
B	0.96126200	-7.41071700	-0.11886700
B	-1.56889200	-7.36941100	-0.01652500
C	-0.33561100	-7.46404200	-0.81391000
C	-0.27553000	-7.47487100	0.67728400
C	-6.12893900	-1.88527500	-4.06873300
C	-6.55159200	-2.64363700	-2.85490400
C	-7.60416800	-0.77225800	0.27859900
C	-7.60773800	0.72003100	0.29169000
C	-6.30948200	-2.69644700	3.28674800

C	-5.79459100	-1.95918300	4.47770600
C	-4.47745400	-5.77132900	2.01339500
C	-3.24481800	-6.24951300	2.70546000
C	-4.62853900	-5.73976600	-1.78082800
C	-3.45512600	-6.20622400	-2.57620400
C	6.87049200	1.26467700	-0.26563300
C	7.55604300	-0.94785800	-0.30147200
N	6.72569900	2.45742000	-0.25053700
N	7.99194800	-2.29616100	-0.35046800
O	8.39177900	-2.70231800	0.72258400
O	6.59588700	3.61600400	-0.23411600

N₂₀(C₂B₂)₃₀(NO₂)₂

B	-2.78148900	4.05013600	-5.18610000
B	-0.74782100	3.25797600	-6.47090900
B	-4.72327900	3.29660500	-3.90323400
B	-5.95022800	1.23591200	-3.09019700
B	-5.95025000	-1.22818900	-3.09279700
B	-4.72332900	-3.28724300	-3.91001400
B	-2.78158300	-4.03785800	-5.19464400
B	-0.74797100	-3.24287400	-6.47780700
B	0.47041100	1.27476900	-7.23219500
B	0.47034100	-1.25809300	-7.23489200
N	-6.38540400	0.00325000	-2.50225900
N	-3.80446600	-4.33109000	-4.23697700
N	0.47208300	-2.65860000	-6.94215000
N	0.47222600	2.67464400	-6.93644600
N	-3.80444800	4.34120800	-4.22785400
B	1.79856400	7.34393600	0.00820300
B	-2.72104500	6.63247800	-1.20974800
B	-3.51558400	5.31390700	-3.21905900
B	1.70010100	3.25894700	-6.49053600
B	3.75695300	4.04281600	-5.23740200
B	3.76581900	6.55222000	-1.21685200
B	4.52974100	5.27082100	-3.26390000
C	4.78867400	5.73723800	-1.89204600
C	3.58447900	6.20890000	-2.63670000
C	0.53355000	7.44350200	0.75456200
C	0.53349900	7.44532600	-0.73783000
C	-3.75644900	5.80890300	-1.85507400
C	-2.56191400	6.26435500	-2.62588500
C	3.12331400	3.08527800	-6.15859500
C	2.38037600	4.29359800	-5.69487000
N	4.80179500	4.32421400	-4.30163800
N	3.19166200	7.01932600	0.00776300

B	-0.73367700	7.38790500	0.00834500
N	-2.13568000	7.10190100	0.00804100
B	-2.72096100	-6.62961600	-1.22439300
B	-3.51554200	-5.30611000	-3.23044300
B	1.69994700	-3.24395000	-6.49758400
B	3.75684400	-4.03074400	-5.24635400
B	3.76592200	-6.54938200	-1.23160900
B	4.52976400	-5.26327100	-3.27572800
C	4.78873200	-5.73281700	-1.90495000
C	3.58455600	-6.20283900	-2.65067300
C	-3.75632500	-5.80436300	-1.86763500
C	-2.56191700	-6.25809100	-2.63965300
C	3.12319800	-3.07112000	-6.16537100
C	2.38020100	-4.28039800	-5.70424000
N	4.80174900	-4.31428400	-4.31131000
B	-0.73354800	-7.38802000	-0.00824300
B	1.79869300	-7.34396200	-0.00836000
C	0.53370700	-7.44536100	0.73780200
C	0.53360500	-7.44355500	-0.75459200
N	-2.13555900	-7.10205700	-0.00778600
N	3.19178200	-7.01931500	-0.00806800
B	5.74072800	3.28129000	-4.02199400
B	7.00454000	-1.22089500	-3.24764400
B	5.74070200	-3.27200100	-4.02935300
C	6.20021700	1.90601900	-4.27474400
C	6.66878100	2.65080300	-3.06936500
C	6.66879700	-2.64366400	-3.07534200
C	6.20020400	-1.89617400	-4.27903200
B	7.00454600	1.22843300	-3.24486100
N	7.46247600	0.00311000	-2.66543400
B	-4.72289900	3.28712400	3.91057400
B	-6.83458100	-0.00165300	1.16060100
B	-6.83501300	0.00169400	-1.16030500
B	-3.51525100	5.30602500	3.23091800
B	-2.72094100	6.62946600	1.22471500
C	-2.56171500	6.25798800	2.63996400
C	-3.75621200	5.80421300	1.86811100
C	-5.18639900	1.90955100	4.14450500
C	-5.60312000	2.64676000	2.91481000
C	-7.29293300	-0.85499500	-0.00092400
C	-7.29310800	0.85492600	0.00140400
N	-3.80402700	4.33097900	4.23747000
B	-5.94984400	1.22815300	3.09318300
N	-6.38495100	-0.00326900	2.50255600

B	-2.72077800	-6.63261200	1.21006500
B	-4.72265700	-3.29656700	3.90350900
B	-5.94963800	-1.23592000	3.09040500
C	-3.75610500	-5.80899400	1.85546900
C	-2.56147300	-6.26440900	2.62615500
C	-5.18624000	-1.91951200	4.14036300
C	-5.60283400	-2.65411100	2.90907400
B	-3.51506800	-5.31394600	3.21940800
N	-3.80382600	-4.34115900	4.22815000
C	-1.41774300	-4.28829600	-5.68664400
C	-2.16298600	-3.06684500	-6.11090100
C	-0.27666600	0.00843100	-7.30204200
C	1.21566700	0.00840600	-7.31673800
C	-2.16287100	3.08115900	-6.10450100
C	-1.41762800	4.30164900	-5.67747900
C	-5.18673800	1.91951600	-4.14005900
C	-5.60353900	2.65414700	-2.90885300
C	-5.18698900	-1.90976000	-4.14412200
C	-5.60342700	-2.64676000	-2.91420300
B	1.70081900	-3.25888600	6.49042900
B	3.75752000	-4.04273800	5.23703400
B	0.47120600	-1.27472000	7.23224800
B	0.47111900	1.25814100	7.23498300
B	1.70062100	3.24401500	6.49754600
B	3.75734800	4.03081100	5.24604000
B	5.74106900	3.27208100	4.02879800
B	7.00485600	1.22099300	3.24695300
B	5.74116900	-3.28119500	4.02142800
B	7.00489800	-1.22833100	3.24417500
N	0.47281800	2.65865600	6.94226500
N	4.80213100	4.31434900	4.31085700
N	7.46275400	-0.00300300	2.66469700
N	4.80226300	-4.32412100	4.30115600
N	0.47299400	-2.67459500	6.93649200
B	-2.78082600	-4.05009100	5.18634800
B	-0.74709900	-3.25791500	6.47105400
B	4.53012600	-5.27074100	3.26345100
B	3.76604500	-6.55218200	1.21648900
C	-2.16216500	-3.08109200	6.10470400
C	-1.41695000	-4.30159600	5.67767600
C	4.78894600	-5.73717200	1.89158000
C	3.58482900	-6.20884800	2.63634900
B	3.76593300	6.54940400	1.23124800
B	4.53001500	5.26332100	3.27529700

B	7.76391800	-0.00141100	1.26600300
B	7.76378600	0.00151900	-1.26677100
C	3.58471700	6.20285600	2.65032900
C	4.78882700	5.73285700	1.90448500
C	7.84125000	-0.74612000	-0.00125000
C	7.84124000	0.74623000	0.00047400
B	-2.78103800	4.03781000	5.19504100
B	-0.74729900	3.24289200	6.47803800
C	-1.41717100	4.28828700	5.68692900
C	-2.16235100	3.06682700	6.11127600
C	6.66905700	2.64375200	3.07467800
C	6.20061500	1.89625800	4.27842500
C	6.20068800	-1.90592900	4.27414300
C	6.66914500	-2.65071000	3.06872200
C	3.12398800	-3.08520900	6.15831000
C	2.38099100	-4.29351700	5.69464700
C	1.21646800	-0.00835300	7.31673900
C	-0.27586700	-0.00838800	7.30219100
C	3.12383300	3.07120000	6.16515700
C	2.38076300	4.28046200	5.70410300
N	-8.36672000	1.85509700	0.00341000
O	-8.76817800	2.23082500	-1.08067100
O	-8.76744400	2.22716500	1.08905800
N	-8.36633800	-1.85537000	-0.00269700
O	-8.76747200	-2.23120800	1.08146100
O	-8.76738300	-2.22727200	-1.08829700

N₂₀(C₂B₂)₃₀CO

B	1.04624200	7.35568000	-0.22529200
B	-1.44093700	7.31744400	0.25399700
B	3.23278900	6.59034700	0.57760500
B	4.39544400	5.25297800	2.38724800
B	4.00413400	3.98463900	4.43735800
B	2.24883000	3.22600100	6.09859500
B	-0.14756200	3.24311900	6.60312000
B	-2.40642600	4.03029800	5.77159000
B	-3.15065600	6.53504400	1.82535000
B	-3.53163000	5.25849400	3.97955600
N	4.85100600	4.27389100	3.32194900
N	1.14117700	2.65684000	6.80418100
N	-3.60996600	4.31407500	5.05134200
N	-2.81159500	7.00043300	0.51550900
N	2.42182500	7.07410700	-0.49839500
B	-0.21730900	3.25425400	-6.60641900
B	3.13232000	5.30875900	-3.94594500

