

Radical(NO) and Nonradical(N₂O) Reagents Convert an Ru^{IV} Nitride to the Same Nitrosyl Complex

Amy Walstrom, Maren Pink, Hongjun Fan, John Tomaszewski and Kenneth G. Caulton*

Department of Chemistry, Indiana University, Bloomington, IN

Experimental:

General Considerations: Preparations from literature sources(see text, ref. 1) were used to synthesize RuN(SiMe₂CH₂P^tBu₂)₂Cl, and standard Schlenk or glovebox techniques in inert (Argon) atmosphere were used for air sensitive manipulations. All solvents, including deuterated NMR solvents, were dried over and distilled from Na / benzophenone and stored in anaerobic conditions. All other reagents were degassed and / or used as received from commercial vendors. ¹H, ¹³C{¹H} and ³¹P{¹H} NMR spectra were recorded on a Varian Unity I400 (400 MHz ¹H, 101 MHz ¹³C{¹H}, 162 MHz ³¹P{¹H}) instrument, and ¹⁵N NMR spectra recorded on a Varian Unity I500 (50 MHz ¹⁵N), with chemical shifts reported in ppm, referenced to protio impurities in each stated solvent, with the exception of ³¹P{¹H} and ¹⁵N spectra which were externally referenced to 85% H₃PO₄ (0 ppm), and neat nitromethane (380.23 ppm), respectively. All FT-IR spectra were recorded on a Nicolet 510P spectrophotometer. Mass spectra (ESI-MS) were acquired on a PE-Sciex API III triple quadrupole spectrometer, and simulated with IsoPro 3.0 isotopic distribution software.

Reaction of PNPRuN with Nitrous oxide (N₂O):

Room Temperature Experiment: A Teflon-closure reaction flask containing 20.1 mg (0.0342 mmol) of PNPRuN in Et₂O, was charged with approximately 2 atm pressure of N₂O. Over 2 days of stirring at room temperature (22 °C), there was a slow but observable color change from deep green to greenish brown, giving quantitatively PNPRuNO. Volatiles were stripped, the solid was redissolved in C₆D₆, and ¹H and ³¹P{¹H} NMR were recorded: ¹H NMR (400 MHz, C₆D₆): δ 1.39 (t, 36H, J_{P-H} = 6.5 Hz, PCMe₃), 1.32 (t, 4H, J_{P-H} = 6 Hz PCH₂Si), 0.167 (s, 12H, SiMe₂). ³¹P{¹H} (162 MHz, C₇D₈): δ 71.5 (s). ¹³C{¹H} (101 MHz, C₆D₆): δ 36.40 (t, J_{C-P} = 6.1 Hz, Si-CH₂-P), 29.88 (t, J_{C-P} = 3.2 Hz, PCMe₃), 9.86 (s, PCMe₃), 6.08 (s, SiMe₂). FT-IR(in Et₂O): ν(N≡O) 1691 cm⁻¹. ESI-MS: m/z 580.2, calculated m/z 580.212.

Reaction of PNPRuN with Nitric oxide (NO):

A J-Young NMR tube containing 10.7 mg (0.171 mmol) of PNPRuN in C₇D₈ was charged with approximately 2.5 mL NO(100 mmHg pressure; less than 1 molar equivalent), to ensure a substoichiometric amount of NO. Upon mixing there occurs a fast distinct color change from green to greenish brown with noticeable gas evolution (N₂O), to give PNPRuN and PNPRuNO only: ¹H NMR (400 MHz, C₇D₈): δ 1.375 (t, J_{P-H} = 6.0 Hz, 36H, PNPRuNO, PCMe₃), 1.302 (t, J_{P-H} = 7.6 Hz, 36H, PNPRuN, PCMe₃), 0.900 (t, J_{P-H} = 6.0 Hz, 4H, PNPRuN, Si-CH₂-P), 0.24 (s, 12H, PNPRuN, SiMe₂), 0.134 (s, 12H, PNPRuNO, SiMe₂). ³¹P{¹H} (162 MHz, C₇D₈): δ 78.34 (s, PNPRuN), 71.44 (s, PNPRuNO). PNPRuN and PNPRuNO are in roughly a 50/50 ratio, supporting the 2:1 stoichiometry of NO to PNPRuN. FT-IR (solution in C₇D₈): 2218 cm⁻¹ (ν N₂O), 1688 cm⁻¹ (ν Ru-NO)

Variable Temperature Experiment: A J-Young NMR tube containing 20.3 mg (0.0342 mmol) of PNPRuN in C₇D₈ was charged with approximately 2.5 mL (at 250 mmHg pressure) NO. The tube was immediately frozen in liquid N₂ and kept frozen until it was inserted into a precooled NMR probe. When placing the sample into the instrument, the sample was briefly shaken vigorously to ensure homogeneity. First spectra were obtained at -60° C, and then repeatedly in 10 degree increments. At every temperature, the only spectroscopically observable species were PNPRuN and PNPRuNO, in differing ratios at every temperature. This shows that there are no NMR observable intermediates (i.e PNPRu(N₂O)) even at -60 °C.

Reaction of (PNP)RuN and organic radicals:

To a J-Young tube containing 10.2 mg (PNP)RuN in C₆D₆, 3.3 mg of TEMPO radical (1 equivalent) or 2.7 mg of galvinoxyl radical (1 equivalent) was added, and NMR spectra obtained immediately. In a different experiment, a J-Young tube containing 10.6 mg (PNP)RuN in C₇D₈ was cooled to -78°C and 3.3 mg of TEMPO radical dissolved in C₇D₈ was then added dropwise to the chilled tube. No reaction between (PNP)RuN and the organic radicals TEMPO or galvinoxyl was observed at either room temperature or low temperature.

¹⁵N labeling experiments:

A. PNPRu¹⁵N(50% ¹⁵N at the nitride site) was synthesized according to literature procedures (see ref. 1 of text), and the following two experiments were carried out.

1. A J-Young NMR tube containing 20.3 mg of PNPRu¹⁵N in C₆D₆ was charged with 2.5 mL at ~ 2 atm of N₂O and allowed to react for 2 days, after which the following spectra were collected: ¹H NMR (400 MHz, C₆D₆): δ 1.39 (t, 36H, J_{P-H} = 6.5 Hz,

PCMe_3), 1.32 (t, 4H, $J_{\text{P-H}} = 6$ Hz PCH_2Si), 0.165 (s, 12H, SiMe_2). $^{31}\text{P}\{\text{H}\}$ (162 MHz, C_7D_8): δ 78.28 (s, $\text{PNPRu}^{14/15}\text{N}$), 71.505 (d, $J_{\text{P-N}} = 6.9$ Hz, $\text{PNPRu}^{15}\text{NO}$), 71.503 (s, $\text{PNPRu}^{14}\text{NO}$). $^{15}\text{N}\{\text{H}\}$ (50 MHz, C_7D_8): δ 846.65 ppm (s, unreacted PNPRuN), 344.12 (t, $J_{\text{P-N}} = 6.9$ Hz), PNPRuNO . FT-IR (in Et_2O): 1691 cm^{-1} ($\text{PNPRu}^{14}\text{NO}$), 1656 cm^{-1} ($\text{PNPRu}^{15}\text{NO}$).

2. A J-Young NMR tube containing 20.1 mg of $\text{PNPRu}^{15}\text{N}$ in C_7D_8 was charged with 250 mmHg pressure of NO and shaken vigorously. The ^1H and $^{31}\text{P}\{\text{H}\}$ NMR spectra acquired immediately showed only a singlet for $(\text{PNP})\text{RuNO}$ in the $^{31}\text{P}\{\text{H}\}$ spectrum which indicates that the final quantitative product is $(\text{PNP})\text{Ru}^{14}\text{NO}$. Of importance, the the $^{15}\text{N}\{\text{H}\}$ NMR spectrum of the same sample showed no signal for $(\text{PNP})\text{Ru}^{15}\text{NO}$, but did show a signal for dissolved N_2O gas (also detected by IR), with a chemical shift appearing at -233 ppm (referenced to CH_3NO_2 at 0 ppm), which corresponds to $^{15}\text{N}_\alpha=^{14}\text{N}_\beta=\text{O}$. No ^{15}N label was incorporated into the N_β position, as a chemical shift of approximately -120 ppm was not detected. The mechanistic conclusion that the overall reaction is not oxygen atom transfer to nitride, but rather $\text{N}(\text{Ru})$ transfer to NO can be made based on these results.

B. Approximately 1 equivalent (2.5 mL at 120 mmHg) of isotopically labeled $^{15}\text{N}=^{15}\text{N}=\text{O}$ was added to a J-Young NMR tube containing 10.1 mg (0.0171 mmol) of $\text{PNPRu}^{14}\text{NO}$ in C_6D_6 and allowed to react over 3 days. ^1H and $^{31}\text{P}\{\text{H}\}$ spectra were then collected in order to detect the presence of $\text{PNPRu}^{15}\text{NO}$. The $^{31}\text{P}\{\text{H}\}$ spectrum showed only a singlet for the PNPRuNO signal at 71.5 ppm, showing that no $\text{PNPRu}^{15}\text{NO}$ was produced.

Computational Details

All calculations were carried out using Density Functional Theory as implemented in the Jaguar 6.0 suite¹ of ab initio quantum chemistry programs. Geometry optimizations were performed with the B3LYP²⁻⁵ functional and the 6-31G** basis set with no symmetry restrictions. Transition metals were represented using the Los Alamos LACVP basis^{6,7}. The bond order is calculated using the definition of Mayer.⁸

The models used in this study consist of up to ~90 atoms, which represent the non-truncated substrates that were also used in the related experimental work. Although a smaller model may also able to reproduce the most important features of the studied reaction qualitatively, we chose to employ the large scale model faithfully construct a realistic model chemistry.

This supporting information includes some structures alluded to, but not pictured in the main text.

