

Long Distance Unconjugated Agostic-Assisted 1,5-H Shift in a Ru-mediated Alder-Ene Type Reaction: Mechanism and Stereoselectivity

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1. Complete reference for Gaussian 09

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J. Gaussian 09, revision D.01; Gaussian, Inc.: Wallingford, CT, **2013**.

2. Computational Methods.

All of the DFT calculations conducted in this study were carried out using the GAUSSIAN 09 series of programs. DFT method B3-LYP^{1,2} with a standard 6-31G(d) basis set (SDD basis set for Ru) was used for the geometry optimizations. The M11-L functional, proposed by Truhlar et al.,³ was used with a 6-311+G(d,p) basis set (SDD basis set for Ru) to calculate the single point energies. The solvent effects were taken into consideration using single point calculations based on the gas-phase stationary points with a SMD continuum solvation model.⁴ The energies presented in this paper are the M11-L calculated Gibbs free energies in acetone solvent with B3-LYP calculated thermodynamic corrections.

Reference

- 1 A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648.
- 2 C. Lee, W. Yang and R. G. Parr, *Physical Review B*, 1988, **37**, 785.
- 3 R. Peverati, D. G. Truhlar, *J. Phys. Chem. Lett.*, **2011**, 2, 2810.
- 4 A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B*, **2009**, 113, 6378.

3. DFT benchmark of different methods of energy between **7-ts** and **22-ts**.

Table S1 DFT benchmark of B3-LYP、 M11-L of energy between **7-ts** and **22-ts** in the gas.

$\Delta G_{\text{gas}}(\text{kcal/mol})$	7-ts	22-ts
M11-L	30.2	27.3
B3-LYP	37.6	39.3

Table S2 DFT benchmark of different methods of energy between **7-ts** and **22-ts** in the solvent.

$\Delta G_{\text{solv}}(\text{kcal/mol})$	7-ts	22-ts
B3-LYP	30.2	34.8
M11-L	24.3	22.6
M11	30.7	26.2
MPWPW91	29.3	27.7
MN12-L	26.4	18.9

we have reoptimized the structures of 1,5-H shift pathway and β -H elimination pathway proposed by Trost at M11-L/6-31+G(d) level in gas phase. As shown in Table S1, the free energy of transition state **7-ts** is higher than that of transition state **22-ts** in M11-L calculated data, which is exactly the opposite of the data obtained by B3-LYP. Computational results suggest that method affects the accuracy of the data. Generally, B3-LYP does not consider the role of dispersion and overestimates the steric hindrance, which could not obtain accurate data. Taking into account the role of dispersion, we

benchmarked different methods including M11, MPWPW91 and MN12-L. Meanwhile, we have also compared B3-LYP calculated results with these methods for solvation single point calculations based on gas-phase stationary points. As shown in Table S2, the free energy of transition state **7-ts** in B3-LYP is lower than that of transition state **22-ts**, which is the opposite of the data obtained by M11-L. Although the free energy obtained by MPWPW91 is higher than that obtained by M11-L, the tendency remains the same. The results indicated that role of dispersion affected accurate energy information. Here are some examples for the combination of B3-LYP with M11-L: Lei, A. *Chem.-Eur. J.* 2014, **20**, 15605; Lan, Y. *Organometallics* 2016, **35**, 1440; Lan, Y. *Acc. Chem. Res.* 2017, **50**, 2799.

In summary, the combination of B3-LYP with M11-L will give accurate energy information. Thus, the data of transition state **7-ts** and **22-ts** given in the manuscript is reliable.

4. Energy difference between pre-catalyst $\text{CpRu}(\text{OC}(\text{CH}_3)_2)_3^+$ and $\text{CpRu}(\text{CH}_3\text{CN})_3^+$.