B	2.75597500	6.61698900	-1.81211900
B	-3.61055700	6.53787600	-0.57744000
B	-4.76350500	5.26431800	-2.43910300
B	-2.62282100	3.25741500	-6.15883000
B	-4.39534900	4.04039900	-4.52804200
C	-3.95477400	3.08426600	-5.55669300
C	-3.13498700	4.29179500	-5.24535200
C	1.24021300	3.07343800	-6.51280800
C	0.59196800	4.29580800	-5.95332000
C	3.64393800	5.80475900	-2.65877300
C	2.31567300	6.25569200	-3.16936900
C	-4.74970800	5.72994500	-1.04291800
C	-3.70915500	6.19571000	-2.00581600
N	-5.23692400	4.32150900	-3.40569300
N	-1.50507900	2.67362700	-6.83437600
B	2.02380600	4.03968200	-5.72616100
N	3.21282200	4.33153500	-4.98678100
B	1.19848200	-1.27366100	7.09747000
B	1.19755800	1.25840500	7.10023600
B	-4.58484200	3.27178400	4.95242800
B	-5.97104400	1.21810900	4.42621400
B	-4.58246200	-3.28631100	4.94510300
B	-5.97016000	-1.23247200	4.42348600
C	-5.67330000	-2.65435400	4.18512900
C	-4.98724100	-1.91188400	5.28287800
C	1.94470800	-0.00727900	7.02841600
C	0.48188100	-0.00813600	7.32497000
C	-5.67520900	2.64073100	4.19103400
C	-4.98861500	1.89630800	5.28712500
N	-6.52973700	-0.00684500	3.94183100
B	-0.14521000	-3.25821800	6.59591400
B	-2.40349700	-4.04511700	5.76255500
C	-0.96437900	-4.29329400	5.94445300
C	-1.60691200	-3.08911700	6.54822400
N	1.14310700	-2.67147900	6.79832800
N	-3.60682700	-4.32811500	5.04165000
B	-6.10452900	3.27889100	-2.95043300
B	-7.56587900	-0.00290800	0.13762100
B	-7.08864700	-0.00557000	2.62492300
C	-6.83177400	2.64659100	-1.83783600
C	-6.60523900	1.90413900	-3.11236400
C	-7.40338300	-0.75048400	1.39502100
C	-7.40391200	0.74191700	1.39671900
B	-7.19591700	1.22458600	-1.94798100

N	-7.53498900	-0.00126700	-1.29278400
B	6.79916900	0.00539200	-2.46666900
B	6.90380400	1.19953200	1.90011800
B	5.72398000	3.23322800	2.86246300
B	5.51486400	1.22475800	-4.19575500
B	4.16706300	3.27730600	-4.82278600
C	4.54498500	1.88123500	-5.08842900
C	5.23534600	2.66033400	-4.01961500
C	7.40639200	-0.71598800	-1.35027000
C	7.40683300	0.72399500	-1.34869100
C	6.15567700	1.83699400	3.00118800
C	6.57174400	2.63956800	1.81628000
N	6.07409500	0.00665700	-3.70558400
B	7.92804400	0.00242700	-0.08976200
N	7.37588600	0.00102500	1.30621500
B	2.25119600	-3.23828200	6.09153300
B	5.72662800	-3.23574600	2.85573500
B	6.90483100	-1.19903000	1.89781200
C	3.56888500	-3.04426800	5.46639700
C	2.75878500	-4.26029000	5.16241000
C	6.57421400	-2.63923300	1.81102500
C	6.15704600	-1.83941200	2.99740800
B	4.00718700	-3.99195500	4.42876000
N	4.85439900	-4.27809500	3.31280800
C	-1.60914300	3.07308000	6.55506000
C	-0.96748300	4.27909400	5.95403600
C	-2.71352300	6.19188200	3.18819600
C	-4.03643000	5.72590600	2.67826300
C	-0.05722000	7.40813800	0.74781200
C	-0.33995700	7.42016200	-0.71736800
C	3.34282800	6.20499200	1.99285900
C	4.37491400	5.76774000	1.00779700
C	2.75563700	4.25047500	5.17176200
C	3.56660900	3.03433300	5.47292500
B	1.05180900	-7.35406500	-0.24179400
B	-1.43541700	-7.31879700	0.23748900
B	2.76098700	-6.61043400	-1.82688200
B	3.13625500	-5.29707700	-3.95774900
B	2.02673300	-4.02492400	-5.73515500
B	-0.21496000	-3.23926200	-6.61373100
B	-2.62046800	-3.24522500	-6.16620400
B	-4.39238400	-4.03325200	-4.53718300
B	-3.60562900	-6.53902400	-0.59222600
B	-4.75957600	-5.26216900	-2.45100900

N	3.21596900	-4.31747500	-4.99640800
N	-1.50315600	-2.65908700	-6.84042100
N	-5.23373200	-4.31754500	-3.41546400
N	-2.80632700	-7.00344400	0.49968200
N	2.42719300	-7.07085900	-0.51422100
B	4.39957700	-5.25531800	2.37579700
B	3.23782500	-6.58910500	0.56292800
B	-3.14578400	-6.54132400	1.81057600
B	-3.52778000	-5.27000700	3.96769300
C	4.37940700	-5.76678500	0.99511400
C	3.34760400	-6.20708600	1.97910700
C	-4.03218400	-5.73480300	2.66531300
C	-2.70894400	-6.20096000	3.17421800
B	-1.56049000	1.27395000	-7.12541900
B	-1.55958100	-1.25879400	-7.12829500
B	-6.10211700	-3.27661100	-2.95784400
B	-7.19501800	-1.22538100	-1.95075800
C	-0.84115200	0.00807900	-7.34077900
C	-2.30772500	0.00723900	-7.06408900
C	-6.82981200	-2.64735700	-1.84381700
C	-6.60384100	-1.90186800	-3.11667200
B	5.51563100	-1.21070900	-4.19845600
B	4.16938100	-3.26286100	-4.83008400
C	4.54625500	-1.86591600	-5.09261000
C	5.23721500	-2.64689200	-4.02555100
C	-3.95254000	-3.07444600	-5.56365600
C	-3.13185200	-4.28207700	-5.25509100
C	-3.70448800	-6.19370200	-2.01982500
C	-4.74542500	-5.73095600	-1.05588500
C	-0.33432500	-7.41840300	-0.73407300
C	-0.05164900	-7.40959600	0.73114100
C	2.32038500	-6.24643000	-3.18331300
C	3.64828100	-5.79556700	-2.67170100
C	0.59509000	-4.28162000	-5.96287900
C	1.24242400	-3.05754600	-6.51968900
C	9.54569700	0.00170700	-0.10235000
O	10.66847900	0.00116400	-0.19204700
AgN₂₀(C₂B₂)₃₀⁺			
B	5.59029200	-0.85671000	-3.66358900
B	5.94833800	1.60070600	-3.04278700
B	5.36941000	-3.23114900	-3.08402400
B	5.27541200	-4.90199500	-1.18948400
B	5.27550400	-4.90148500	1.19015000
B	5.36972700	-3.23002600	3.08414500

B	5.59077400	-0.85535300	3.66299000
B	5.94884300	1.60184800	3.04125200
B	6.27234900	3.19809800	-1.27171800
B	6.27274100	3.19862400	1.26958500
N	4.97185600	-5.62194000	0.00049600
N	5.21509500	-2.16691300	4.02380200
N	5.97091100	2.96315600	2.63117300
N	5.97044500	2.96216000	-2.63320700
N	5.21448000	-2.16835400	-4.02400000
B	-0.87296700	1.17571100	-7.26200300
B	2.08135400	-2.42184000	-6.41205100
B	4.21331400	-2.31278300	-5.05188900
B	5.09063900	3.89098300	-3.30511600
B	3.08763100	5.21734000	-4.10005900
B	-0.58383900	3.49124600	-6.53369200
B	0.95936100	5.06765100	-5.29059900
C	-0.39217000	4.72013500	-5.74361600
C	0.78568400	3.92559100	-6.19903000
C	-1.02589400	-0.28644800	-7.33452300
C	0.33287600	0.32898200	-7.30148500
C	3.11364900	-3.10336300	-5.60452100
C	3.27546900	-1.66668600	-5.97363600
C	4.23181200	5.06725500	-3.17291200
C	4.05962100	4.12142600	-4.31422400
N	1.80354700	5.76272900	-4.36003100
N	-1.45260300	2.45091300	-6.97977700
B	0.17046600	-1.13104600	-7.22449200
N	0.74904300	-2.40354100	-6.90789900
B	2.08249200	-2.41944200	6.41267100
B	4.21414400	-2.31098200	5.05197500
B	5.09130000	3.89227500	3.30293700
B	3.08842400	5.21898300	4.09762700
B	-0.58258200	3.49376200	6.53249800
B	0.96034400	5.06973900	5.28852000
C	-0.39109400	4.72233600	5.74189100
C	0.78687000	3.92805300	6.19746200
C	3.11455400	-3.10129700	5.60512400
C	3.27653900	-1.66450000	5.97370100
C	4.23252300	5.06855500	3.17041800
C	4.06038900	4.12310700	4.31204900
N	1.80437900	5.76448100	4.35755400
B	0.17178900	-1.12830000	7.22503800
B	-0.87157200	1.17849900	7.26178500
C	-1.02452300	-0.28362300	7.33494400

C	0.33426000	0.33175800	7.30144400
N	0.75028600	-2.40091700	6.90878200
N	-1.45124800	2.45358500	6.97913400
B	1.16899600	6.50191000	-3.30592100
B	-0.04462900	7.29548100	1.22571300
B	1.16965400	6.50324200	3.30325800
C	1.22302500	6.99613300	-1.92132600
C	-0.07311300	6.93836800	-2.65708300
C	-0.07258600	6.93939800	2.65447000
C	1.22340300	6.99685200	1.91843400
B	-0.04487500	7.29499900	-1.22846700
N	-0.75655600	7.45695700	-0.00133700
B	-1.87994500	-6.47615300	-3.26014500
B	1.44669300	-7.37969600	0.00121800
B	3.80779600	-6.46753600	0.00077300
B	-1.67202900	-5.02344600	-5.22317400
B	-0.12783000	-3.45372400	-6.47470800
C	-1.49083900	-3.89252200	-6.14996800
C	-0.31207500	-4.67148900	-5.67174900
C	-1.93180600	-7.02380700	-1.89471500
C	-0.63876700	-6.96808300	-2.63612900
C	2.66242500	-6.99798300	0.74698600
C	2.66225100	-6.99826100	-0.74498100
N	-2.50750900	-5.70884400	-4.28999800
B	-0.67350700	-7.37867700	-1.22351900
N	0.03876100	-7.59464600	0.00141900
B	-0.12669800	-3.45122400	6.47610800
B	-1.87928000	-6.47482500	3.26291500
B	-0.67323300	-7.37818200	1.22642700
C	-0.31107200	-4.66929700	5.67363300
C	-1.48975300	-3.89010500	6.15170200
C	-1.93141000	-7.02306900	1.89773100
C	-0.63821200	-6.96694700	2.63884200
B	-1.67110500	-5.02137600	5.22537200
N	-2.50670200	-5.70713000	4.29256600
C	5.61246900	0.56433800	3.99111500
C	6.00237900	0.15228400	2.60711800
C	6.17780100	3.91085000	-0.00120700
C	6.00189800	0.15132200	-2.60816000
C	5.61187800	0.56288100	-3.99229900
C	5.79505100	-3.62520400	-1.73042000
C	4.99447300	-4.55261800	-2.58693200
C	5.79512600	-3.62446700	1.73056900
C	4.99476000	-4.55165700	2.58752800