References

1. Jaguar, version 6.0, *Schrödinger, L.L.C, New York, NY, 2005*.
2. Becke, A. D., *Phys. Rev. A* **1988**, 38, 3098.
3. Becke, A. D., *J. Chem. Phys.* **1993**, 98, 5648.
4. Lee, C. T.; Yang, W. T.; Parr, R. G., 1988 *Phys. Rev. B*, 37, 785.
5. Vosko, S. H.; Wilk, L.; Nusair, M., *Can. J. Phys.* **1980**, 58, 1200.
6. Hay, P. J.; Wadt, W. R., *J. Chem. Phys.* **1985**, 82, 270.
7. Wadt, W. R.; Hay, P. J., *J. Chem. Phys.* **1985**, 82, 284.
8. I. Mayer, *Chem. Phys. Lett.* 97, 270 (1983).

S1. Free N₂O:

Bond lengths (Å) and bond angles (°).

N-N 1.135

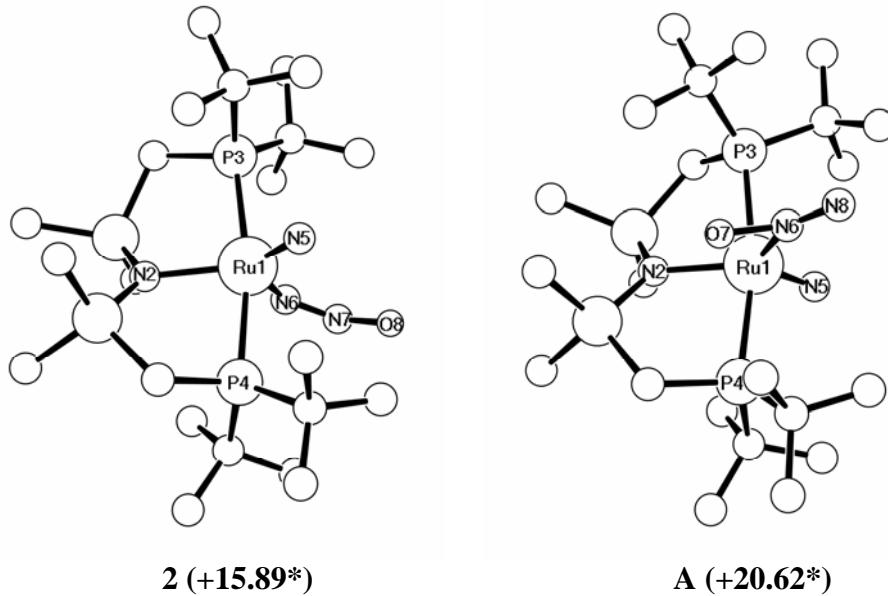
N-O 1.193

N-N-O 180.0

Coordinates:

N	0.000000000	0.000000000	1.207212787
N	0.000000000	0.000000000	0.072551275
O	0.000000000	0.000000000	-1.120395531

S2. Simple adducts between (PNP)Ru(N) and N₂O.

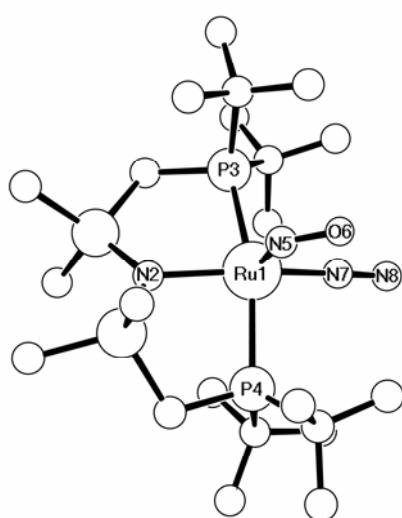


* Relative E(SCF) energy in kcal/mol (compare to (PNP)Ru(N) + N₂O).

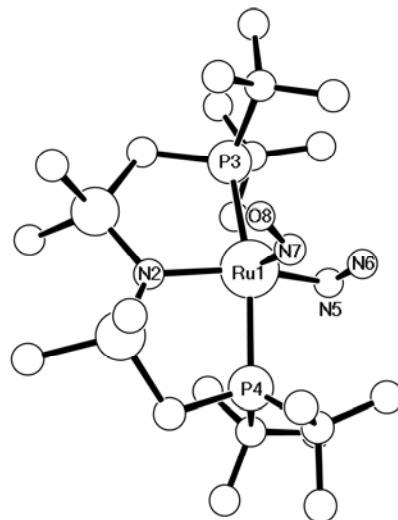
Select bond lengths (Å) and bond angles (°).

	2	A	
Ru1-P3:	2.569	Ru1-P3:	2.536
Ru1-P4:	2.544	Ru1-P4:	2.567
Ru1-N2:	2.142	Ru1-N2:	2.148
Ru1-N5	1.635	Ru1-N5	1.642
Ru1-N6	2.113	Ru1-N6	2.198
N6-N7	1.203	N6-N8	1.169
N7-O8	1.255	N6-O7	1.317
P3-Ru1-P4:	170.5	P3-Ru1-P4:	168.5
P3-Ru1-N2:	86.4	P3-Ru1-N2:	84.4
P4-Ru1-N2:	84.4	P4-Ru1-N2:	86.0
N5-Ru1-N6	120.1	N5-Ru1-N6	113.4
Ru1-N6-N7	126.7	Ru1-N6-N8	139.1
N6-N7-O8	133.6	Ru1-N6-O7	82.2
N2-Ru1-N5	134.1	N2-Ru1-N5	123.4
N2-Ru1-N6	105.8	N2-Ru1-N6	123.2
		Ru1-O7	2.405

S3. Possible intermediates for (PNP)Ru(N) + N₂O →(PNP)Ru(NO) + N₂.



B (-58.90*)



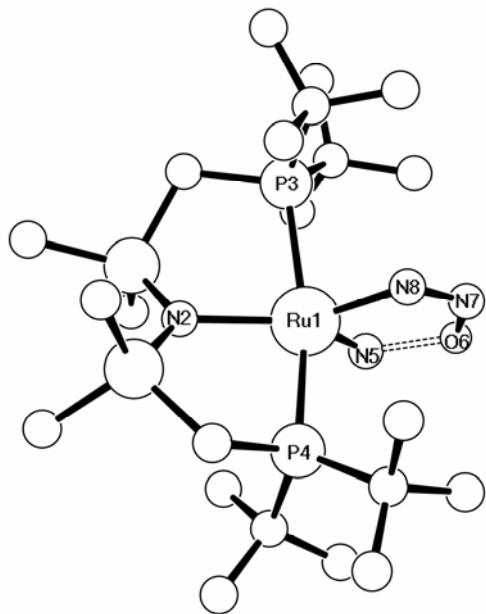
C (-34.61*)

* Relative E(SCF) energy in kcal/mol (compare to (PNP)Ru(N) + N₂O).

Select bond lengths (Å) and bond angles (°).

	B	C
Ru1-P3:	2.510	2.527
Ru1-P4:	2.486	2.505
Ru1-N2:	2.172	2.123
Ru1-N5	1.887	2.279
Ru1-N7	1.958	1.922
N7-N8	1.126	2.446
N5-O6	1.203	1.132
P3-Ru1-P4:	161.9	165.1
P3-Ru1-N2:	86.3	88.1
P4-Ru1-N2:	85.8	86.1
N5-Ru1-N7	92.7	104.2
Ru1-N7-N8	178.0	84.5
Ru1-N5-O6	126.1	121.0
N2-Ru1-N5	98.7	152.6
N2-Ru1-N7	168.5	102.7

S4. Transition state.



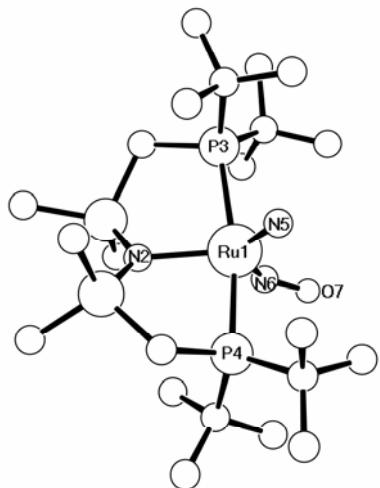
3 (+21.26*)

* Relative E(SCF) energy in kcal/mol (compare to (PNP)Ru(N) + N₂O).

Select bond lengths (Å) and bond angles (°).

Ru1-P3:	2.533
Ru1-P4:	2.497
Ru1-N5:	1.735
Ru1-N8	2.032
Ru1-N2	2.194
N8-N7	1.239
N5-O6	1.638
N7-O6	1.347
P3-Ru1-P4:	162.0
P3-Ru1-N2:	83.8
P4-Ru1-N2:	83.4
N5-Ru1-N8	82.2
Ru1-N5-O6	114.9
Ru1-N8-O7	116.5
N5-O6-N7	108.6
N8-N7-O6	117.7
N2-Ru1-N5	137.8
N2-Ru1-N8	139.9

S5. Optimized structure of (PNP)Ru(NO)(N) (Doublet, **1**).



1 (-12.64*)

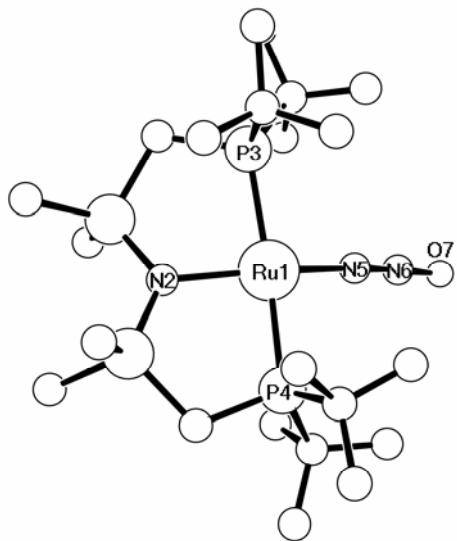
* Relative E(SCF) energy in kcal/mol (compare to (PNP)Ru(N) + NO).

Spin density: Ru1 0.06, N5 0.84, N6 0.00, O7 0.02, P3 0.03, P4 0.03.

Select bond lengths (\AA) and bond angles ($^\circ$).

Ru1-P3:	2.554
Ru1-P4:	2.517
Ru1-N2:	2.172
Ru1-N5	1.739
Ru1-N6	1.858
N6-O7	1.199
P3-Ru1-P4:	168.7
P3-Ru1-N2:	85.9
P4-Ru1-N2:	85.1
N5-Ru1-N6	118.8
Ru1-N6-O7	141.7
N2-Ru1-N5	124.5
N2-Ru1-N6	116.6

S6. Optimized structure of (PNP)Ru(N₂O) (Doublet).