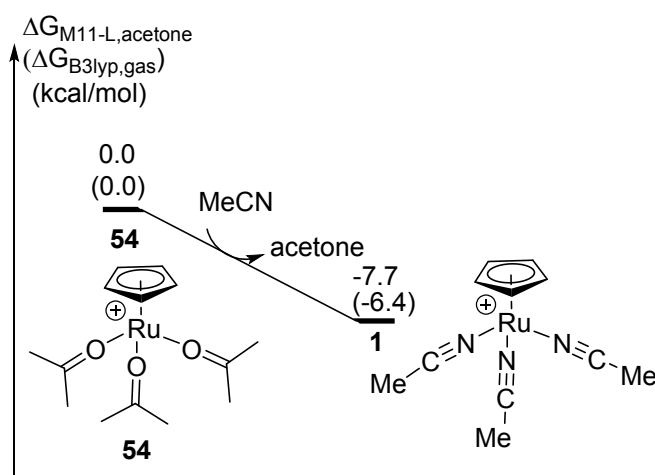


Fig. S1 Free energy profiles for ligand exchange of the precatalyst between $\text{CpRu}(\text{OC}(\text{CH}_3)_2)_3^+$ and $\text{CpRu}(\text{CH}_3\text{CN})_3^+$.

As shown Figure S1, ligand exchange with acetonitrile forms active catalyst **1** in an exothermic process with 7.7 kcal/mol free energy and simultaneously releases three molecules of acetone. Therefore, the results show that the coordination ability of acetonitrile is indeed stronger than acetone. The acetonitrile-coordinated ruthenium was employed as a pre-catalyst in the revised manuscript.

5. DFT benchmark of different methods of 1,5-H shift pathway.

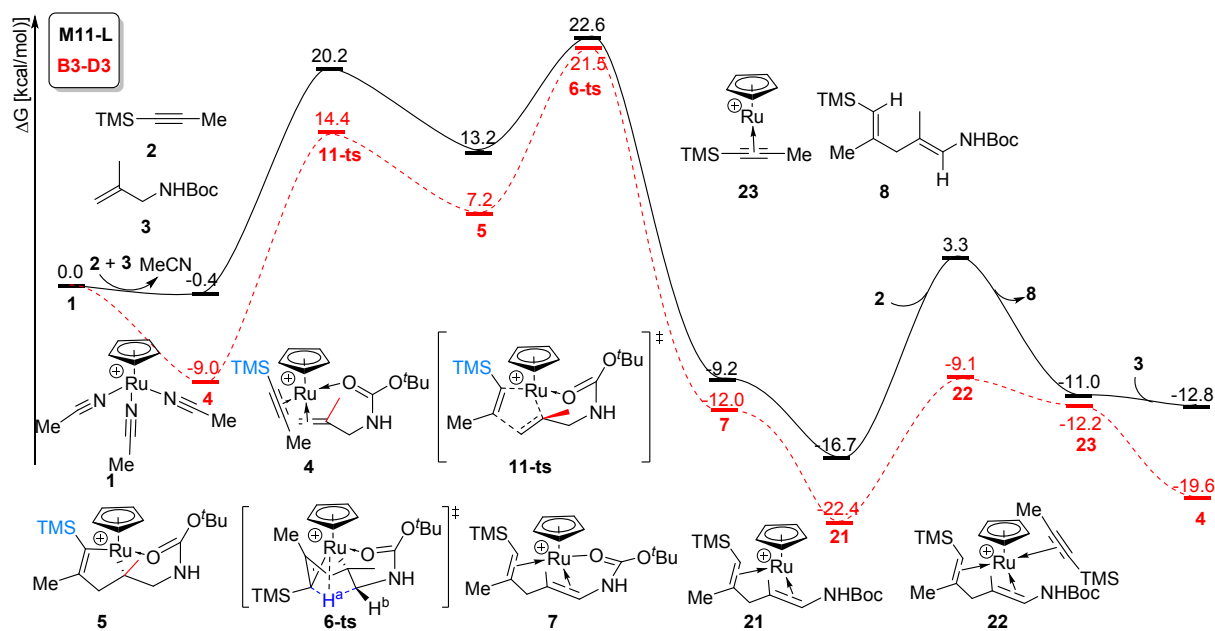


Fig. S2 Free energy profiles of Ru-catalyzed alkene and alkyne coupling reaction at the M11-L, B3-D3 level of theory.