B	-6.79347200	-1.54629200	3.24862600
B	-6.48708600	0.84297600	4.03111700
B	-6.98168300	-2.97365900	1.26736100
B	-6.98195800	-2.97415400	-1.26523200
B	-6.79413200	-1.54751200	-3.24703500
B	-6.48793600	0.84151300	-4.03035500
B	-6.18221700	3.15249400	-3.27448300
B	-5.97530400	4.62617000	-1.22519900
B	-6.18156300	3.15367000	3.27437300
B	-5.97507300	4.62660100	1.22450900
N	-6.70445100	-2.85063000	-2.66367500
N	-6.05659200	2.17690600	-4.31343800
N	-5.62418200	5.27861300	-0.00049100
N	-6.05569000	2.17846300	4.31366400
N	-6.70389500	-2.84961000	2.66569300
B	-3.79395800	-5.14004100	4.01627300
B	-5.78592000	-3.77973900	3.24415400
B	-4.99887900	2.34930700	5.25893000
B	-2.81283200	2.48056200	6.52951400
C	-4.89872300	-4.94216300	3.06690200
C	-4.76979100	-4.07009400	4.27028200
C	-3.85127500	3.14479500	5.72949500
C	-4.03153800	1.73558800	6.18525800
B	-2.81411500	2.47808600	-6.52996800
B	-4.99996500	2.34737200	-5.25898900
B	-4.47080700	6.12047800	-0.00074600
B	-2.16033800	7.15816800	-0.00113200
C	-4.03276700	1.73325800	-6.18520200
C	-3.85244600	3.14266300	-5.73008900
C	-3.34325500	6.70798200	0.74489500
C	-3.34336700	6.70767000	-0.74680400
B	-3.79471300	-5.14160800	-4.01375700
B	-5.78655900	-3.78098100	-3.24191100
C	-4.77058100	-4.07176800	-4.26806500
C	-4.89933000	-4.94332800	-3.06429400
C	-5.68001000	4.38593800	-2.64681700
C	-6.59523100	3.47512800	-1.89962000
C	-6.59485400	3.47579500	1.89947100
C	-5.67950700	4.38688900	2.64615500
C	-7.06995300	-0.11114400	3.07528400
C	-6.34030800	-0.59982800	4.28119200
C	-7.35898900	-2.32616400	0.00098000
C	-6.74277400	-3.68485100	0.00117600
C	-7.07058700	-0.11231000	-3.07409800

C	-6.34120300	-0.60136900	-4.28000100
C	6.57076800	2.47575800	-0.00096100
Ag	6.27416000	0.01913400	-0.00040800
(CO₂) AgN₂₀(C₂B₂)₃₀⁺			
B	5.46432700	-0.21189300	3.75546000
B	5.36054400	-2.67606000	3.09635300
B	5.64506700	2.15039000	3.13675600
B	5.82562700	3.77315900	1.19825500
B	5.82583600	3.77413200	-1.19814500
B	5.64486100	2.15229200	-3.13734700
B	5.46341900	-0.20971000	-3.75659600
B	5.35937600	-2.67417600	-3.09856100
B	5.35418400	-4.25481200	1.27221900
B	5.35352800	-4.25408800	-1.27530400
N	5.65075500	4.52036600	0.00034800
N	5.32084700	1.15495900	-4.10217500
N	5.11554000	-4.00172100	-2.64611800
N	5.11665900	-4.00340200	2.64326500
N	5.32176400	1.15269700	4.10145300
B	-1.29674800	-1.03691800	7.26498200
B	2.25885400	1.97921300	6.45015200
B	4.35207000	1.48302400	5.11644600
B	4.08195200	-4.76854700	3.29946400
B	1.87339100	-5.71931300	4.08778500
B	-1.42498000	-3.36588600	6.53003900
B	-0.19040800	-5.19250600	5.28478200
C	-1.45738500	-4.60887800	5.73989500
C	-0.15591900	-4.03858400	6.19435000
C	-1.18635100	0.42895300	7.34175500
C	0.04064800	-0.41898900	7.31417200
C	3.40096500	2.46057300	5.64608000
C	3.30891000	1.02352900	6.03617400
C	3.01913500	-5.76272000	3.15207100
C	3.03224100	-4.82724400	4.31435100
N	0.51243100	-6.02572000	4.35049100
N	-2.09399900	-2.18701700	6.97671700
B	0.14225000	1.04668800	7.24237500
N	0.93920600	2.19714900	6.93230800
B	2.25722200	1.98243100	-6.44965800
B	4.35069700	1.48564400	-5.11660300
B	4.08072500	-4.76654600	-3.30254700
B	1.87212500	-5.71700900	-4.09115500
B	-1.42674100	-3.36248500	-6.53159500
B	-0.19193100	-5.18975200	-5.28751400

C	-1.45898800	-4.60589200	-5.74209500
C	-0.15760800	-4.03534900	-6.19648600
C	3.39952600	2.46344400	-5.64565000
C	3.30730800	1.02654800	-6.03624800
C	3.01814200	-5.76103500	-3.15581200
C	3.03074500	-4.82447400	-4.31722200
N	0.51116000	-6.02345800	-4.35384100
B	0.14045000	1.05036900	-7.24194400
B	-1.29866300	-1.03314200	-7.26538400
C	-1.18820400	0.43276100	-7.34138500
C	0.03875700	-0.41526000	-7.31453600
N	0.93750600	2.20064900	-6.93147400
N	-2.09585500	-2.18338300	-6.97753800
B	-0.24734700	-6.63780200	3.29812000
B	-1.58897900	-7.20258700	-1.22817900
B	-0.24832700	-6.63615400	-3.30160400
C	-0.28633500	-7.13562000	1.91448500
C	-1.54922600	-6.84571500	2.65293300
C	-1.55000600	-6.84444000	-2.65612800
C	-0.28687800	-7.13461500	-1.91818900
B	-1.58865000	-7.20318700	1.22483800
N	-2.31926600	-7.23580800	-0.00158000
B	-0.91094400	6.66124000	3.26741300
B	2.51933300	6.91425500	0.00142200
B	4.66247000	5.56795900	0.00074900
B	-0.97239800	5.20182600	5.23493700
B	0.26388000	3.38450300	6.49309700
C	-0.99836000	4.05781300	6.16257600
C	0.30169200	4.61492500	5.68912400
C	-0.86135600	7.20520600	1.90033000
C	0.39948600	6.91244400	2.64127300
C	3.63967300	6.30653600	-0.74483400
C	3.63976100	6.30593600	0.74705000
N	-1.66867500	6.02509400	4.29865700
B	0.43984000	7.31792800	1.22757000
N	1.17920700	7.39419000	0.00169000
B	0.26231900	3.38779300	-6.49148500
B	-0.91174100	6.66288500	-3.26389400
B	0.43955200	7.31856000	-1.22405900
C	0.30030600	4.61781100	-5.68691100
C	-0.99985200	4.06094500	-6.16036500
C	-0.86180800	7.20614400	-1.89654500
C	0.39884900	6.91379500	-2.63796000
B	-0.97368100	5.20449200	-5.23216000

N	-1.66972800	6.02727800	-4.29528600
C	5.20755600	-1.61151700	-4.07358600
C	5.70967700	-1.26396300	-2.70911700
C	5.12639900	-4.92787600	-0.00168500
C	5.71039100	-1.26560700	2.70736800
C	5.20898300	-1.61388500	4.07192000
C	6.13142700	2.43804700	1.77165700
C	5.48550700	3.49925300	2.59756900
C	6.13164900	2.43936100	-1.77230900
C	5.48526600	3.50087100	-2.59747900
B	-6.63427800	2.71251700	-3.24618500
B	-6.76097300	0.30740300	-4.02945800
B	-6.56342500	4.15006700	-1.26435200
B	-6.56313300	4.14944100	1.26800800
B	-6.63351600	2.71090900	3.24913400
B	-6.75992600	0.30538000	4.03117300
B	-6.87571000	-2.02229200	3.27384100
B	-6.93929900	-3.50911300	1.22472900
B	-6.87664200	-2.02067800	-3.27337500
B	-6.93965700	-3.50853900	-1.22500200
N	-6.31219700	3.97730700	2.66628900
N	-6.57519100	-1.08580200	4.31302600
N	-6.71228100	-4.21359300	-0.00033700
N	-6.57637100	-1.08363300	-4.31212700
N	-6.31280600	3.97861900	-2.66277400
B	-3.03828800	5.70363900	-4.01728400
B	-5.24318300	4.72837000	-3.24197500
B	-5.56663300	-1.44193100	-5.25656200
B	-3.43948800	-1.96562000	-6.52625200
C	-4.15864400	5.70943400	-3.06583300
C	-4.19342700	4.83029100	-4.27034000
C	-4.58043300	-2.43109500	-5.72559800
C	-4.50440100	-1.01325600	-6.18299600
B	-3.43773100	-1.96901500	6.52584700
B	-5.56519300	-1.44459900	5.25699000
B	-5.73042400	-5.25046000	-0.00071000
B	-3.64569100	-6.68872200	-0.00127700
C	-4.50271100	-1.01644100	6.18337600
C	-4.57888900	-2.43403400	5.72523600
C	-4.72808000	-6.03190200	-0.74678200
C	-4.72789900	-6.03223000	0.74477600
B	-3.03731000	5.70161300	4.02083400
B	-5.24241100	4.72675200	3.24559700
C	-4.19239500	4.82814700	4.27374800