E (-28.78*)

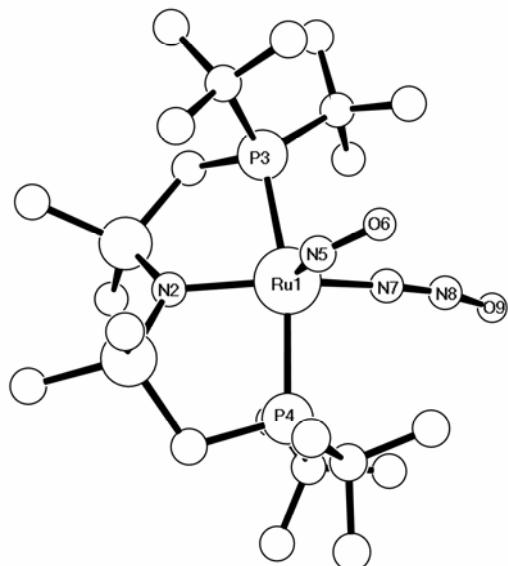
* Relative E(SCF) energy in kcal/mol (compare to (PNP)Ru(N) + NO).

Spin density: Ru1: 1.049; N2O: -0.04

Select bond lengths (Å) and bond angles (°).

Ru1-P3:	2.432
Ru1-P4:	2.431
Ru1-N2:	2.140
Ru1-N5	1.998
N5-N6	1.145
N6-O7	1.217
P3-Ru1-P4:	166.2
P3-Ru1-N2:	85.8
P4-Ru1-N2:	88.1
N2-Ru1-N5	162.2
Ru1-N5-N6	172.2
N5-N6-O7	176.1
P2-Ru1-N5	96.6
P3-Ru1-N5	93.0

S7. Optimized structure of (PNP)Ru(N₂O)(NO).



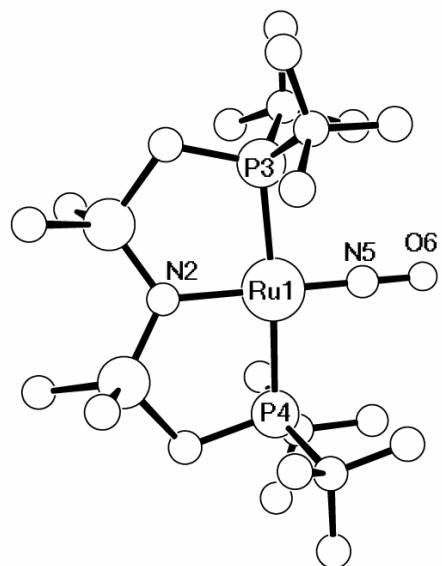
F (-59.17*)

* Relative E(SCF) energy in kcal/mol (compare to (PNP)Ru(N) + 2NO).

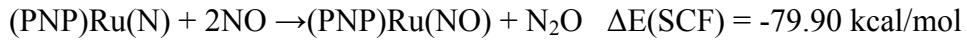
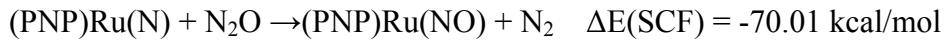
Select bond lengths (Å) and bond angles (°).

Ru1-P3:	2.474
Ru1-P4:	2.517
Ru1-N2:	2.168
Ru1-N5	1.886
Ru1-N7	2.040
N5-O6	1.207
N7-N8	1.140
N8-O9	1.211
P3-Ru1-P4:	167.1
P3-Ru1-N2:	82.9
P4-Ru1-N2:	85.7
N5-Ru1-N7	92.0
Ru1-N5-O6	124.4
Ru1-N7-N8	173.9
N7-N8-O9	178.7
N2-Ru1-N5	108.9
N2-Ru1-N7	159.1

S8. Optimized structure of (PNP)Ru(NO).



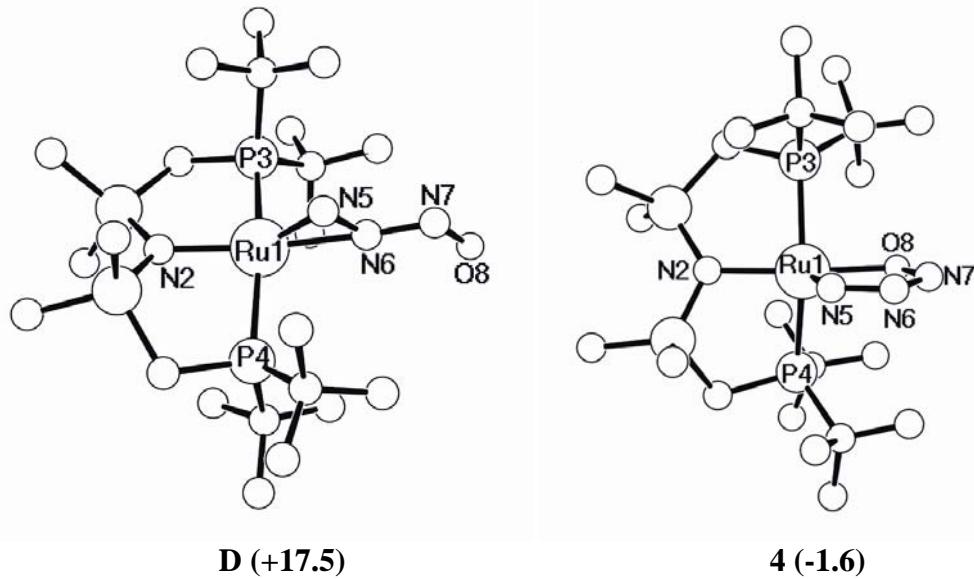
G



Select bond lengths (\AA) and bond angles ($^\circ$).

Ru1-P3:	2.449
Ru1-P4:	2.448
Ru1-N2:	2.119
Ru1-N5	1.742
N5-N6	1.189
P3-Ru1-P4:	175.5
P3-Ru1-N2:	87.7
P4-Ru1-N2:	87.8
N2-Ru1-N5	179.7
Ru1-N5-N6	179.8

S9. Structures that are unlikely in the pathway for $(\text{PNP})\text{Ru}(\text{N}) + \text{N}_2\text{O} \rightarrow (\text{PNP})\text{Ru}(\text{NO}) + \text{N}_2$.



* Relative E(SCF) energy in kcal/mol (compare to $(\text{PNP})\text{Ru}(\text{N}) + \text{N}_2\text{O}$).

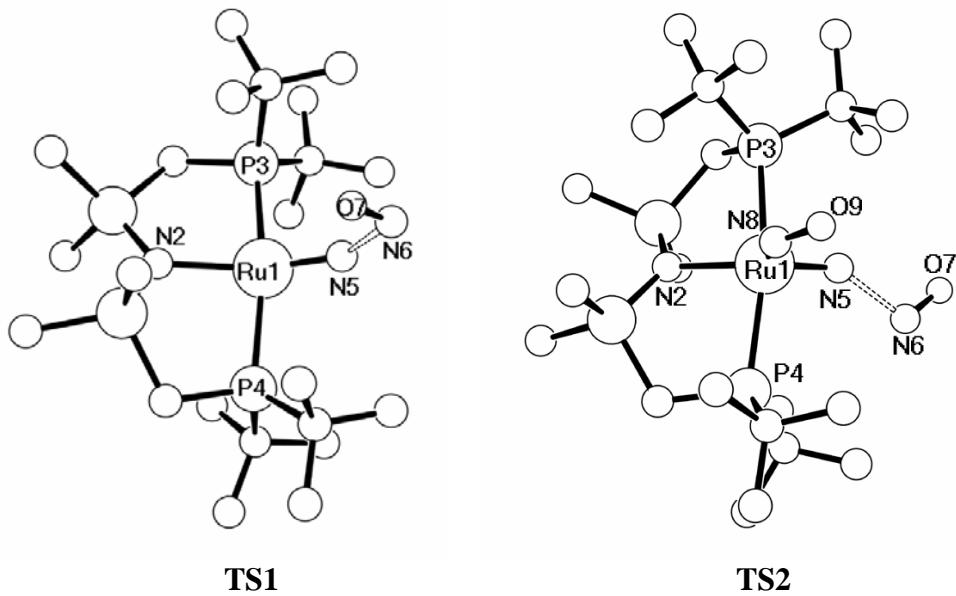
Select bond lengths (\AA) and bond angles ($^\circ$).

D		4	
Ru1-P3:	2.47	Ru1-P3:	2.47
Ru1-N2:	2.07	Ru1-N2:	2.12
Ru1-N5	1.88	Ru1-N5	1.82
Ru1-N6	2.23	Ru1-O8	2.08
N5-N6	1.26	N5-N6	1.35
N6-N7	1.42	N6-N7	1.29
N7-O8	1.21	N7-O8	1.30
P3-Ru1-P4:	163.9	P3-Ru1-P4:	149.1
N2-Ru1-N6:	168.7	N2-Ru1-N5:	115.8
N5-Ru1-N6:	88.0	N2-Ru1-O8:	168.9
N2-Ru1-N5	134.4	Ru1-N5-N6	121.6
N5-N6-N7	117.3	Ru1-O8-N7	114.1
Ru1-N6-N7	174.8	N5-N6-N7	115.3
N6-N7-O8	112.7	N6-N7-O8	113.7

Comment:

E is a candidate for the unknown species found by NMR at low temperature.

S10. TS for (PNP)Ru(N) + NO → (PNP)Ru(NNO) and **1** + NO → (PNP)Ru(NO) + N₂O.



Relative E(SCF) energy in kcal/mol for **TS1** (compare to (PNP)Ru(N) + NO): 8.7

Relative free energy in kcal/mol for **TS1** (compare to (PNP)Ru(N) + NO): 20.6

Relative E(SCF) energy in kcal/mol for **TS2** (compare to (PNP)Ru(N) + 2NO): -4.2

Relative free energy in kcal/mol for **TS2** (compare to (PNP)Ru(N) + 2NO): 17.8

Select bond lengths (Å) and bond angles (°).