Generally, B3-LYP does not consider the role of dispersion and overestimates the steric hindrance, which could not obtain accurate data. However, M11-L functional has considered the dispersion effect. As shown Figure S2, although the free energies obtained by Grimme's D3 are lower than the obtained by M11-L, the total activation free energy obtained by Grimme's D3 is 6.4 kcal/mol higher than the obtained by M11-L. The overall trend of free energy profiles is almost the same.

As shown Figure S3, all energies are with respect to acetonitrile-coordinated Ru complex **1**. The Ru involved [3+2] cyclometallation proceeded through transition state **11-ts** with an energy barrier of 20.6 kcal/mol to yield ruthenacyclopentene **5**. The followed agostic-assisted 1,5-H Shift takes places via transition state **6-ts** with an energy barrier of 23.0 kcal/mol to form intermediate **7**. Ligand exchange would occur to regenerate active catalyst **4** by endothermic 3.9 kcal/mol. The results shows that the overall activation free energy is 26.9 kcal/mol, which is lower 14.7 kcal/mol and 8.6 kcal/mol than the energy obtained by M06 and M06-L, respectively. Therefore, it could be concluded that the computational methods M11-L/B3-LYP used in this work is reliable to give accurate results.

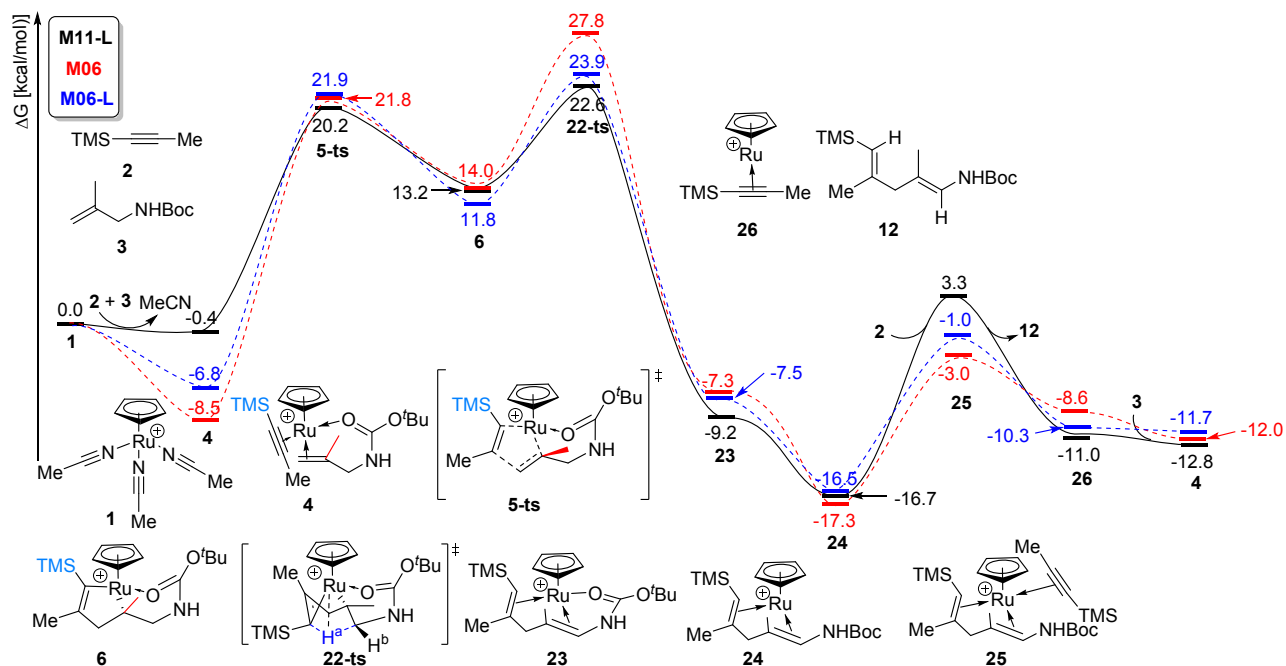


Fig. S3 Free energy profiles of Ru-catalyzed alkene and alkyne coupling reaction at the M11-L, M06 or M06-L level of theory.