C	-4.15790500	5.70788800	3.06966700
C	-6.60453800	-3.32587300	2.64602200
C	-7.34141200	-2.26535100	1.89953000
C	-7.34196800	-2.26444200	-1.89906400
C	-6.60529000	-3.32458100	-2.64629700
C	-7.16331600	1.35027600	-3.07324900
C	-6.35803200	1.70058400	-4.27889900
C	-7.04996500	3.57993300	0.00174300
C	-6.20141700	4.80668700	0.00194800
C	-7.16258400	1.34875100	3.07564000
C	-6.35694700	1.69843700	4.28123500
C	5.76833800	-3.58659700	-0.00142700
Ag	6.11518700	-1.19597600	-0.00085100
C	8.32856500	1.48716800	-0.00009300
O	8.69973500	2.58196600	-0.00020600
O	8.01149000	0.36061900	0.00013800
(N ₂ O) AgN ₂₀ (C ₂ B ₂) ₃₀ ⁺			
B	-5.46801500	-0.17659400	-3.76049900
B	-5.37542600	-2.64201900	-3.10400200
B	-5.63263100	2.18640300	-3.13487600
B	-5.79999800	3.80465000	-1.19166100
B	-5.79903600	3.80084800	1.20533000
B	-5.63022300	2.17656000	3.14340300
B	-5.46544700	-0.18844300	3.76166800
B	-5.37354100	-2.65207500	3.09841600
B	-5.37180500	-4.22383100	-1.27961700
B	-5.37078200	-4.22893500	1.26999100
N	-5.61789700	4.54799500	0.00794900
N	-5.31346100	1.17496100	4.10754300
N	-5.13435500	-3.97959200	2.64150000
N	-5.13588400	-3.97055400	-2.65042000
N	-5.31649400	1.18789000	-4.10245500
B	1.29333400	-1.03084500	-7.27021500
B	-2.24716400	2.00213200	-6.44744300
B	-4.34376400	1.51449900	-5.11593100
B	-4.10507300	-4.74006400	-3.30859700
B	-1.90202100	-5.70082600	-4.10001500
B	1.40968000	-3.36115800	-6.53739100
B	0.16537900	-5.18335100	-5.29531100
C	1.43554200	-4.60520100	-5.74841900
C	0.13716700	-4.02872200	-6.20420000
C	1.18983700	0.43553200	-7.34512400
C	-0.04122900	-0.40658700	-7.31817300
C	-3.38674600	2.48797200	-5.64263500

C	-3.30310000	1.05140900	-6.03684700
C	-3.04798700	-5.74055500	-3.16442300
C	-3.05624700	-4.80177400	-4.32428900
N	-0.54258100	-6.01395100	-4.36253300
N	2.08481100	-2.18515000	-6.98217600
B	-0.13576200	1.05948900	-7.24352200
N	-0.92628500	2.21340500	-6.92953000
B	-2.24317800	1.98262600	6.45359900
B	-4.34026200	1.49854500	5.12156300
B	-4.10321300	-4.75059300	3.29734100
B	-1.89976300	-5.71335900	4.08527000
B	1.41345800	-3.38045100	6.52743300
B	0.16827400	-5.19906600	5.28099200
C	1.43871800	-4.62223300	5.73494300
C	0.14067000	-4.04701500	6.19319500
C	-3.38317600	2.47061200	5.65068700
C	-3.29904000	1.03288800	6.04053500
C	-3.04596400	-5.75050000	3.14979700
C	-3.05407900	-4.81521900	4.31245400
N	-0.54015200	-6.02702200	4.34621500
B	-0.13152200	1.03814600	7.24652600
B	1.29757500	-1.05224400	7.26695300
C	1.19412200	0.41392200	7.34605000
C	-0.03695400	-0.42811900	7.31716100
N	-0.92223400	2.19283700	6.93594300
N	2.08888800	-2.20576200	6.97521700
B	0.21285500	-6.63211400	-3.31042400
B	1.55067700	-7.21114900	1.21611400
B	0.21481000	-6.64196200	3.29188400
C	0.24806400	-7.13183400	-1.92721900
C	1.51306900	-6.84900700	-2.66497800
C	1.51467000	-6.85665900	2.64500000
C	0.24926700	-7.13758600	1.90719800
B	1.54988500	-7.20762500	-1.23715900
N	2.28040000	-7.24526300	-0.01080600
B	0.95251500	6.66085700	-3.25802100
B	-2.47340400	6.92498300	0.01068300
B	-4.62327800	5.58938000	0.00925200
B	1.00401800	5.20423000	-5.22830200
B	-0.24380700	3.39602300	-6.48841500
C	1.02256100	4.06227300	-6.15877400
C	-0.27380500	4.62491800	-5.68173700
C	0.90784100	7.20274800	-1.88982900
C	-0.35561200	6.91889600	-2.63001200

C	-3.59650400	6.32163200	0.75613400
C	-3.59695000	6.32395400	-0.73596200
N	1.70552000	6.02201400	-4.29126800
B	-0.39206100	7.32120200	-1.21529500
N	-1.13062600	7.39833700	0.01103100
B	-0.24014200	3.37686100	6.49803700
B	0.95436000	6.65139900	3.27677300
B	-0.39142400	7.31762100	1.23674200
C	-0.27075300	4.60802500	5.69482800
C	1.02592100	4.04444500	6.16997000
C	0.90887700	7.19721100	1.91016800
C	-0.35414600	6.91120300	2.65025900
B	1.00677800	5.18902700	5.24273900
N	1.70785400	6.00960300	4.30783800
C	-5.20960900	-1.59209500	4.07503300
C	-5.72714300	-1.24172200	2.71751700
C	-5.14439000	-4.89840900	-0.00621900
C	-5.72886500	-1.23269900	-2.71884700
C	-5.21212800	-1.57930300	-4.07759300
C	-6.11629100	2.47576600	-1.77032700
C	-5.46087900	3.53343200	-2.59288800
C	-6.11458800	2.47000500	1.77993300
C	-5.45924400	3.52534000	2.60554100
B	6.65474200	2.67389700	3.25039100
B	6.76761400	0.26715400	4.03117800
B	6.59063500	4.11523800	1.27076000
B	6.58976400	4.11869600	-1.26179200
B	6.65268900	2.68322400	-3.24579900
B	6.76540000	0.27882400	-4.03381900
B	6.86662200	-2.05018300	-3.27939600
B	6.91934600	-3.53996900	-1.23190200
B	6.86837300	-2.05955000	3.26973900
B	6.91994100	-3.54346800	1.21793300
N	6.33839200	3.95027300	-2.66046200
N	6.57268400	-1.11085600	-4.31805400
N	6.68815800	-4.24501800	-0.00793700
N	6.57498300	-1.12336900	4.31137600
N	6.34010400	3.94272100	2.66910600
B	3.07534700	5.68058900	4.03048000
B	5.27539100	4.69750400	3.25107600
B	5.56326200	-1.47806400	5.25513300
B	3.43329400	-1.99378900	6.52350600
C	4.19558800	5.68436300	3.07865100
C	4.22702100	4.80161200	4.28060100

C	4.57171500	-2.46331200	5.72137200
C	4.50341000	-1.04623300	6.18278900
B	3.42949100	-1.97451100	-6.53068600
B	5.56036900	-1.46266200	-5.26226600
B	5.70178100	-5.27756900	-0.00915400
B	3.61010100	-6.70574200	-0.01044800
C	4.49984500	-1.02798500	-6.18781200
C	4.56851400	-2.44648200	-5.73084100
C	4.69591800	-6.05565100	0.73597800
C	4.69538100	-6.05349800	-0.75577700
B	3.07310500	5.69217900	-4.01538300
B	5.27347600	4.70689700	-3.23964400
C	4.22475800	4.81406400	-4.26850800
C	4.19363600	5.69314100	-3.06387400
C	6.58632200	-3.35277100	-2.65324800
C	7.32952700	-2.29784500	-1.90494000
C	7.33046300	-2.30324500	1.89427700
C	6.58774200	-3.36032300	2.63997900
C	7.17599800	1.30875800	3.07603000
C	6.37304600	1.66248700	4.28222400
C	7.07261300	3.54379000	0.00354100
C	6.23280600	4.77653000	0.00551400
C	7.17407000	1.31760000	-3.07574900
C	6.37065300	1.67490600	-4.28055800
C	-5.78488400	-3.55718600	-0.00331200
Ag	-6.17810000	-1.19093500	-0.00072100
N	-7.99942700	0.41376100	0.00319300
N	-8.31547000	1.49110400	0.00505300
O	-8.66200400	2.61375800	0.00682200
CuN₂₀(C₂B₂)₃₀⁺			
B	-5.42940900	1.81714600	-3.36789400
B	-6.22760300	-0.57776500	-2.89872000
B	-4.84675100	4.19779900	-2.91208700
B	-4.51471400	5.99667600	-1.17541500
B	-4.51471500	5.99673700	1.17514800
B	-4.84675000	4.19794400	2.91190600
B	-5.42940600	1.81731300	3.36781800
B	-6.22759500	-0.57762200	2.89874500
B	-6.94222300	-2.17095200	-1.26758400
B	-6.94221500	-2.17088600	1.26768000
N	-4.09103900	6.68410200	-0.00015100
N	-4.84065300	3.04020600	3.75006900
N	-6.53737000	-1.93228600	2.59899700
N	-6.53738000	-1.93241700	-2.59891300

N	-4.84065500	3.04002400	-3.75019800
B	0.51404700	-1.28909900	-7.22320300
B	-1.78280300	2.72969400	-6.23792800
B	-3.84926500	2.98191900	-4.79691600
B	-5.82113900	-2.97458100	-3.29998900
B	-4.06851900	-4.61171600	-4.10628800
B	-0.15124400	-3.52992100	-6.52345100
B	-1.94131500	-4.82457300	-5.28781000
C	-0.55034300	-4.71172500	-5.73889600
C	-1.57531500	-3.72665200	-6.19231200
C	0.90269200	0.12906000	-7.28153400
C	-0.53736500	-0.25632500	-7.22017000
C	-2.66531900	3.57885300	-5.41315200
C	-3.05489700	2.17312000	-5.72563600
C	-5.19468400	-4.29169400	-3.19959500
C	-4.81995800	-3.34927300	-4.29416000
N	-2.89671600	-5.36858100	-4.36353900
N	0.87800800	-2.64688500	-6.96578800
B	-0.13616600	1.15585200	-7.12896900
N	-0.49220400	2.50110600	-6.78872700
B	-1.78279000	2.72998900	6.23780200
B	-3.84925700	2.98214800	4.79678400
B	-5.82113100	-2.97441800	3.30012200
B	-4.06851100	-4.61151500	4.10649800
B	-0.15123200	-3.52960200	6.52360200
B	-1.94130300	-4.82431100	5.28802200
C	-0.55032900	-4.71143500	5.73909100
C	-1.57530200	-3.72634500	6.19246800
C	-2.66530400	3.57910600	5.41298200
C	-3.05488100	2.17338800	5.72553200
C	-5.19468100	-4.29153900	3.19979400
C	-4.81995300	-3.34906600	4.29431400
N	-2.89670600	-5.36836600	4.36378100
B	-0.13615400	1.15619200	7.12893300
B	0.51406000	-1.28875300	7.22327600
C	0.90270200	0.12941000	7.28157900
C	-0.53735400	-0.25597900	7.22022900
N	-0.49219200	2.50142800	6.78861400
N	0.87802000	-2.64654800	6.96590500
B	-2.40186500	-6.20732500	-3.30917300
B	-1.33930400	-7.18556200	1.22788700
B	-2.40185800	-6.20716100	3.30945400
C	-2.53891700	-6.68006100	-1.92264100
C	-1.25191800	-6.84502300	-2.65762000