	TS1	TS2
Ru1-P3:	2.463	2.536
Ru1-P4:	2.491	2.601
Ru1-N2:	2.130	2.180
Ru1-N5	1.675	1.758
N5-N6	1.835	1.857
N6-O7	1.193	1.847
P3-Ru1-P4:	165.6	1.188
N2-Ru1-N5	151.4	1.195
Ru1-N5-N6	140.3	168.8
N5-N6-O7	109.3	128.3
		N2-Ru1-N8
		118.1
		Ru1-N5-N6
		146.2
		Ru1-N8-O9
		139.7
		N5-N6-O7
		112.1
		N5-Ru1-N8
		112.9

S11. Coordinates

2				
Ru	14.698307089	1.517976631	18.272663832	C 18.652719505 1.827672327 19.910868318
P	15.888283685	-0.517515750	19.292906398	C 18.597645015 0.820945331 17.629459156
P	13.449853677	3.648182212	17.659519803	C 12.214128969 5.578144104 16.261022142
Si	14.832974013	1.340426657	21.573137741	C 12.141317712 3.082330263 16.255824081
Si	12.226991238	2.425524778	20.269173387	C 14.014163189 4.278530936 15.085170448
N	13.857584040	1.833361811	20.217151665	C 15.889484040 5.536046694 19.543299600
C	16.209256015	2.571905018	21.986994679	C 16.689622648 4.991524688 17.240412092
H	15.782531503	3.502641118	22.378646517	H 19.672006241 2.159032047 19.674765303
H	16.805294329	2.827765391	21.106662074	H 18.598559392 1.678059011 20.992091272
H	16.885005851	2.173041278	22.753890410	H 17.966308807 2.638191214 19.646095890
C	13.874149193	1.031058989	23.185533512	H 20.335942589 -0.202562554 19.547652268
H	13.527408167	1.961136504	23.646801086	H 19.241976557 -1.470702212 18.998263381
H	14.534425007	0.540339288	23.911741945	H 19.119699843 -0.845889000 20.653078579
H	13.004000301	0.381053351	23.041196053	H 19.641497478 1.130609665 17.490618392
C	15.617639136	-0.350680158	21.115989090	H 17.956980864 1.629612958 17.264428912
H	16.542474983	-0.541403605	21.669277706	H 18.428201396 -0.052821014 16.996426224
H	14.903635630	-1.119596626	21.427514323	H 16.316525928 -3.720627189 19.553293914
C	14.976665168	-2.149064650	18.831564673	H 16.287855599 -2.584557212 20.899708560
C	17.786596889	-0.669940002	19.029888947	H 17.738321417 -2.737733497 19.903550732
C	11.830737094	3.587539215	21.722199770	H 16.200073109 -2.978687360 17.180166003
H	12.552657296	4.404736316	21.824387091	H 17.680776167 -2.060007574 17.436216250
H	11.797040124	3.053863400	22.677024619	H 16.256801379 -1.275106236 16.736212348
H	10.841763433	4.038356513	21.572081590	H 14.239607929 -2.787677259 18.643628786
C	10.933012124	1.038913825	20.311367480	H 14.088857144 -1.073711754 18.201546357
H	11.068556867	0.351786987	19.468542999	H 14.124446218 -1.549582155 19.900639366
H	9.911527115	1.436230735	20.260607993	H 16.793043864 6.153957847 19.622581907
H	11.010493480	0.449692871	21.232536663	H 16.101783826 4.550145067 19.964309815
C	11.907959758	3.398695923	18.642198833	H 15.120207353 6.004898914 20.163790766
H	11.254807927	2.766403538	18.033408960	H 17.507767523 5.712458517 17.365947671
H	11.366043130	4.332667001	18.818574118	H 16.478613255 4.914012382 16.171056595
C	14.169737082	5.339377356	18.250571604	H 17.049785563 4.015903954 17.583841820
C	13.062391070	6.386593136	18.499219376	H 11.594357933 5.549022926 15.355559901
H	13.542992680	7.337199108	18.761950667	H 12.804819241 6.494134316 16.221017448
H	12.419466418	6.112076552	19.340199470	H 11.534848910 5.651910230 17.114709963
H	12.430585221	6.570142670	17.628857822	H 13.412208601 4.202446782 14.170981637
C	12.897722749	3.754881846	15.812532788	H 14.698169259 3.425734154 15.102147747
C	15.327863893	-3.331491761	19.759474255	H 14.611446047 5.191133146 15.002548766
C	15.276748232	-2.531424166	17.369761288	H 11.546450720 3.125517537 15.334763524
C	13.462600224	-1.871609456	18.973529616	H 11.440023825 3.064890900 17.096526423
C	18.374151192	-2.002057617	19.536448004	H 12.690444748 2.138517007 16.263678744
C	18.464216429	0.473994400	19.819311062	N 15.104870698 1.199707710 16.673197766
C	18.116242310	-0.504051341	17.530611657	N 14.993012788 0.671985221 15.663218241
C	12.068806596	5.020714942	15.513919802	O 14.825930294 0.054824437 14.627334821
C	12.011584954	2.526888799	15.505114646	=====
C	14.128592072	3.696875959	14.883500141	F
C	14.914391742	5.120327355	19.584343501	=====
C	15.177866917	5.896139148	17.223428183	Ru 14.720127127 1.574178775 18.339548307
H	19.538404407	0.452644301	19.598405944	P 15.715289429 -0.514597551 19.330213388
H	18.356092679	0.354183539	20.901374626	P 13.352737928 3.550339438 17.752749776
H	18.083129193	1.454024416	19.531949679	Si 14.866087233 1.391694239 21.630471455
H	19.468879895	-1.933352329	19.502568798	Si 12.237723466 2.440680332 20.409993240
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			C 16.326847791 2.542797608 21.991040910	
			H 15.960230298 3.476690917 22.433374375	

H	18.087522651	-2.850980792	18.911165376	H	16.879714969	2.803020247	21.084679089
H	18.094451971	-2.219643784	20.572495402	H	17.028658813	2.096238438	22.706441945
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H	17.705430199	0.413260112	17.106153952	H	13.677133552	2.123806964	23.744047885
H	17.753824914	-1.343356307	16.932206923	H	14.625544210	0.662955495	24.008040448
H	14.689924668	-4.183229678	19.493394772	H	13.056446817	0.556303332	23.204725977
H	15.140442246	-3.106801295	20.813519645	C	15.467497898	-0.367438004	21.161147335
H	16.362871376	-3.657582678	19.662441308	H	16.341905266	-0.720077859	21.717665069
H	14.614544982	-3.353305024	17.070370568	H	14.636256473	-1.022966571	21.440851381
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H	13.120040365	-1.110434449	18.271075573	H	12.498804051	4.523495919	21.849563197
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H	15.262235828	6.095787902	19.948048412	H	10.804658263	4.044144041	21.686585470
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H	14.271600880	4.687865876	20.353039529	H	11.060510033	0.313430292	19.760892220
H	15.703039887	6.744920873	17.678617221	H	9.947484346	1.402006738	20.605454082
H	14.688761826	6.268598370	16.319780657	H	11.131707920	0.463303099	21.520416336
H	15.930444432	5.160801220	16.931301273	C	11.816901803	3.293204454	18.741848351
H	11.689922843	4.958043157	14.486018829	H	11.205544901	2.578749101	18.181715909
H	12.660416292	5.936375612	15.581872265	H	11.218448733	4.201560159	18.858629270
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H	13.780635123	3.589132123	13.848467393	C	12.891446889	6.270661831	18.646366319
H	14.786211643	2.856588799	15.118463015	H	13.338710025	7.240216507	18.899447378
H	14.732541860	4.603987242	14.930841299	H	12.293686063	5.960865927	19.507896397
H	11.790459734	2.526179074	14.431126906	H	12.217633448	6.433200189	17.803311247
H	11.051656450	2.557165545	16.029110233	C	12.761025305	3.683392143	15.920855870
H	12.510927608	1.583703245	15.738784443	C	14.946764608	-3.283750520	19.882052255
N	14.221046959	0.687304257	16.947397940	C	15.202419093	-2.661380972	17.470375092
N	16.522458331	2.584981668	18.252799523	C	13.287452707	-1.752272809	18.804418078
N	17.155761026	2.907942655	17.282892220	C	18.131623271	-2.102108640	19.640234125
O	17.030607324	2.685039930	16.054209278	C	18.318596728	0.375287041	19.896289477