6. Free energy profiles for the ligand exchange of substrate in path a, b and d.

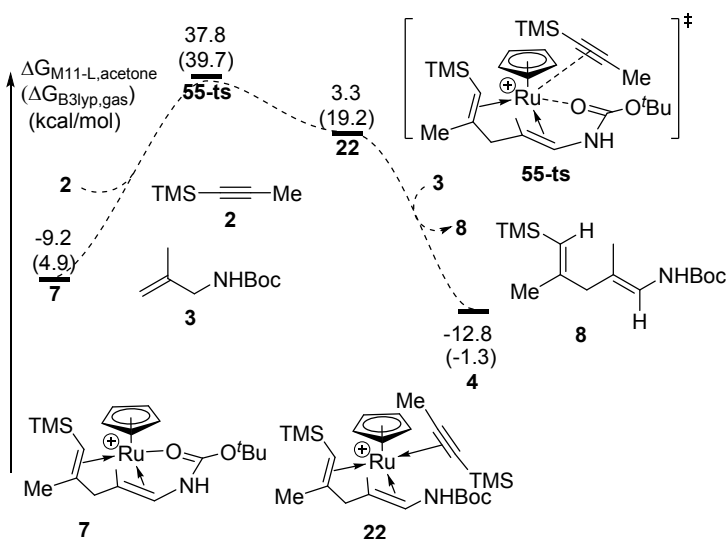


Fig. S4 Free energy profiles for the ligand exchange of 2+3 through the associative replacement pathway in path a.

We also have considered the associative replacement pathway of the ligand exchange in path a. As shown in Fig. S4, the associative replacement pathway involves a concerted substitution with intermediate 7 by alkyne 2 via a concerted transition state 55-ts with an activation barrier of 47.0 kcal/mol. The activation free energy of associative replacement pathway is 27.0 kcal/mol higher than

that of dissociative pathway. Therefore, the associative replacement pathway is energetically unfavorable.

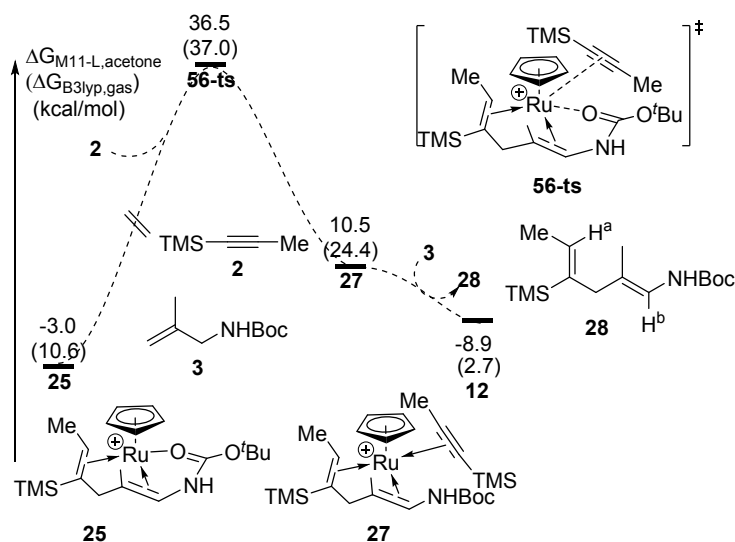


Fig. S5 Free energy profiles for the ligand exchange of **2+3** through the associative replacement pathway in path b.