C	-1.25191200	-6.84489100	2.65793000
C	-2.53891300	-6.67996500	1.92294600
B	-1.33930700	-7.18562200	-1.22756000
N	-0.66421600	-7.46021400	0.00017000
B	2.83146300	6.12454300	-3.25022600
B	-0.27612500	7.66966200	-0.00017600
B	-2.77503900	7.26468200	-0.00016600
B	2.35906100	4.70802000	-5.19167500
B	0.55368900	3.40053900	-6.39275600
C	1.97692800	3.61616900	-6.10422200
C	0.95088800	4.57895700	-5.60930200
C	2.97973000	6.66130400	-1.88793400
C	1.70042600	6.83981900	-2.63349400
C	-1.54387300	7.54745100	0.74574900
C	-1.54387200	7.54741000	-0.74609400
N	3.31024100	5.25064300	-4.27558600
B	1.80658500	7.24621400	-1.22305500
N	1.14708500	7.59718600	-0.00017400
B	0.55370100	3.40084800	6.39260900
B	2.83147000	6.12470500	3.24994500
B	1.80659000	7.24628100	1.22272400
C	0.95090200	4.57924200	5.60911900
C	1.97694200	3.61647700	6.10408300
C	2.97974000	6.66141800	1.88763400
C	1.70043900	6.83997400	2.63318900
B	2.35907100	4.70827100	5.19146400
N	3.31024600	5.25084500	4.27534000
C	-5.69045500	0.44055200	3.75960100
C	-6.00350800	0.83183900	2.34854000
C	-7.01228200	-2.88632500	0.00006700
C	-6.00351400	0.83171700	-2.34857500
C	-5.69046000	0.44037000	-3.75962100
C	-5.27330600	4.82390400	-1.65769000
C	-4.23486300	5.46658400	-2.51861700
C	-5.27331000	4.82399200	1.65748300
C	-4.23486000	5.46670800	2.51837400
B	6.81931000	0.41042000	3.24599400
B	6.11526500	-1.89380800	4.02720800
B	7.25316400	1.78432300	1.26604300
B	7.25316200	1.78426200	-1.26614200
B	6.81929800	0.41026500	-3.24602500
B	6.11525200	-1.89400100	-4.02713300
B	5.42353300	-4.12124200	-3.27149900
B	4.95935200	-5.53792500	-1.22426600

B	5.42353600	-4.12108000	3.27167400
B	4.95935000	-5.53786200	1.22450900
N	6.95542400	1.70974600	-2.66386500
N	5.46727100	-3.13883100	-4.31062900
N	4.49936600	-6.11970800	0.00013600
N	5.46728000	-3.13862300	4.31076000
N	6.95542900	1.70987300	2.66377100
B	4.48126000	4.47035900	4.00372000
B	6.21083900	2.78522800	3.23976300
B	4.39804300	-3.13166800	5.25740900
B	2.21836200	-2.90080800	6.52410400
C	5.54121700	4.08486100	3.06097700
C	5.25420000	3.24607800	4.26045400
C	3.13630000	-3.72865600	5.72965000
C	3.54275200	-2.36594700	6.18057200
B	2.21835200	-2.90112500	-6.52398100
B	4.39803500	-3.13192300	-5.25727800
B	3.22078800	-6.75478400	0.00015200
B	0.76994000	-7.39581000	0.00016800
C	3.54274000	-2.36624600	-6.18047500
C	3.13629500	-3.72893800	-5.72949600
C	2.01085500	-7.14621900	0.74586200
C	2.01085500	-7.14625600	-0.74553900
B	4.48125900	4.47017300	-4.00393700
B	6.21083800	2.78507600	-3.23990800
C	5.25420300	3.24588500	-4.26062100
C	5.54122500	4.08472300	-3.06118400
C	4.71468200	-5.25026800	-2.64647800
C	5.77017800	-4.51060700	-1.89566000
C	5.77017300	-4.51050700	1.89585100
C	4.71467500	-5.25012900	2.64670500
C	6.84929300	-1.05071600	3.07136200
C	6.21272500	-0.44702500	4.27762800
C	7.51261500	1.08109700	-0.00003300
C	7.14233300	2.52604100	-0.00006700
C	6.84927100	-1.05086200	-3.07132000
C	6.21270200	-0.44722800	-4.27761400
C	-7.12483300	-1.40368400	0.00002900
Cu	-6.34740300	0.65538800	0.00000700
(CO₂) CuN₂₀(C₂B₂)₃₀⁺			
B	5.57270900	2.26798000	3.62522800
B	5.49449300	-0.18446200	4.25715200
B	5.68540400	3.81452800	1.75408600
B	5.81057200	3.92713400	-0.77793400

B	5.88295100	2.55739500	-2.79073300
B	5.87546400	0.17315000	-3.66628900
B	5.79896000	-2.18400100	-3.03843500
B	5.65592800	-3.86832000	-1.10676800
B	5.48638800	-2.47130800	3.39938700
B	5.53910900	-3.97592900	1.31884800
N	5.63313200	3.81922500	-2.18981600
N	5.63528300	-1.19177600	-4.02565700
N	5.37347100	-4.61985600	0.06376000
N	5.22357000	-1.57843000	4.45582000
N	5.37258200	3.58468000	3.12548800
B	-1.40618200	3.12529800	6.62895200
B	2.12534400	5.40061300	4.43921600
B	4.32238900	4.37227400	3.71619600
B	4.17007300	-1.94134300	5.37445600
B	1.96325100	-2.42204600	6.51689200
B	-1.45265300	0.76150900	7.26530500
B	-0.14035200	-1.40394400	7.22762800
C	-1.43365100	-0.71184300	7.27725900
C	-0.15964400	0.05904200	7.36537600
C	-1.33393900	4.40138100	5.89929700
C	-0.08866100	3.73641600	6.38083900
C	3.29972100	5.40815200	3.54464200
C	3.23560400	4.46153900	4.69601000
C	3.12009100	-2.89992000	5.72717500
C	3.10443700	-1.51361300	6.27845800
N	0.60442500	-2.58634200	6.89809700
N	-2.16393200	1.96760200	6.98855300
B	-0.01536400	4.93208600	5.52631800
N	0.76761200	5.76648900	4.66401300
B	2.59310400	-1.81870000	-6.46404900
B	4.67702900	-1.45971600	-5.07344600
B	4.36962300	-5.66004700	-0.03189900
B	2.21147400	-6.96889200	-0.19914100
B	-1.00944200	-6.43750200	-3.61544400
B	0.19572800	-7.25624500	-1.54429900
C	-1.05815900	-7.05251300	-2.27746800
C	0.25353800	-6.78131900	-2.93409400
C	3.70120500	-0.94162300	-6.02942900
C	3.67202300	-2.37521600	-5.61697600
C	3.30607900	-6.41044000	0.62845300
C	3.37929400	-6.34103000	-0.86049900
N	0.86962600	-7.41671700	-0.28614400
B	0.51425800	-3.09710000	-6.62173700

B	-0.88774500	-4.88827200	-5.50747200
C	-0.79962500	-3.70600900	-6.37994800
C	0.44038700	-4.36009100	-5.87071200
N	1.27849700	-1.94021300	-6.98759400
N	-1.67631700	-5.71265900	-4.64767000
B	-0.11573400	-3.70043700	6.35457100
B	-1.32850200	-6.74276700	2.92140800
B	0.07556100	-7.37116600	0.90999200
C	-0.11171000	-4.88872500	5.48675900
C	-1.39778400	-4.27911700	5.93304800
C	-1.24448300	-7.23016900	1.53342800
C	-0.00394500	-7.02835000	2.33693800
B	-1.39640500	-5.37553100	4.95115900
N	-2.09508700	-6.11382800	3.94708200
B	-1.01309300	7.33675700	-0.91275000
B	2.52297900	5.76656300	-3.64265900
B	4.64239600	4.66443900	-2.80578300
B	-1.13420300	7.22535400	1.53073100
B	0.08568800	6.47098200	3.61815300
C	-1.17656600	6.78487400	2.93504700
C	0.13028400	7.05148200	2.26740500
C	-0.91501800	7.02691300	-2.34907800
C	0.31865800	7.22314900	-1.53410200
C	3.65590700	4.84730800	-3.87433400
C	3.60521800	5.68590800	-2.64144900
N	-1.80455400	7.36224900	0.27631700
B	0.40932900	6.76946300	-2.93006300
N	1.19321500	6.15970700	-3.96451700
B	0.56360000	-0.72840500	-7.27453000
B	-0.77013300	3.72962800	-6.37360900
B	0.50103400	5.41479600	-4.97397900
C	0.55227800	0.74106000	-7.27442100
C	-0.72134600	-0.02793100	-7.38299700
C	-0.77293700	4.93082700	-5.52333000
C	0.51528000	4.30514800	-5.94028400
B	-0.74718600	1.43778400	-7.23342400
N	-1.48584800	2.61621400	-6.91366000
C	5.53678400	-3.52257200	-2.50721200
C	6.08028900	-2.49325200	-1.58875800
C	5.28507400	-3.75559100	2.72531000
C	5.97161900	0.86818100	3.34198800
C	5.22553800	1.21254200	4.58814600
C	6.18344300	3.24359700	0.48170300
C	5.45433400	4.54275400	0.50238900

C	6.26452200	1.12922800	-2.60725100
C	5.63117500	1.59673900	-3.87261800
B	-6.43239200	0.27569500	-4.32056400
B	-6.48687100	-2.16690100	-3.65386100
B	-6.45653700	2.56778700	-3.45588400
B	-6.54753600	3.95996700	-1.34230900
B	-6.66678600	3.84592700	1.10114900
B	-6.77476700	2.26266000	3.07480600
B	-6.82423500	-0.10007100	3.72001500
B	-6.80306400	-2.46974300	2.82669900
B	-6.59454800	-3.69920300	-1.74478700
B	-6.71793000	-3.81735600	0.78202600
N	-6.34654600	4.59393300	-0.07568000
N	-6.57292600	1.26183400	4.07791100
N	-6.52719100	-3.72571300	2.19727400
N	-6.26753500	-3.47712300	-3.12021800
N	-6.15373500	1.66394600	-4.52373500
B	-2.85964200	2.45893300	-6.53498800
B	-5.07622800	2.00529500	-5.39757200
B	-5.21746700	-4.25973900	-3.68881800
B	-3.03829000	-5.32411000	-4.41751600
C	-4.01110400	2.95321400	-5.76721100
C	-3.99444000	1.55683500	-6.29152000
C	-4.19884500	-5.31101400	-3.51667300
C	-4.12852600	-4.37402700	-4.67520100
B	-3.49339200	1.85138500	6.46510000
B	-5.58697600	1.51523100	5.08057600
B	-5.53359600	-4.56259000	2.78986600
B	-3.43019100	-5.69966400	3.62375900
C	-4.56799000	2.42014600	5.63932200
C	-4.59441100	0.98049000	6.02873900
C	-4.49842300	-5.59790600	2.62007800
C	-4.54469100	-4.77289200	3.86196000
B	-3.15540400	6.89218200	0.18778900
B	-5.31237000	5.57567900	0.02065200
C	-4.30869200	6.26469000	0.84941800
C	-4.23516900	6.33317500	-0.63879400
C	-6.51582800	-1.52593000	3.91833800
C	-7.24271000	-1.07217600	2.69742100
C	-7.10984600	-3.16255200	-0.47570500
C	-6.33067500	-4.43421600	-0.49713000
C	-6.94353800	-0.78553100	-3.43841600
C	-6.09948000	-1.12681800	-4.61992600
C	-6.97885000	2.77176500	-2.09585300