A

Ru	14.688197595	1.583597324	18.243654107	C	11.830220685	4.879408698	15.643121610
P	15.998555967	-0.371610293	19.267338297	C	11.965573641	2.391040792	15.619373273
P	13.433141101	3.718609496	17.697487718	C	13.976694580	3.748529542	14.967142717
Si	14.689828000	1.309603376	21.588340983	C	14.841133875	5.075062912	19.642315941
Si	12.152119509	2.366712792	20.205111068	C	14.978676850	5.890207656	17.295930110
N	13.791607550	1.802136355	20.183325467	H	19.396458683	0.316578723	19.700134176
C	15.524603850	2.744877007	22.503424683	H	18.179328397	0.279575744	20.976432001
H	14.790674176	3.463937125	22.884776208	H	17.976691664	1.366312166	19.591436516
H	16.205389444	3.284176421	21.836929368	H	19.228842616	-2.097402764	19.612123918
H	16.105429344	2.382206037	23.361287217	H	17.798212874	-2.947935161	19.033936799
C	13.663649193	0.371785604	22.893404931	H	17.835193978	-2.282858145	20.678434809
H	12.887642675	1.004036453	23.338557736	H	19.076964670	-0.686668599	17.516362185
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H	13.169182951	-0.521049503	22.496263928	H	17.539662736	-1.370967099	16.990395624
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H	16.241663434	-0.706044358	21.703260387	H	15.976855792	-3.632775798	19.965365060
C	14.956563620	-1.991649410	19.251126183	H	14.534387813	-3.480906978	17.176669551
C	17.808550537	-0.736516444	18.688193258	H	16.220113621	-3.060405433	17.467302313
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				H	12.687518987	-2.639258769	18.563974078
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H	12.336735318	4.297757843	21.851184735	H	12.928647490	-1.356935760	19.759454185
H	11.716516267	2.849557470	22.646007997	H	15.156554819	6.062457619	20.004042970
H	10.658751541	3.797200166	21.604772758	H	15.734367370	4.470957899	19.477740820
C	10.857723627	0.979875498	20.121207813	H	14.262876148	4.593380910	20.430547302
H	11.002639898	0.354262607	19.233472631	H	15.465915235	6.765105370	17.744631459
H	9.840051663	1.388633987	20.080334937	H	14.452324684	6.241701115	16.405221150
H	10.913325760	0.325192286	20.998315900	H	15.765865801	5.197228063	16.989608116
C	11.865991242	3.426078025	18.621743633	H	11.441867220	4.804687227	14.618829940
H	11.223782192	2.828232163	17.968417066	H	12.348355426	5.838171304	15.720218400
H	11.325476811	4.353362789	18.833651512	H	10.968669554	4.896092581	16.318494667
C	14.103056759	5.406899549	18.349133504	H	13.642886461	3.555304530	13.940109846
C	12.989439182	6.470675456	18.468594370	H	14.745919910	3.016469135	15.218338503
H	13.449813506	7.405324144	18.811840120	H	14.452127985	4.729737935	14.972281151
H	12.237411721	6.196967834	19.213747514	H	11.792598586	2.319757054	14.538987105
H	12.480676639	6.684125483	17.528460012	H	10.985261663	2.391448142	16.104495750
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C	15.340968045	-2.967476412	20.383903136	N	14.916325494	0.813826877	16.457206588
C	15.084830956	-2.689621375	17.881404882	N	16.340596806	2.528296146	18.194347604
C	13.470180208	-1.622098856	19.444416446	O	16.848882793	2.853547058	17.149330401
C	18.371979161	-2.069855536	19.220375484	N	14.978712957	0.286461465	15.447940834
C	18.738203320	0.384192720	19.212456728	O	15.043979488	-0.297173510	14.389155285
C	17.846055221	-0.732505673	17.144445256	<hr/> <hr/> <hr/> <hr/>			
C	12.256207713	5.146227036	15.447344939	G			
C	12.041235412	2.666157798	15.473060949	Ru	15.454990457	2.178625749	18.594105129
C	14.272281980	3.690958964	14.992903563	P	16.609703469	0.186400873	19.426342651
C	14.691754625	5.189160845	19.758322061	P	14.207502861	4.179002242	17.929152859
C	15.227247032	5.939231020	17.436203698	Si	15.119349394	1.425576674	21.849597579
H	19.702382546	0.299465014	18.697022127	Si	13.101101301	3.327072061	20.699426623
H	18.936017758	0.272701935	20.283442024	N	14.504785416	2.316096146	20.482703186
H	18.346761779	1.388091089	19.042832715	C	16.240123817	2.459940348	22.982277832
H	19.431468996	-2.133385952	18.940990949	H	15.643178614	3.199924293	23.526581456
H	17.875921047	-2.946717782	18.798854144	H	17.003491589	3.005190652	22.420203039
H	18.323445128	-2.130914674	20.312321743	H	16.747566093	1.837504632	23.730215845
H	18.876257404	-0.916212979	16.814562114	C	13.784210488	0.670367749	22.982710920
H	17.532382651	0.229202119	16.734108089	H	13.183873673	1.420513960	23.506980439
H	17.218829326	-1.512016253	16.706320645	H	14.260388576	0.046530252	23.749934098
H	14.722077912	-3.868622428	20.291647095	H	13.096121410	0.029873214	22.419197217
H	15.139213867	-2.542631121	21.371455609	C	16.056847803	-0.093825595	21.169168227
H	16.383589959	-3.283595488	20.353871136	H	16.878415526	-0.428049078	21.811385920
H	14.361355771	-3.513113962	17.836429760	H	15.323673831	-0.906815443	21.154758260
H	16.074992006	-3.119148518	17.713089126	C	16.106180614	-1.439289658	18.521915139
H	14.855316627	-2.006359409	17.057811598	C	18.521984891	0.350280283	19.541397155
H	12.888827152	-2.550811200	19.508785297	C	13.059004658	4.292470918	22.343627035
H	13.085253789	-1.037943516	18.607876260	H	13.968216851	4.889350539	22.479481739
H	13.294171475	-1.054804734	20.358923493	H	12.950444792	3.650141199	23.223163531
H	15.033242575	6.160077328	20.139819928	H	12.207815778	4.985245745	22.344286900
H	15.538192410	4.503901736	19.735122975	C	11.459030518	2.376831557	20.605920761
H	13.951738590	4.801199319	20.460461004	H	11.403780833	1.736485825	19.720874604
H	15.674251709	6.818945861	17.915330786	H	10.597961792	3.056870793	20.588116732
H	14.860635405	6.258374786	16.457204187	H	11.346332876	1.732180432	21.484386477
H	16.024777505	5.207630799	17.288233552	C	13.166312859	4.695057379	19.368316680
H	11.943443800	5.081708857	14.397574821	H	12.179110238	5.049224633	19.053937992
H	12.896197968	6.026540750	15.537784045	H	13.663017610	5.545243585	19.846973313
H	11.353692541	5.306864397	16.045953851	C	15.318296733	5.717431760	17.592331893
H	14.008415429	3.696618949	13.928024600	C	14.569379101	7.065081079	17.646059503

H	14.980827081	4.503825558	15.159989342	H	15.299217968	7.879465289	17.552874984
H	11.924577169	2.635439816	14.383066085	H	14.041617370	7.213742771	18.592175218
H	11.041702809	2.791488069	15.900208374	H	13.848007818	7.181081897	16.835745270
H	12.438904144	1.697790736	15.786878858	C	12.952616305	3.905987384	16.498417556
N	14.041142132	0.664671214	17.046727772	C	16.417069267	-2.726294708	19.313216386
N	16.563763697	2.572719312	17.665586952	C	16.764835786	-1.527522140	17.131588110
O	16.631496182	2.805293305	18.960012731	C	14.575426340	-1.342896807	18.329329728
N	17.185869402	2.792631553	16.701158470	C	19.236194944	-0.946185206	19.969050443

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Ru	14.932166158	1.536291194	17.958084457	C	18.803307342	1.445258494	20.592583182
P	16.344531598	-0.262137730	18.992038402	C	19.104670527	0.838607934	18.199484074
P	13.879568622	3.739941350	17.490831286	C	12.229910843	5.189834943	16.047820408
Si	14.602567309	0.991552849	21.302366192	C	11.905926230	2.900563602	17.025580423
Si	12.346108994	2.394959725	19.817660708	C	13.648940491	3.256385865	15.284895815
N	13.893728311	1.622808051	19.863347227	C	16.383901064	5.705248206	18.712164097
C	15.277585813	2.329445270	22.479872152	C	16.038832608	5.592609543	16.235717125
H	14.479180305	2.968127005	22.873485172	H	19.877771318	1.668364001	20.596500754
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H	15.792741203	1.884225182	23.340974125	H	18.267120647	2.369651092	20.356091529
C	13.471854108	-0.118213656	22.361870309	H	20.289526574	-0.723466825	20.183058053
H	12.693813588	0.461998757	22.869036093	H	19.221454195	-1.702793942	19.180181707
H	14.051261566	-0.626684288	23.143117810	H	18.805886135	-1.384900244	20.875030693
H	12.969791851	-0.886667366	21.764629095	H	20.188300007	0.972097659	18.311275578
C	16.143173577	-0.043206210	20.818276340	H	18.676666493	1.799552811	17.906864417
H	17.013642416	0.520689871	21.169389390	H	18.944827610	0.133754496	17.381457781
H	16.174771234	-1.006577996	21.338924116	H	15.997957284	-3.584465217	18.772497242
C	15.756147437	-2.060724896	18.643623426	H	15.966909126	-2.723581387	20.309846138
C	18.258176139	-0.120405179	18.753400800	H	17.487314005	-2.905176448	19.427323609
C	11.660145950	2.993757837	21.492407609	H	16.312363618	-2.356486592	16.572701042
H	12.357889443	3.649380984	22.024656263	H	17.837294451	-1.732387322	17.195905036
H	11.400316993	2.167195570	22.161718058	H	16.621247910	-0.616482997	16.544808393
H	10.739444499	3.566359129	21.321793722	H	14.219820885	-2.242439315	17.810402425
C	10.978009014	1.323306782	19.062575891	H	14.304473838	-0.463915648	17.738468699
H	11.306604429	0.829848390	18.144560560	H	14.039916220	-1.279377717	19.282392757
H	10.070158473	1.899660604	18.845294040	H	17.062420961	6.556924847	18.573880087
H	10.702235365	0.536967833	19.776214173	H	16.968562364	4.781514061	18.693858823
C	12.620668848	4.009388357	18.819527270	H	15.939811850	5.796741386	19.708978222
H	11.710507680	4.471921700	18.425434814	H	16.797105041	6.382173258	16.158592949
H	13.040162066	4.713741129	19.545377442	H	15.354353996	5.721786716	15.392411324
C	15.137884175	5.185648830	17.725724121	H	16.549316388	4.632613371	16.122495013
C	14.481672968	6.548588921	18.028831586	H	11.416099024	4.923178667	15.361197269
H	15.272455956	7.281355408	18.234031370	H	12.896213525	5.868581716	15.508880434
H	13.836936764	6.516959031	18.911088171	H	11.783422252	5.737445120	16.883993836
H	13.892814572	6.930554087	17.194108396	H	12.900722798	3.071076597	14.503628440
C	12.906956044	3.942591805	15.841541894	H	14.100154176	2.298327135	15.551032097
C	16.608271493	-3.140424171	19.339032805	H	14.426343506	3.887692392	14.850091555
C	15.737744245	-2.339664867	17.125549250	H	11.238790082	2.615249027	16.202390171
C	14.310593096	-2.158117268	19.178938552	H	11.284451515	3.320179834	17.820760650
C	19.071428105	-0.848633094	19.845640934	H	12.383959919	1.991322970	17.403546671
C	18.596310379	1.385480007	18.842159171	N	16.240862935	2.071507107	17.043562923
C	18.704318939	-0.648114237	17.374944068	O	16.778882208	2.001630246	15.985402016