As shown in Fig. S5, for the path b, the associative replacement pathway involves a concerted substitution with intermediate **25** by alkyne **2** via a concerted transition state **56-ts**, with an activation barrier of 39.5 kcal/mol. The activation free energy of associative replacement pathway is 19.1 kcal/mol higher than the corresponding dissociative pathway. Therefore, the associative replacement pathway is also energetically unfavorable.

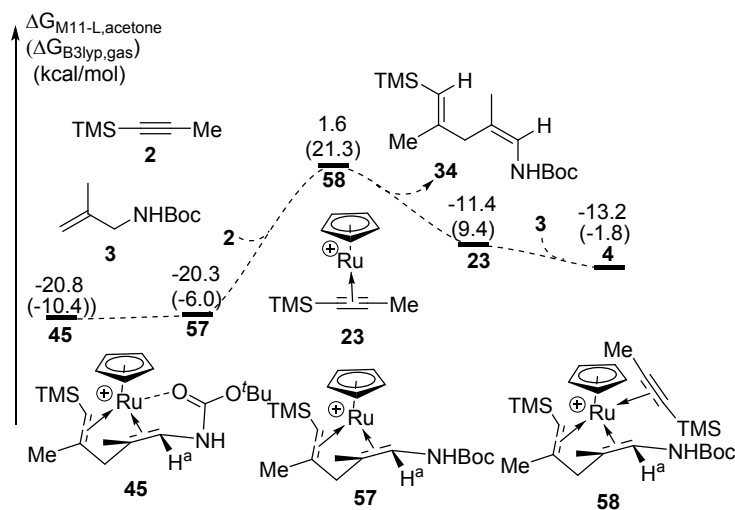


Fig. S6 Free energy profiles for the ligand exchange of **2+3** through the dissociative pathway in path d.

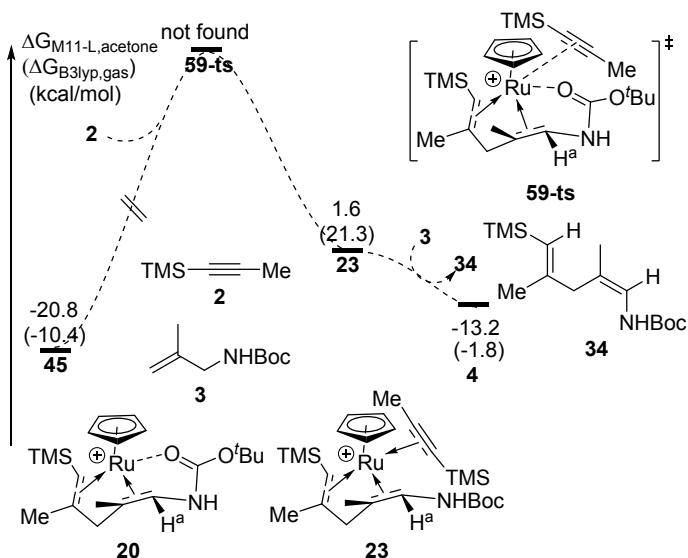


Fig. S7 Free energy profiles for the ligand exchange of **2+3** through the dissociative pathway in path d.

We also have carried out calculation on the ligand exchange steps for the **path d** (Fig 4 in manuscript). As shown in Fig. S6, the dissociative pathway involves oxygen atom dissociation in intermediate **45** to form diene-coordinated complex **57**, which is slightly endergonic by 0.5 kcal/mol. The alkyne **2** coordinates to the vacancy to form 18e intermediate **58** with 18.7 kcal/mol endothermic, which can be attributed to entropy loss. Subsequently, alkyne-coordinated ruthenium complex **26** is formed with the release of product **34**, which could be coordinated by propene **3** to regenerate the active species **4**. Alternatively, we have considered the corresponding associative replacement pathway for this process. Unfortunately, the concerted transition state **59-ts** could not be located after many efforts (Fig. S7).