C	-6.15092600	3.82397300	-2.75326800
C	-7.16362400	2.59469000	1.69533600
C	-6.40833300	3.57747500	2.52506300
C	5.90580900	-2.64882000	1.95877100
C	8.12013200	1.17253600	-0.28923900
O	8.70118400	2.01062700	-0.82773200
O	7.59234800	0.29739500	0.28500400
Cu	6.47650100	-1.49847200	0.26504500

(N₂O) CuN₂₀(C₂B₂)₃₀⁺

B	5.78472000	-1.92866600	3.18322100
B	5.63388600	-3.78180200	1.41343400
B	5.88286500	0.47409200	3.63687500
B	5.90815500	2.78684700	2.59021000
B	5.83018900	3.97298100	0.46887800
B	5.68982500	3.63012600	-2.04058800
B	5.56878700	1.92387100	-3.77050900
B	5.48886000	-0.57171000	-4.21010800
B	5.52375300	-4.11498500	-0.98840500
B	5.47783000	-2.78824600	-3.18656000
N	5.65823300	3.99456000	1.88572300
N	5.37317200	3.27838800	-3.38583500
N	5.21642900	-1.97619700	-4.30644000
N	5.35292700	-4.64097600	0.31854100
N	5.62689600	-0.86062000	4.08941200
B	-0.90906000	-4.41192000	5.88989900
B	2.58409700	-1.28259500	6.57228100
B	4.66572500	-1.04287600	5.15265200
B	4.34433800	-5.66404800	0.50595800
B	2.18063000	-6.94510000	0.78058700
B	-1.03938400	-6.11543700	4.13681900
B	0.16258900	-7.11014100	2.14238900
C	-1.09058600	-6.83999900	2.85494500
C	0.22218700	-6.52108300	3.48762700
C	-0.81464800	-3.16017000	6.65856300
C	0.42175800	-3.85904100	6.20270400
C	3.69576100	-0.44793700	6.06933300
C	3.65614700	-1.90824100	5.76590100
C	3.27991600	-6.46594900	-0.08958800
C	3.34911900	-6.26594500	1.38774200
N	0.83678200	-7.37830600	0.90276200
N	-1.70241600	-5.30368400	5.10474800
B	0.50191800	-2.53706400	6.84345400
N	1.27107500	-1.35650800	7.10905500
B	2.14146700	4.99514400	-4.86148300

B	4.32941700	4.01792500	-4.04587700
B	4.16129100	-2.40430800	-5.19499800
B	1.95176600	-2.96585600	-6.29443200
B	-1.45338000	0.15779400	-7.30317100
B	-0.14876700	-2.00166500	-7.08579400
C	-1.43958000	-1.31156900	-7.19288400
C	-0.16284100	-0.55513100	-7.34434300
C	3.31411500	5.07200000	-3.96809800
C	3.24514700	4.02902900	-5.03262700
C	3.10878100	-3.38455000	-5.47190000
C	3.09563000	-2.04456800	-6.12785600
N	0.59214900	-3.15553500	-6.66009500
B	0.00074500	4.45030000	-5.91196500
B	-1.39751300	2.56543000	-6.86402700
C	-1.31994400	3.89713100	-6.24250900
C	-0.07726200	3.18843300	-6.66492600
N	0.78672100	5.34940900	-5.12043400
N	-2.16008500	1.38521400	-7.12767700
B	0.04396500	-7.42856400	-0.29396700
B	-1.41841900	-5.76539200	-4.48744100
B	-0.13191400	-4.21817400	-6.02594000
C	-0.03321400	-7.20344600	-1.74432500
C	-1.27508200	-7.33343200	-0.92815700
C	-1.41595000	-4.75436600	-5.55709500
C	-0.13207400	-5.33008800	-5.06219800
B	-1.35618300	-6.96095800	-2.35144200
N	-2.11987300	-6.41498800	-3.42566300
B	-0.75864100	4.25250000	6.04154100
B	2.54286600	6.05515600	3.15919200
B	4.66537000	4.88797800	2.42440700
B	-0.74189500	2.03769100	7.08421200
B	0.56148200	-0.12276400	7.29872400
C	-0.72080300	0.58893700	7.35254200
C	0.55520400	1.34189800	7.17931400
C	-0.75823800	5.37982900	5.09553400
C	0.52830400	4.78852300	5.56450300
C	3.62659400	5.88964700	2.17034200
C	3.67694800	5.16197900	3.47176200
N	-1.47731600	3.18860300	6.67034500
B	0.51741800	5.81513900	4.51032200
N	1.21200900	6.47333300	3.44389900
B	0.10724200	6.14293000	-4.13861000
B	-0.99031800	7.39261800	0.30207300
B	0.42995100	6.99449200	2.36099600

C	0.15340300	6.83460200	-2.84146200
C	-1.15415400	6.51903800	-3.48598000
C	-0.89369700	7.20409100	1.75931800
C	0.34080600	7.32952300	0.93172800
B	-1.11077400	7.07565000	-2.12342500
N	-1.78124700	7.32004800	-0.88551900
C	5.22389200	0.79568500	-4.64747800
C	5.96317300	0.54822200	-3.37450500
C	5.27045000	-4.01115500	-2.40866700
C	6.06227900	-2.37053000	1.76680200
C	5.51162500	-3.30823200	2.77529700
C	6.29857500	1.35301300	2.52526400
C	5.63669300	1.90990000	3.73823300
C	6.18597700	3.17315100	-0.72417000
C	5.47176200	4.47378000	-0.86126200
B	-6.65601200	3.76446900	-1.41832000
B	-6.76974300	2.02272400	-3.25327600
B	-6.53661100	4.08103500	1.00719000
B	-6.44959200	2.86931200	3.22924900
B	-6.43319000	0.65698300	4.28113700
B	-6.49815200	-1.83234700	3.81977700
B	-6.61208000	-3.51830200	2.04515000
B	-6.73460700	-3.84607100	-0.46312600
B	-6.82760600	-0.38533300	-3.69978000
B	-6.81438400	-2.67264400	-2.61267100
N	-6.14923500	2.05620300	4.36832100
N	-6.28458400	-3.18351500	3.39740300
N	-6.54291600	-3.87294800	-1.88099000
N	-6.57148100	0.94117000	-4.16964500
N	-6.33337300	4.60667400	-0.30774500
B	-3.13368100	6.86355100	-0.75914900
B	-5.29555100	5.57332000	-0.48467900
B	-5.58464200	1.10662200	-5.18950700
B	-3.48998500	1.31824300	-6.59678900
C	-4.21604100	6.37941000	0.11024700
C	-4.28879800	6.18701900	-1.36711100
C	-4.59458400	0.49102400	-6.09014300
C	-4.56190100	1.95782000	-5.82101400
B	-3.06301000	-4.93019300	4.84391800
B	-5.23788500	-3.92054600	4.02968400
B	-5.55223900	-4.75957800	-2.40167100
B	-3.45322500	-5.96996800	-3.13782400
C	-4.14884800	-3.95704400	5.02183500
C	-4.22432600	-4.98729900	3.94573800

C	-4.56414000	-5.06183100	-3.45238400
C	-4.52084800	-5.78099800	-2.14629000
B	-2.85167000	3.00472200	6.30616400
B	-5.07019900	2.46529300	5.21071500
C	-3.98928500	2.08899000	6.13829700
C	-4.00215200	3.43734900	5.50053400
C	-6.35040000	-4.35576300	0.86326700
C	-7.12471400	-3.08734400	0.73536600
C	-7.24931900	-1.26773800	-2.60014200
C	-6.52392800	-1.82376600	-3.77890900
C	-7.15737900	2.46984500	-1.90642700
C	-6.39855400	3.37742400	-2.81487800
C	-6.97170900	2.96115700	1.85700300
C	-6.14018300	4.06175100	2.42459900
C	-6.94899300	-0.47174400	3.49018500
C	-6.10604100	-0.71720400	4.69603500
C	5.90234000	-2.85050000	-1.73817900
N	7.64281300	0.20211300	-0.19039900
N	8.15803300	1.12533200	0.18481000
O	8.70721900	2.08551100	0.56981200
Cu	6.50851400	-1.53924500	-0.18512800
AuN₂₀(C₂B₂)₃₀⁺			
B	-5.24146300	1.05167100	-3.27272800
B	-5.78770000	-1.43754100	-2.80910400
B	-4.97893900	3.49832900	-2.85545900
B	-4.91945500	5.37224900	-1.17078300
B	-4.91988800	5.37327200	1.16749600
B	-4.97998100	3.50047200	2.85338900
B	-5.24252100	1.05402600	3.27153200
B	-5.78816000	-1.43542900	2.80856600
B	-6.39139200	-3.17082200	-1.25091600
B	-6.39148000	-3.16969300	1.25108600
N	-4.59793100	6.12285800	-0.00191900
N	-4.81024300	2.33390100	3.66283800
N	-5.94219900	-2.81605700	2.55464400
N	-5.94206600	-2.81811600	-2.55474700
N	-4.80907900	2.33140800	-3.66433500
B	1.03371600	-1.23227200	-7.22792800
B	-1.76979700	2.42907500	-6.19607000
B	-3.82788900	2.39656900	-4.72192100
B	-5.05305400	-3.72090800	-3.25050400
B	-3.08622800	-5.08498600	-4.07414300
B	0.66209000	-3.53269400	-6.51976500
B	-0.95098700	-5.02715800	-5.26652500