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Ru	15.152875484	1.961188166	18.481219694
P	16.583845131	0.157479588	19.373908739
P	14.151101523	4.175920642	17.950076872

C	16.003369909	4.786334856	18.942034268	Si	15.224673444	1.568154475	21.807691864
C	16.060435880	5.333800110	16.499955694	Si	12.892418959	3.061995516	20.506481130
H	19.683901753	1.513516650	18.773523107	N	14.433232610	2.243391893	20.405841212
H	18.276800041	1.827458465	19.792158043	C	16.038581328	2.905664682	22.884619480
H	18.140660577	1.957539962	18.032170448	H	15.301000512	3.580383796	23.331601251
H	20.139027258	-0.670928240	19.663387987	H	16.732068989	3.517885154	22.296695350
H	18.916313304	-1.928046285	19.841308962	H	16.607153970	2.452630850	23.706738190
H	18.850346102	-0.479603342	20.850443801	C	14.102580103	0.553343273	22.965939373
H	19.750000624	-0.362734999	17.202913937	H	13.458852909	1.198825012	23.572378964
H	18.114108840	-0.237806583	16.553065725	H	14.707995076	-0.038042236	23.664389387
H	18.657449436	-1.739103694	17.321835581	H	13.453568426	-0.138898351	22.420457324
H	16.105407689	-4.110199137	19.232777249	C	16.655547177	0.453818081	21.201440424
H	16.734708730	-2.957870835	20.410830061	H	17.582490901	1.000799687	21.403343370
H	17.597991393	-3.241455549	18.886232072	H	16.722768984	-0.483447650	21.764144753
H	15.302517506	-3.332945948	16.956898891	C	15.887660764	-1.631070241	19.203531106
H	16.738100920	-2.347681309	16.688543067	C	18.432514767	0.235167607	18.826758631
H	15.132238717	-1.617696648	16.577871489	C	12.455087791	3.779250483	22.214385716
H	13.891809077	-3.129011834	18.886329478	H	13.215825891	4.476067233	22.582247620
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H	14.276199956	-2.103157982	20.270301149	H	11.513889018	4.337776614	22.132713820
H	16.724201487	5.586831479	19.152677966	C	11.464248827	1.922252029	20.005353274
H	16.564137099	3.866175785	18.749942287	H	11.638114867	1.474943173	19.021387475
H	15.405921993	4.627531455	19.844993119	H	10.502525498	2.449692912	19.978864410
H	16.857395969	6.050039143	16.737191274	H	11.368151512	1.100565254	20.725300143
H	15.530851603	5.721072925	15.625271573	C	12.958376374	4.554300411	19.319531530
H	16.539041293	4.391878010	16.222158310	H	11.966820662	4.767108936	18.911250726
H	11.791950008	5.402491236	14.703796735	H	13.269583733	5.448953481	19.867668153
H	13.298530835	6.053463591	15.344654050	C	15.514346249	5.530692785	18.067861135
H	11.902206868	5.819450684	16.415658030	C	15.013390780	6.962920563	17.808319812
H	13.182748496	3.557992484	13.731288147	H	15.808206134	7.674890994	18.065702911
H	14.001215875	2.378758036	14.761160688	H	14.138658946	7.217715281	18.415473120
H	14.689842092	3.996072738	14.536316689	H	14.764252676	7.127580967	16.757205531
H	11.129415186	3.095773293	14.955831809	C	13.081786815	4.393187851	16.357526665
H	10.931668528	3.415363919	16.679090447	C	16.816706215	-2.711365951	19.790605620
H	11.872453239	2.016988930	16.137230986	C	15.584031657	-1.971982803	17.730504069
N	13.691164355	0.483481507	17.003583361	C	14.550401290	-1.650079576	19.974526109
N	16.124367085	1.699679388	16.413008587	C	19.399560255	-0.484812640	19.789294929
O	13.762692724	0.183051359	15.840674727	C	18.799089337	1.736249539	18.801432903
N	16.832611784	1.817736223	15.545708215	C	18.621389604	-0.327556635	17.404871341
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Ru	14.876422807	1.750035824	18.391416653	C	12.103291506	3.197293635	16.326186097
P	15.841280183	-0.452605291	19.092072010	C	13.961167365	4.353880921	15.091373376
P	13.352062141	3.621158162	17.642704962	C	16.088857900	5.460957170	19.500829564
Si	14.558660835	0.883003267	21.557554567	C	16.655955015	5.191776969	17.087091354
Si	12.435485642	2.735929456	20.510655392	H	19.851988776	1.845258940	18.511370345
N	13.799871878	1.697431777	20.220046933	H	18.678500015	2.212648785	19.780523855
C	15.881429616	1.878852103	22.484663091	H	18.186160931	2.282781688	18.080595074
H	15.413120527	2.717604564	23.013221284	H	20.428585828	-0.308587263	19.451018868
H	16.641763803	2.301714881	21.824973260	H	19.246632537	-1.564755558	19.813895352
H	16.382247869	1.256641366	23.237875984	H	19.329080872	-0.109807730	20.814088240
C	13.350778894	0.294237901	22.908565565	H	19.642620744	-0.109777542	17.067328434
H	12.867958233	1.120816878	23.441060372	H	17.937497744	0.128661140	16.685189293
H	13.905217294	-0.286544417	23.656735816	H	18.496577143	-1.413338630	17.369843407
H	12.562462651	-0.350788441	22.506047883	H	16.277456824	-3.666950970	19.821362882
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C	15.304701785	-0.721755432	20.841645957	H	15.161467922	-2.983998637	17.685756869
H	16.105104527	-1.152751457	21.450844354	H	16.473607011	-1.962967748	17.097594331
H	14.485679487	-1.447430644	20.841269349	H	14.850751177	-1.287034827	17.299857732
C	15.045498327	-1.951368591	18.158234186	H	14.046563740	-2.606591019	19.787790330
C	17.760882816	-0.640540756	19.123637374	H	13.883915016	-0.846815546	19.647071265
C	12.707093920	4.010970347	21.896949778	H	14.694457015	-1.563158049	21.054350455
H	13.613806683	4.601013147	21.730731130	H	16.951818780	6.135163784	19.567983544
H	12.806783612	3.526462666	22.875043243	H	16.423941435	4.451509582	19.753570995
H	11.859514878	4.704674488	21.966881087	H	15.368078257	5.775807654	20.261101257
C	10.837875584	1.792471175	20.937509233	H	17.489702052	5.885964096	17.250981475
H	10.625644511	1.027901576	20.180268253	H	16.354681110	5.282582141	16.041586381
H	9.982078230	2.479400900	20.965143418	H	17.024412368	4.174254281	17.241869733
H	10.886088692	1.290361100	21.908131789	H	11.620001793	5.679224677	15.429749715
C	11.995038014	3.662864647	18.898638465	H	12.853141655	6.591181093	16.296945643
H	11.143843573	3.123182021	18.471274937	H	11.564345873	5.771869979	17.186811677
H	11.645802947	4.683913300	19.085939765	H	13.313438448	4.277805870	14.209120106
C	14.060829558	5.412674425	17.598685955	H	14.639653597	3.499825012	15.077301351
C	13.122238585	6.462317230	16.973778398	H	14.553917016	5.265575975	14.976209974
H	13.558340128	7.457623825	17.130356702	H	11.470364089	3.283322442	15.434158480
H	12.131994618	6.467297699	17.440559854	H	11.439473214	3.186621848	17.196691178
H	12.998389981	6.332742318	15.895778936	H	12.620138696	2.236571206	16.281634313
C	12.369165147	3.285001096	16.002061969	N	14.540662655	1.014935963	16.971865437
C	15.120783754	-3.285220300	18.931659188	N	15.564107914	1.418944023	16.357829330
C	15.666655664	-2.163992020	16.762956255	N	15.723858994	0.997247456	15.011332791
C	13.554364217	-1.583654498	17.985754197	O	16.738190109	1.421485771	14.506581578

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Ru	15.140698282	1.929541308	18.445066469
P	16.778513404	0.368552651	19.431092267
P	14.382228348	4.276747332	18.054466089
Si	15.217343961	1.661601248	21.826984963
Si	12.866723665	3.060481637	20.426146861
N	14.391932398	2.222055277	20.410000636
C	15.888596663	3.056973202	22.933770577
H	15.088228950	3.671388025	23.359200519
H	16.558470006	3.723501491	22.379193457
H	16.457459574	2.639408844	23.774574490
C	14.190272599	0.551946470	22.983567223
H	13.481259144	1.152164749	23.564300791
H	14.834071798	0.034302408	23.705635402
H	13.613770490	-0.204733247	22.443551949
C	16.787779986	0.726728998	21.243655199
H	17.626868320	1.406120575	21.427820913
H	16.987552181	-0.175536386	21.830889417
C	16.221879797	-1.470232201	19.301130361
C	18.619447929	0.569746595	18.886596831
C	12.257389003	3.644128591	22.131956424
H	12.980346949	4.281394584	22.650568633
H	12.014818941	2.805446305	22.792294556
H	11.336663061	4.227747017	22.007214445
C	11.463401423	2.031469373	19.689529324
H	11.766362509	1.542086675	18.760195205
H	10.564906648	2.629932959	19.496875731
H	11.184313405	1.243992228	20.400132883
C	13.195435220	4.659139127	19.423095059

H	16.124092826	4.726802364	17.281282252	H	12.295118724	5.148776261	19.041864382
H	10.536341952	3.777986998	14.971811706	H	13.666392589	5.362170896	20.117833023
H	11.249390205	5.177932869	15.768443539	C	15.806961529	5.555887306	18.262043562
H	10.391267832	3.960465457	16.718019881	C	15.331233299	7.010843841	18.447279847
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H	14.188007523	3.011824342	14.782285635	H	14.613262923	7.115113000	19.267253146
H	13.443634633	4.607209433	14.608113561	H	14.880377503	7.428457076	17.545866910
H	11.357018112	1.570545874	15.142418762	C	13.363573388	4.599646947	16.449546366
H	11.366420211	1.538385133	16.906977063	C	17.230257922	-2.441794452	19.945668288
H	12.834987987	1.132970777	16.005512301	C	15.982510503	-1.890727971	17.837649368
N	15.232555142	1.105886168	16.234756102	C	14.879031528	-1.578937865	20.052238593
N	16.486465558	2.680879437	18.876316300	C	19.618027831	-0.002915435	19.913510785
N	16.108552699	1.822108389	16.279377850	C	18.867698011	2.087276593	18.763957896
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Ru	14.618724663	1.751249698	18.939366148	C	14.145199123	4.191840867	15.184759398
P	15.487854035	-0.425505634	19.898587147	C	16.563710693	5.140490390	19.542291688
P	13.093199620	3.619433658	18.292273447	C	16.773809207	5.469824247	17.064907528
Si	14.521225511	1.371284311	22.228403170	H	19.915716422	2.258311331	18.483931262
Si	11.973380209	2.519354252	20.979442274	H	18.696904256	2.612334144	19.709805166
N	13.592947170	1.918240789	20.871790321	H	18.229119429	2.528457373	17.996512913
C	15.938347302	2.542469802	22.688647200	H	20.636821135	0.210816919	19.565460001
H	15.532699663	3.481837461	23.083051933	H	19.534586054	-1.083697613	20.031737959
H	16.564346668	2.793910355	21.827503976	H	19.512376676	0.454754710	20.900444313
H	16.584043551	2.114312094	23.465565289	H	19.879011328	0.217941248	17.167981396
C	13.554439176	1.063519184	23.840244270	H	18.159361124	0.276048984	16.761917369
H	13.219346278	1.991784429	24.314042829	H	18.853424088	-1.161239245	17.549647568
H	14.203771547	0.552733199	24.562642645	H	16.773494725	-3.437917901	19.995069938
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C	15.195485748	-0.345428576	21.723486061	H	18.146040392	-2.537148276	19.357447884
H	16.083978539	-0.657476456	22.281141026	H	15.648786947	-2.936147682	17.830492234
H	14.403245482	-1.056055506	21.976699687	H	16.880903039	-1.831784998	17.221658896
C	14.511094559	-1.985514463	19.321233224	H	15.201778699	-1.294837826	17.365213033
C	17.386757118	-0.669509890	19.715045908	H	14.472581249	-2.585765815	19.898922883
C	11.638020073	3.791818310	22.355547687	H	14.147305328	-0.857813985	19.679740543
H	12.349495696	4.624880081	22.345183824	H	14.997290873	-1.435823585	21.128750427
H	11.678223005	3.337577182	23.350679729	H	17.401041757	5.831623247	19.700255628
H	10.632532669	4.214843306	22.237124277	H	16.966638900	4.128638006	19.459241133
C	10.664409906	1.156197808	21.184549611	H	15.929600561	5.177988254	20.432924467
H	10.735982183	0.416358138	20.379229701	H	17.701847149	6.001055566	17.310378782
H	9.649596309	1.573606760	21.165064724	H	16.358481876	5.944799390	16.171773488
H	10.777684692	0.621132394	22.134223942	H	17.028805461	4.435380424	16.816490144
C	11.578375389	3.365231315	19.306173115	H	12.177524520	6.145433720	15.517761927
H	10.952431512	2.663538076	18.747027573	H	13.762010004	6.720740933	16.022760124
H	10.997307021	4.285102886	19.419729598	H	12.480252218	6.477840423	17.223982633
C	13.820895610	5.321344047	18.834417813	H	13.533828858	4.438744451	14.307493058
C	12.715244280	6.324842118	19.221598575	H	14.346468806	3.122610556	15.153686887
H	13.183091041	7.290113213	19.451757097	H	15.092931458	4.721210484	15.077827084
H	12.169652563	6.009777914	20.115282613	H	11.542600644	3.825183053	15.590809928
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C	12.439185785	3.689747570	16.477823040	H	12.337429426	2.664682953	16.664157919
C	14.627524969	-3.170780631	20.303593943	N	14.083542195	0.956070593	17.334118312
C	14.956695046	-2.459248386	17.923611889	N	14.453186842	0.681320839	16.069195972
C	13.031284166	-1.550214506	19.244302215	N	15.605427878	1.146376581	15.718366244
O	16.200015853	1.837589329	16.653977305	O	16.200015853	1.837589329	16.653977305