C	0.41353600	-4.74978900	-5.72805400
C	-0.72556300	-3.89689600	-6.17743300
C	1.22924000	0.22548600	-7.28422200
C	-0.14631800	-0.34901100	-7.21661600
C	-2.74969000	3.14908400	-5.35779900
C	-2.94252500	1.70061200	-5.65858500
C	-4.25986100	-4.94638600	-3.18391500
C	-3.98533800	-3.91768100	-4.22912400
N	-1.82858000	-5.68577200	-4.34130800
N	1.57160500	-2.53059400	-6.97214600
B	0.06381700	1.10285400	-7.11979500
N	-0.47009700	2.38526700	-6.76771600
B	-1.77102500	2.43241000	6.19461200
B	-3.82909000	2.39944900	4.72042400
B	-5.05336000	-3.71854700	3.25104300
B	-3.08699300	-5.08257400	4.07584600
B	0.66075500	-3.52938200	6.52161800
B	-0.95209900	-5.02444200	5.26881200
C	0.41232600	-4.74687900	5.73049500
C	-0.72684300	-3.89373400	6.17921300
C	-2.75087600	3.15214700	5.35605500
C	-2.94374500	1.70377900	5.65732600
C	-4.26023000	-4.94410600	3.18506400
C	-3.98605700	-3.91515300	4.23012000
N	-1.82950600	-5.68337800	4.34364300
B	0.06244500	1.10651000	7.11909800
B	1.03227400	-1.22858700	7.22861700
C	1.22783000	0.22920300	7.28417500
C	-0.14772900	-0.34529800	7.21659800
N	-0.47136200	2.38879100	6.76636700
N	1.57019700	-2.52705700	6.97363100
B	-1.23068900	-6.46696400	-3.29641300
B	-0.04591100	-7.31470400	1.22809500
B	-1.23139100	-6.46515800	3.29931500
C	-1.30199100	-6.96430100	-1.91385400
C	-0.00657700	-6.95810700	-2.65254200
C	-0.00717600	-6.95673100	2.65599100
C	-1.30241300	-6.96322500	1.91700000
B	-0.04564200	-7.31536500	-1.22447100
N	0.66105600	-7.50366100	0.00194500
B	2.34726300	6.43092600	-3.24860100
B	-0.93539900	7.57641700	-0.00209300
B	-3.36488600	6.86525800	-0.00206000
B	2.06244000	4.96080200	-5.18631100

B	0.44538000	3.42040500	-6.37909700
C	1.82730100	3.82875600	-6.09976900
C	0.68229200	4.64103200	-5.59571200
C	2.42401100	6.98504100	-1.88735300
C	1.13293400	6.99589500	-2.63386800
C	-2.17871100	7.29863400	0.74384100
C	-2.17857100	7.29809000	-0.74806000
N	2.93536200	5.62533900	-4.27296400
B	1.18499400	7.41567700	-1.22436700
N	0.48544500	7.68145700	-0.00198900
B	0.44419600	3.42370300	6.37734000
B	2.34664400	6.43261100	3.24561800
B	1.18476300	7.41632300	1.22065700
C	0.68125000	4.64392400	5.59337100
C	1.82616800	3.83187200	6.09799600
C	2.42364800	6.98601800	1.88410000
C	1.13242600	6.99725100	2.63036200
B	2.06146700	4.96347700	5.18402900
N	2.93455000	5.62755500	4.27050500
C	-5.36715700	-0.34094200	3.63537600
C	-5.68026100	0.00707100	2.21573000
C	-6.23795400	-3.91258000	0.00042900
C	-5.67958000	0.00509200	-2.21666000
C	-5.36620400	-0.34336700	-3.63613600
C	-5.51036400	4.09765500	-1.62997600
C	-4.54897600	4.84760600	-2.49439900
C	-5.51118000	4.09915300	1.62750200
C	-4.54966300	4.84942700	2.49150900
B	7.04755700	1.28457800	3.24642000
B	6.65586800	-1.09266800	4.02831500
B	7.29676200	2.70306000	1.26600500
B	7.29700400	2.70241100	-1.26611400
B	7.04821100	1.28291300	-3.24585200
B	6.65670600	-1.09474600	-4.02658900
B	6.26273400	-3.39314300	-3.26974500
B	5.98343900	-4.85734200	-1.22225600
B	6.26206800	-3.39146600	3.27260200
B	5.98320000	-4.85672300	1.22581300
N	7.01153500	2.58918000	-2.66384400
N	6.17991300	-2.41448000	-4.31025200
N	5.60270000	-5.49392600	0.00190100
N	6.17902300	-2.41225200	4.31257900
N	7.01102000	2.59054600	2.66373800
B	4.19803800	5.00652600	4.00054600

B	6.13238400	3.55968300	3.23893300
B	5.12112400	-2.54720800	5.26236300
B	2.93246000	-2.60555100	6.53299200
C	5.29983900	4.76149500	3.05897900
C	5.12291300	3.89300200	4.25856300
C	3.94941300	-3.30493700	5.73582700
C	4.17549900	-1.90182700	6.18947500
B	2.93378200	-2.60887600	-6.53120400
B	5.12220300	-2.54991100	-5.26018200
B	4.41889300	-6.29243900	0.00199500
B	2.07395900	-7.25134600	0.00201600
C	4.17677100	-1.90499200	-6.18781700
C	3.95056600	-3.30785800	-5.73347300
C	3.27137600	-6.83996700	0.74770500
C	3.27151900	-6.84035000	-0.74364400
B	4.19879400	5.00445000	-4.00244200
B	6.13299700	3.55800700	-3.23970600
C	5.12371600	3.89078700	-4.25970000
C	5.30040900	4.75990300	-3.06053300
C	5.70658500	-4.60490700	-2.64532600
C	6.65384100	-3.73257500	-1.89267500
C	6.65347800	-3.73161400	1.89579100
C	5.70606400	-4.60355600	2.64869500
C	7.27068600	-0.15962900	3.07176900
C	6.56067900	0.35448700	4.27846400
C	7.64648400	2.03974300	0.00014900
C	7.08962000	3.42356900	-0.00025900
C	7.27133100	-0.16120200	-3.07040700
C	6.56156200	0.35227800	-4.27751100
C	-6.86457300	-2.55376000	-0.00020600
Au	-5.79771600	0.12399000	-0.00033600

(CO₂) AuN₂₀(C₂B₂)₃₀⁺

B	5.31975200	0.33710700	4.01299500
B	5.40501100	-2.08160100	3.24501100
B	5.20814400	2.65562600	3.27259100
B	5.13617900	4.16402800	1.22960600
B	5.13660300	4.17115200	-1.20701000
B	5.20904300	2.67400200	-3.25820100
B	5.32055900	0.35930600	-4.01044100
B	5.40538000	-2.06331900	-3.25483400
B	5.41490900	-3.53584300	1.28323900
B	5.41517500	-3.52837900	-1.30067200
N	4.86521800	4.85188700	0.01326400
N	5.01720300	1.71477700	-4.29695000

N	5.20622900	-3.36188200	-2.68153900
N	5.20577500	-3.37718400	2.66503400
N	5.01628000	1.69107400	4.30636900
B	-1.45649400	-1.11473100	7.27562900
B	1.80504200	2.24264100	6.53664500
B	3.97978300	1.94714200	5.27545200
B	4.23285100	-4.25537100	3.27851100
B	2.13314000	-5.44120700	4.04497200
B	-1.35916800	-3.44116500	6.52299800
B	0.04053000	-5.13494300	5.26478500
C	-1.27477100	-4.67864000	5.72732500
C	-0.03249200	-3.98822600	6.18060100
C	-1.48877600	0.35414800	7.36064700
C	-0.18569300	-0.37150300	7.34567500
C	2.90531500	2.82552600	5.74185300
C	2.97043500	1.40323600	6.18759600
C	3.25435000	-5.32495800	3.08364200
C	3.21616700	-4.46666400	4.30377700
N	0.81390600	-5.88665800	4.31623400
N	-2.13828500	-2.33426700	6.97406300
B	-0.22439100	1.09803100	7.28236800
N	0.45722200	2.32303800	6.98469200
B	1.80606900	2.27800200	-6.52445000
B	3.98073800	1.97589800	-5.26469700
B	4.23337700	-4.23684000	-3.29985000
B	2.13394500	-5.41869000	-4.07321600
B	-1.35801300	-3.40583500	-6.54141100
B	0.04159800	-5.10610800	-5.29189500
C	-1.27364600	-4.64749200	-5.75227700
C	-0.03134200	-3.95456900	-6.20164200
C	2.90635500	2.85672600	-5.72665600
C	2.97138600	1.43673100	-6.17967100
C	3.25494300	-5.30755100	-3.11103000
C	3.21691500	-4.44260600	-4.32645900
N	0.81484600	-5.86281600	-4.34720100
B	-0.22328800	1.13737300	-7.27638900
B	-1.45530500	-1.07543800	-7.28169500
C	-1.48763900	0.39387000	-7.35885700
C	-0.18453000	-0.33180100	-7.34752800
N	0.45826200	2.36078900	-6.97215000
N	-2.13710100	-2.29660900	-6.98675600
B	0.10963200	-6.56722200	3.26739000
B	-1.17930300	-7.26477300	-1.24355200
B	0.11039200	-6.54917200	-3.30226400

C	0.11349500	-7.07024600	1.88548700
C	-1.16807900	-6.90846300	2.63155600
C	-1.16745200	-6.89401100	-2.66865000
C	0.11394300	-7.05980700	-1.92315700
B	-1.17958700	-7.27144000	1.20445500
N	-1.90572600	-7.37878400	-0.01994200
B	-1.80835400	6.56409200	3.29325900
B	1.57676800	7.03523600	0.01916200
B	3.79434600	5.81550000	0.01587900
B	-1.73806900	5.11517600	5.26546600
B	-0.33123600	3.43260000	6.53184500
C	-1.65356200	3.97322200	6.19178900
C	-0.41387000	4.66066400	5.72762900
C	-1.80549000	7.10583600	1.92435100
C	-0.52351900	6.91541500	2.66275700
C	2.72898300	6.49212300	-0.72826700
C	2.72874900	6.48769200	0.76372800
N	-2.50754900	5.86802100	4.32698800
B	-0.51869000	7.31453700	1.24698500
N	0.21194300	7.43948000	0.02012700
B	-0.33022600	3.46788900	-6.51341200
B	-1.80777100	6.58177800	-3.25801900
B	-0.51845000	7.32124200	-1.20753000
C	-0.41296400	4.69158200	-5.70257600
C	-1.65260000	4.00660400	-6.17050900
C	-1.80513800	7.11608700	-1.88619400
C	-0.52304900	6.92979000	-2.62544600
B	-1.73720400	5.14354900	-5.23805000
N	-2.50680100	5.89127200	-4.29558300
C	5.10242700	-1.06916100	-4.27609500
C	5.76949000	-0.64869800	-3.00888800
C	5.22521500	-4.16382700	-0.01058000
C	5.76888300	-0.66570000	3.00636600
C	5.10187200	-1.09274100	4.27142300
C	5.63332300	2.92277500	1.87897200
C	4.84640300	3.92817000	2.64657600
C	5.63402600	2.93362000	-1.86313700
C	4.84720900	3.94316700	-2.62535800
B	-7.13214300	2.12621300	-3.24238300
B	-7.02354900	-0.27771200	-4.03172200
B	-7.19784000	3.55946300	-1.25718600
B	-7.19810100	3.55268300	1.27535200
B	-7.13274600	2.10877300	3.25282400
B	-7.02421800	-0.29939800	4.02910300