C	17.871785307	-1.986762378	20.354534899
C	18.061101589	0.519776646	20.432788066
C	17.822423898	-0.639395695	18.236425170
C	11.428835076	4.838537537	16.281859523
C	11.721807955	2.346271891	16.203047407
C	13.578765179	3.835897563	15.446868652
C	14.726967073	5.090223279	20.062537389
C	14.699107765	5.925061338	17.720348599
H	19.147162807	0.436742844	20.302482907
H	17.861346470	0.534374430	21.507644424
H	17.747657146	1.475674196	20.004322873
H	18.969019235	-1.993920309	20.358282764
H	17.547167042	-2.861858164	19.785907636
H	17.541785721	-2.105742149	21.391197409
H	18.915505374	-0.730512480	18.197808097
H	17.550548198	0.294594435	17.744329521
H	17.408202167	-1.465079489	17.655971350
H	14.041938608	-4.007130930	19.901981627
H	14.222993079	-2.945561525	21.293800994
H	15.652871641	-3.522454397	20.428818288
H	14.254738442	-3.228763526	17.578057823
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H	14.947787439	-1.648749245	17.193222742
H	12.416715419	-2.425622120	18.998553700
H	12.885157694	-0.797734336	18.466497316
H	12.667284544	-1.146025521	20.193885978
H	15.075790929	6.065802057	20.425267982
H	15.601638248	4.489238421	19.803471445
H	14.210312196	4.586438328	20.880462590
H	15.258970309	6.770750460	18.138475287
H	14.108550099	6.310847008	16.885711028
H	15.428713952	5.206307228	17.336466605
H	10.983103669	4.750238277	15.282950677
H	11.901052458	5.823411791	16.337222702
H	10.610346432	4.804797852	17.007753631
H	13.157356352	3.693885149	14.444018738
H	14.365944845	3.095927261	15.581504186
H	14.035529929	4.825438160	15.463100712
H	11.425293065	2.326296370	15.147422921
H	10.806647799	2.229729717	16.790861930
H	12.373546855	1.488017761	16.383809077
N	14.452122799	0.763737680	17.171455483
N	15.325099617	0.995083636	16.323762894
O	16.282614706	1.888472576	16.638424024
N	16.034850901	2.399213706	18.174716583
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Ru	14.847164467	1.644853857	18.350672994
P	15.872352090	-0.496889823	19.290155465
P	13.436348461	3.620371518	17.684877579
Si	14.849702329	1.313001898	21.617233982
Si	12.241016906	2.388471664	20.308696901
N	13.882055851	1.846580481	20.286392782
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H	15.819454642	3.451776406	22.467026062
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P	13.424743502	3.674424389	17.706389105
Si	14.871910495	1.365945587	21.563379766
Si	12.222575053	2.359639691	20.273026797
N	13.872450890	1.841536320	20.236358647
C	16.266137124	2.588734694	21.965555904
H	15.854006396	3.528288470	22.351182327
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H	16.930986943	2.182771511	22.738578856
C	13.955697939	1.066882612	23.204131896
H	13.609159706	2.000043998	23.659735121
H	14.631259499	0.588722411	23.924602062
H	13.087053150	0.409650093	23.083421146
C	15.623542298	-0.327436600	21.088597784
H	16.543192668	-0.564897938	21.633416850
H	14.878041962	-1.060838742	21.409727391
C	15.046895857	-2.265341423	18.921481126
C	17.764923023	-0.645016462	19.013062769
C	11.728205732	3.453720755	21.749304269
H	12.391053051	4.315159403	21.885550668
H	11.717816752	2.891896576	22.688405032
H	10.712930907	3.840352908	21.595226248
C	10.990669616	0.917334307	20.228977342
H	11.170872381	0.278823863	19.356878613
H	9.952178008	1.268109268	20.179794950
H	11.082447673	0.288530127	21.122454968
C	11.887129011	3.378356638	18.672167545
H	11.253414910	2.748035041	18.041011064
H	11.327004532	4.298529300	18.865338986
C	14.173522669	5.322100928	18.376142045
C	13.092288060	6.393512718	18.633992171
H	13.587308163	7.311041565	18.975621807
H	12.400381342	6.091126078	19.425041069
H	12.509935595	6.646832150	17.747576091
C	12.902609342	3.887457775	15.861941779
C	15.330605406	-3.303691337	20.030172994
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C	13.524469484	-2.012882662	18.879350474
C	18.397335381	-1.908519182	19.630744056
C	18.406031041	0.577669796	19.706868998
C	18.094670439	-0.591399638	17.505479473
C	12.231088500	5.243314205	15.562706337
C	11.881208543	2.784344696	15.502445070
C	14.148991843	3.700494421	14.968664408
C	14.879208794	5.038704084	19.718215981
C	15.237831344	5.878076795	17.405125364
H	19.482023890	0.574523081	19.493666499
H	18.290749441	0.544700624	20.793750090
H	18.002750585	1.526188559	19.350204464
H	19.489395823	-1.823009720	19.563853291
H	18.112649306	-2.821658657	19.104009171
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H	16.842959608	2.794058428	21.187849096	H	19.184642817	-0.560832274	17.381697456
H	16.912099777	2.107890056	22.820517070	H	17.681860223	0.296210106	17.023221037
C	13.893966295	0.981333923	23.228884351	H	17.728372089	-1.467884960	16.968134248
H	13.528832913	1.904803525	23.689968122	H	14.834841947	-4.241297176	19.749785574
H	14.554525155	0.497012343	23.958986901	H	14.928088596	-3.010276208	21.002858530
H	13.033750679	0.320007367	23.075865492	H	16.391735420	-3.522176158	20.154806537
C	15.628053752	-0.372378025	21.124330830	H	14.876939586	-3.718534453	17.333891343
H	16.558094638	-0.580370387	21.663051897	H	16.540446696	-3.212283846	17.615624463
H	14.915313128	-1.145494390	21.428434297	H	15.407140073	-2.141408902	16.754505355
C	14.932163232	-2.107613617	18.810183228	H	13.007794220	-2.973701245	18.762017072
C	17.766471421	-0.684797998	19.020515910	H	13.248440729	-1.373056086	18.040024928
C	11.779472482	3.554028501	21.742781712	H	13.157879935	-1.552660318	19.802973886
H	12.460431922	4.405807089	21.843404528	H	15.267230442	5.986942556	20.112362845
H	11.769572483	3.026149647	22.701962976	H	15.719004732	4.353108623	19.598993529
H	10.769900901	3.954793644	21.587580578	H	14.206330824	4.614135372	20.463945080
C	10.973501754	0.974375650	20.360086289	H	15.730802613	6.733650163	17.883328520
H	11.120941813	0.281551009	19.524386710	H	14.813930797	6.235839853	16.464651671
H	9.944906489	1.352938318	20.305218876	H	16.013147212	5.142380416	17.177002438
H	11.059313215	0.395300191	21.286979186	H	11.881741238	5.233805220	14.522493877
C	11.899748736	3.321284230	18.658233404	H	12.907959201	6.093897087	15.665358317
H	11.290308144	2.640609951	18.056064152	H	11.354582160	5.416643414	16.195584122
H	11.307029845	4.229929582	18.802682832	H	13.846351532	3.777626691	13.917032413
C	14.095922644	5.335187519	18.264683193	H	14.597473020	2.716087800	15.118914571
C	12.970835523	6.377746768	18.439668804	H	14.915546748	4.458007124	15.144390311
H	13.424171392	7.332933345	18.732572784	H	11.699867718	2.827277297	14.421678425
H	12.275371453	6.098180405	19.235884876	H	10.916614249	2.939096105	15.995679246
H	12.396552476	6.554061877	17.529213821	H	12.250159435	1.784333742	15.735905398
C	12.920029234	3.693195907	15.831501411	N	14.040055013	0.860451426	16.830672811
C	15.264197715	-3.313100235	19.714946039	N	16.366480897	2.447354010	17.905207745
C	15.207386884	-2.474589821	17.338889938	O	17.073568796	2.710125968	16.978083002
C	13.426171765	-1.797435788	18.967812789	N	13.930851397	-0.643678379	15.764545883
C	18.344264141	-2.020468933	19.527838050	O	13.154792774	-0.505211966	14.875804335
C	18.461674774	0.456383100	19.797368005	=====	=====	=====	=====
C	18.090388794	-0.524636337	17.519006755	TS1	=====	=====	=====
C	12.173553778	4.982533399	15.437503028	Ru	15.338130253	2.089690422	18.485633013
C	11.979423038	2.499796693	15.545168943	P	16.727673475	0.277468237	19.408874464
C	14.186140380	3.520334187	14.964034560	P	14.251190198	4.268288376	17.961043619
C	14.783570105	5.153233466	19.635228010	Si	15.240821555	1.600276676	21.819433147
C	15.153929087	5.876462170	17.279262420	Si	12.887221982	3.016527804	20.433030935
H	19.531830333	0.439960128	19.557420279	N	14.463422071	2.276531286	20.418714078
H	18.370432383	0.337204829	20.880636739	C	15.918546787	2.942885604	22.981216969
H	18.079884957	1.442512180	19.528805165	H	15.115403946	3.533516646	23.434761789
H	19.440097578	-1.965822649	19.499146808	H	16.571831874	3.635208220	22.437572065
H	18.048549392	-2.863954793	18.899729044	H	16.502818228	2.501774840	23.798745934
H	18.055388256	-2.237916116	20.561142520	C	14.173434520	0.455202425	22.903708193
H	19.179394099	-0.555059211	17.386741084	H	13.365223868	1.009137866	23.393431668
H	17.733554353	0.425692685	17.119149839	H	14.785113833	0.011607820	23.699619009
H	17.665730367	-1.327754709	16.913616466	H	13.712985229	-0.365898749	22.345380158
H	14.599758859	-4.142649885	19.442699970	C	16.778817696	0.615076249	21.224891414
H	15.096722968	-3.103637695	20.775425152	H	17.640400084	1.265304901	21.405156306
H	16.288551772	-3.666564637	19.598176547	H	16.944931744	-0.291703274	21.813365618
H	14.525768763	-3.280775986	17.039476604	C	15.971589392	-1.486326538	19.242399798
H	16.226182572	-2.843848170	17.190743807	C	18.552786540	0.308353765	18.804067071
H	15.033582288	-1.622868092	16.676065208	C	12.314103499	3.671520890	22.125788548
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H	13.166818342	-1.494577243	19.986834689	H	12.159710161	2.873966003	22.860005768
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H	15.652305787	4.496568450	19.573039771	C	11.534149023	1.845781736	19.816015174
H	14.109412048	4.743105183	20.388296584	H	11.805147939	1.378694374	18.864955579
H	15.607405116	6.776045255	17.713828956	H	10.570910425	2.355541284	19.689167116
H	14.728184635	6.164699817	16.315306636	H	11.384052318	1.039258834	20.544134283
H	15.958863462	5.158695329	17.102277726	C	13.023602991	4.569517067	19.318091877
H	11.831655700	4.886219034	14.398999945	H	12.060197364	4.896654500	18.915080432
H	12.802567984	5.874236905	15.487437532	H	13.387906243	5.382495635	19.954815740
H	11.285458931	5.148335839	16.056167504	C	15.489802193	5.733618618	18.088728430
H	13.894590583	3.508597559	13.906306999	C	14.828085183	7.120835253	18.201261639
H	14.687091150	2.575934912	15.189289277	H	15.605185430	7.870613852	18.396213817
H	14.905504254	4.331157662	15.095860210	H	14.112145586	7.176474415	19.026658697
H	11.821761493	2.439733182	14.461123493	H	14.312274329	7.417785280	17.287109425
H	10.995250599	2.630043852	16.005664394	C	13.212100378	4.347099371	16.343273105
H	12.411720717	1.552948397	15.877068494	C	16.473704588	-2.467647490	20.322287318
N	14.207280773	0.724937683	17.021320702	C	16.252870508	-2.077863753	17.846213254
N	16.440223959	2.571803856	18.113481908	C	14.442622044	-1.337627017	19.396244851
O	17.264771731	2.829361562	17.281528486	C	19.414841136	-0.813983699	19.411503041

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Ru	15.100812087	1.959552322	18.521069787	C	19.139784435	1.674593016	19.223087989
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P	14.098242884	4.097988780	17.940895343	C	12.567839144	5.727218569	16.102621941
Si	15.356624107	1.694121075	21.878229578	C	12.086207834	3.299644790	16.493919461
Si	13.100518461	3.368438725	20.756599692	C	14.060950881	3.964683148	15.114018680
N	14.538759167	2.419953028	20.533539873	C	16.308380851	5.479099383	19.374409284
C	16.566132395	2.863775485	22.766741503	C	16.457931891	5.712404546	16.890273944
H	16.009391695	3.655019703	23.281961669	H	20.127886577	1.791362367	18.762233417
H	17.262739381	3.352054163	22.078589665	H	19.275967520	1.764572484	20.304841598
H	17.156809619	2.334965273	23.525559377	H	18.507220709	2.500297316	18.881452048
C	14.208393121	1.015068760	23.242171965	H	20.464982982	-0.657887029	19.132579229
H	13.638011643	1.794076971	23.757804326	H	19.127528982	-1.802070007	19.042540608
H	14.800674969	0.493316172	24.004757918	H	19.365094271	-0.826254393	20.505543415
H	13.489673559	0.294802560	22.834522010	H	19.640740417	0.396815107	16.936456139
C	16.275105904	0.139923131	21.243397330	H	17.986068442	1.026517039	16.812608951
H	17.219849687	-0.058828287	21.761150985	H	18.274601500	-0.715258363	16.864957874
H	15.611039485	-0.696420006	21.485960718	H	16.041466790	-3.456131323	20.122625380
C	16.086137720	-1.669437138	18.902047371	H	16.150588368	-2.178043771	21.326207370
C	18.342906656	0.535042098	19.124733174	H	17.559768263	-2.582085349	20.331251068
C	13.087505541	4.468815770	22.313430980	H	15.639748425	-2.978919941	17.719762222
H	13.947624109	5.147493186	22.334080466	H	17.296743660	-2.379854184	17.723746809
H	13.099391751	3.894515087	23.245169642	H	15.987023123	-1.386038665	17.042671139
H	12.180031922	5.085304542	22.328071839	H	13.987509224	-2.335855487	19.356708237
C	11.523581461	2.309026218	20.804015776	H	14.009001366	-0.734040187	18.597308557
H	11.426276491	1.726316662	19.880165999	H	14.164938795	-0.886051011	20.350574545
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H	11.543757563	1.597554066	21.636785114	H	16.846379378	4.528147578	19.319741491
C	12.890431465	4.554730814	19.266729553	H	15.683638946	5.457995562	20.272655283
H	11.879233544	4.418498961	18.870427028	H	17.295788568	6.392482207	17.088295332
H	12.973976190	5.608782486	19.551985400	H	15.978915252	6.049473322	15.967167388
C	15.465548779	5.451492480	18.059126799	H	16.869106199	4.711910152	16.721915427
C	15.035115892	6.856022878	17.599630202	H	11.835921087	5.637810180	15.289976652
H	15.827273439	7.574906670	17.847169974	H	13.300877699	6.475961436	15.792356745
H	14.122959094	7.194083049	18.101786931	H	12.035260049	6.107662095	16.979950562
H	14.843934807	4.695149271	14.899896402	H	13.403958121	3.924150487	14.235820099
H	14.523171293	2.982358638	15.227208777	H	14.843934807	4.695149271	14.899896402

H	14.875074165	6.912283316	16.519717722	H	11.519902312	3.258946921	15.555149946
C	13.085173692	4.305963371	16.314429955	H	11.378607284	3.555868447	17.287369926
C	16.647343127	-2.725378665	19.877313687	H	12.474611201	2.297596832	16.686369076
C	16.590066437	-1.998730543	17.483178375	N	15.338988965	1.484420086	16.923914179
C	14.543879636	-1.768248050	18.913018446	N	14.352969659	0.383492441	15.836268734
C	19.302199226	-0.567253688	19.610240328	O	13.361281892	0.048822866	16.409223910