B	-6.91768800	-2.62515500	3.26659800
B	-6.85010000	-4.10664500	1.21364000
B	-6.91718000	-2.60758700	-3.28186400
B	-6.84992900	-4.10010600	-1.23690200
N	-6.93414200	3.40166200	2.67367400
N	-6.70464200	-1.66677400	4.30725400
N	-6.56157800	-4.78489100	-0.01342600
N	-6.70396000	-1.64355400	-4.31725500
N	-6.93361700	3.41596200	-2.65625200
B	-3.83887000	5.44178800	-4.01656600
B	-5.94091900	4.26456400	-3.23635700
B	-5.66247500	-1.89938100	-5.26066100
B	-3.49442600	-2.20985500	-6.53192600
C	-4.95165100	5.34157800	-3.06130000
C	-4.90951800	4.46633200	-4.26841200
C	-4.58370900	-2.78614300	-5.73102000
C	-4.64708300	-1.36697500	-6.18585800
B	-3.49551500	-2.24503900	6.51942900
B	-5.66331400	-1.92772400	5.24942500
B	-5.48925100	-5.72745600	-0.01585500
B	-3.27936400	-6.96383800	-0.01897300
C	-4.64811400	-1.40030500	6.17769500
C	-4.58463200	-2.81699000	5.71519700
C	-4.41866800	-6.41092900	-0.76342600
C	-4.41877500	-6.41487900	0.72823500
B	-3.83960500	5.42011300	4.04538700
B	-5.94154500	4.24713000	3.25850900
C	-4.91028900	4.44330300	4.29179300
C	-4.95225000	5.32507700	3.08943200
C	-6.52898500	-3.89659900	2.63443500
C	-7.36308100	-2.90707900	1.89288000
C	-7.36286100	-2.89692500	-1.90977000
C	-6.52859200	-3.88240500	-2.65648900
C	-7.52623900	0.71845900	-3.07329300
C	-6.75855100	1.14861300	-4.27766400
C	-7.62792100	2.94241000	0.00739600
C	-6.89999700	4.24426700	0.01095700
C	-7.52683600	0.70195800	3.07605100
C	-6.75927000	1.12557000	4.28281600
C	5.77994500	-2.78695800	-0.00643800
C	7.78679300	2.29475100	0.00620900
O	8.05100400	3.41700900	0.00964200
O	7.60718700	1.13692600	0.00253900
Au	6.43059500	-0.82525700	-0.00201000

(N₂O) AuN₂₀(C₂B₂)₃₀⁺

B	5.30475500	0.43205000	3.99956200
B	5.42337500	-1.99409300	3.25599000
B	5.17527600	2.75121500	3.24515800
B	5.09921300	4.24975000	1.19500300
B	5.09878600	4.23525900	-1.24340000
B	5.17404400	2.71331900	-3.27632300
B	5.30331800	0.38587200	-4.00566600
B	5.42216300	-2.03221500	-3.23647900
B	5.46255100	-3.47984500	1.31132900
B	5.46186800	-3.49554100	-1.27565200
N	4.81797700	4.92321800	-0.02817700
N	4.98317300	1.73604900	-4.30001500
N	5.23956200	-3.33107600	-2.65441800
N	5.24071800	-3.29919400	2.68816900
N	4.98471200	1.78526300	4.27960000
B	-1.45720400	-1.06244700	7.28431900
B	1.76782700	2.32010600	6.50794900
B	3.94229000	2.03613800	5.24357900
B	4.26872700	-4.17573300	3.30675800
B	2.17887500	-5.37255800	4.08337800
B	-1.33493600	-3.39288900	6.54981200
B	0.08369400	-5.07912800	5.30282300
C	-1.23656300	-4.63511000	5.76308200
C	-0.00214400	-3.92676500	6.21019400
C	-1.50465000	0.40661300	7.35688700
C	-0.19413400	-0.30566000	7.34603400
C	2.86068500	2.90761800	5.70663800
C	2.93928300	1.48862200	6.16073800
C	3.30026500	-5.25613300	3.12200400
C	3.25172700	-4.38415600	4.33205500
N	0.86484400	-5.82973700	4.35964500
N	-2.12621300	-2.29173000	6.99347800
B	-0.24809500	1.16278800	7.26966800
N	0.42075400	2.39169200	6.96011800
B	1.76584700	2.24632300	-6.53348900
B	3.94057100	1.97639100	-5.26647300
B	4.26726800	-4.21438500	-3.26271600
B	2.17692900	-5.41959200	-4.02486700
B	-1.33752800	-3.46673600	-6.51140500
B	0.08125000	-5.13941900	-5.24646700
C	-1.23911100	-4.70019800	-5.71102200
C	-0.00472000	-3.99718000	-6.16653800
C	2.85879900	2.84268100	-5.73885900

C	2.93740400	1.41879000	-6.17736900
C	3.29873000	-5.29248900	-3.06533600
C	3.24985000	-4.43429300	-4.28519100
N	0.86268700	-5.87962800	-4.29535300
B	-0.25030300	1.08064000	-7.28190500
B	-1.45967100	-1.14448800	-7.27150800
C	-1.50695800	0.32367600	-7.36038300
C	-0.19652200	-0.38858000	-7.34194400
N	0.41869000	2.31288100	-6.98620700
N	-2.12875400	-2.37037600	-6.96686400
B	0.16709900	-6.52839100	3.31842200
B	-1.11783600	-7.28063500	-1.18279500
B	0.16535600	-6.56624900	-3.24587900
C	0.17463400	-7.04488800	1.94154600
C	-1.10763700	-6.88992600	2.68791800
C	-1.10907800	-6.92038300	-2.61056900
C	0.17359400	-7.06696400	-1.86319400
B	-1.11716000	-7.26653000	1.26437400
N	-1.84308900	-7.39265000	0.04167900
B	-1.88773500	6.57936700	3.23809000
B	1.49534300	7.05603300	-0.04002900
B	3.72978600	5.86700200	-0.03355500
B	-1.80345700	5.14890300	5.22258400
B	-0.37910300	3.49015600	6.50052900
C	-1.70702900	4.01537500	6.15805200
C	-0.47453400	4.71119700	5.68718000
C	-1.88911400	7.10813500	1.86417500
C	-0.60592800	6.93729500	2.60527100
C	2.65427100	6.52179500	-0.78316300
C	2.65459500	6.53053700	0.70879500
N	-2.58063500	5.88612200	4.27806700
B	-0.60375500	7.32306400	1.18577700
N	0.12568400	7.44448900	-0.04199400
B	-0.38105100	3.41648600	-6.53888800
B	-1.88887000	6.54246800	-3.31143000
B	-0.60419400	7.30920200	-1.26805700
C	-0.47630600	4.64665200	-5.73938100
C	-1.70890600	3.94559200	-6.20214700
C	-1.88978400	7.08669000	-1.94355800
C	-0.60684500	6.90743400	-2.68309500
B	-1.80513500	5.08965100	-5.27957600
N	-2.58209000	5.83757200	-4.34331400
C	5.09128500	-1.04722600	-4.25909400
C	5.77883500	-0.61393000	-3.00874600

C	5.26868400	-4.11519500	0.02178900
C	5.77990000	-0.57827200	3.01306300
C	5.09286900	-0.99830300	4.26819300
C	5.61804600	3.02828400	1.86059400
C	4.79424600	4.01530300	2.61086500
C	5.61684900	3.00580100	-1.89485100
C	4.79381900	3.98475300	-2.65646600
B	-7.16731300	2.03263900	-3.25798800
B	-7.03437300	-0.37664400	-4.02710600
B	-7.24758300	3.48144600	-1.28477600
B	-7.24711500	3.49567200	1.24771200
B	-7.16614600	2.06914700	3.23708600
B	-7.03293600	-0.33131600	4.03327900
B	-6.90274000	-2.66220700	3.29011400
B	-6.82008400	-4.16018400	1.24970400
B	-6.90390900	-2.69903200	-3.25777600
B	-6.82051900	-4.17396500	-1.20067600
N	-6.98123500	3.35916700	2.64716000
N	-6.69953100	-1.69306700	4.32270000
N	-6.52482100	-4.84572200	0.02827900
N	-6.70107200	-1.74158000	-4.30128000
N	-6.98220500	3.32922300	-2.68269200
B	-3.90928900	5.37671200	-4.06011300
B	-5.99865000	4.18359900	-3.26997800
B	-5.65749300	-1.99483000	-5.24307600
B	-3.48685100	-2.29400000	-6.51258200
C	-5.02082400	5.27235400	-3.10378900
C	-4.96976500	4.38809200	-4.30395300
C	-4.56986600	-2.87452600	-5.70623900
C	-4.64810700	-1.46012700	-6.17347200
B	-3.48448400	-2.22055900	6.53886500
B	-5.65560500	-1.93570400	5.26689900
B	-5.44303700	-5.77734900	0.03333100
B	-3.22086200	-6.99154500	0.03973900
C	-4.64592300	-1.39059800	6.19091400
C	-4.56774500	-2.81011600	5.73944600
C	-4.36584200	-6.45631200	-0.70888700
C	-4.36550400	-6.44782200	0.78274200
B	-3.90790000	5.42206300	4.00045300
B	-5.99749000	4.22010100	3.22446300
C	-4.96829300	4.43625500	4.25575300
C	-5.01970800	5.30689900	3.04569300
C	-6.50113100	-3.93493000	2.66864500
C	-7.34526800	-2.96025100	1.91885900

C	-7.34593300	-2.98162600	-1.88309200
C	-6.50206500	-3.96468800	-2.62216800
C	-7.54692500	0.62236100	-3.07690300
C	-6.78401500	1.05018000	-4.28512400
C	-7.67069200	2.87029800	-0.01498000
C	-6.95687600	4.17993900	-0.02246700
C	-7.54581700	0.65691300	3.07204300
C	-6.78249800	1.09832700	4.27509800
C	5.85587700	-2.75516600	0.01307900
N	7.47486400	1.16872300	-0.00582700
N	7.75811400	2.25184400	-0.01263200
O	8.06383900	3.38090800	-0.01967100
Au	6.55122000	-0.81810500	0.00435100