7. B3-LYP and M11-L calculated absolute energies, enthalpies, and free energies of all structures.

Geometry	$E_{\text{(elec-B3-LYP)}}^1$	$H_{\text{(corr-B3-LYP)}}^2$	$G_{\text{(corr-B3-LYP)}}^3$	$E_{\text{(solv-M11-L)}}^4$	IF ⁵
1	-686.579006	0.246154	0.177306	-686.813783	-
2	-525.346289	0.171181	0.123999	-525.369209	-
3	-558.402103	0.269949	0.212297	-558.458435	-
MeCN	-132.751485	0.050181	0.021629	-132.765914	-
4	-1372.050273	0.536976	0.440869	-1372.318220	-
5	-1372.033442	0.537511	0.445211	-1372.30092	-
6-ts	-1372.001866	0.531408	0.440292	-1372.281007	-707.5

7	-1372.064260	0.537973	0.447905	-1372.339297	-
8	-1083.789420	0.445069	0.360494	-1083.853311	-
9	-1372.014596	0.534324	0.438239	-1372.290430	-
10	-1372.028549	0.533892	0.436963	-1372.296876	-
11-ts	-1372.018862	0.536522	0.445245	-1372.289782	-213.4
12	-1372.050674	0.537190	0.441395	-1372.318678	-
13-ts	-1372.021313	0.536285	0.443686	-1372.286503	-227.7
14	-1372.033357	0.536980	0.443913	-1372.303446	-
15	-1372.048490	0.537022	0.440164	-1372.316895	-
16-ts	-1371.993186	0.535230	0.442958	-1372.264758	-400.0
17	-1372.015011	0.536838	0.444362	-1372.288381	-
18	-1372.046023	0.537337	0.442058	-1372.316454	-
19-ts	-1371.99254	0.535267	0.442764	-1372.267835	-421.1
20	-1372.016958	0.537081	0.443931	-1372.287444	-
21	-1372.058623	0.536544	0.439476	-1372.342795	-
22	-1897.408524	0.712877	0.592715	-1897.710811	-
23	-813.602784	0.262880	0.200948	-813.848970	-
24-ts	-1371.994083	0.531363	0.440238	-1372.272271	-807.7
25	-1372.054843	0.538138	0.447450	-1372.328928	-
26	-1372.052959	0.537201	0.442760	-1372.33525	-
27	-1897.400024	0.713269	0.592326	-1897.698865	-
28	-1083.783799	0.445307	0.360705	-1083.846811	-
29	-1504.817516	0.589615	0.481647	-1505.092326	-
30-ts	-1504.784838	0.588887	0.484571	-1505.06555	-189.4
31	-1504.788721	0.589924	0.484407	-1505.068898	-
32-ts	-1504.776363	0.585464	0.482109	-1505.059401	-424.0

33	-1504.849700	0.590630	0.488108	-1505.132361	-
34	-1083.789846	0.445010	0.360130	-1083.853618	-
35-ts	-1372.003575	0.534840	0.439200	-1372.277190	-166.5
36-ts	-1372.014842	0.532437	0.438242	-1372.289085	-122.0
37-ts	-1372.024482	0.532335	0.436900	-1372.29748	-494.9
38-ts	-1372.020460	0.536721	0.446293	-1372.289102	-155.5
39	-1372.031168	0.537271	0.442928	-1372.298490	-
40-ts	-1372.002483	0.535007	0.442141	-1372.275833	-173.3
41	-1372.014080	0.534682	0.439494	-1372.288766	-
42-ts	-1372.013459	0.532153	0.437557	-1372.286852	-226.1
43	-1372.025461	0.533830	0.437897	-1372.294163	-
44-ts	-1372.024530	0.532408	0.437586	-1372.297749	-432.5
45	-1372.086449	0.537986	0.445642	-1372.355566	-
46	-541.089385	0.258413	0.200489	-541.123079	-
47	-959.579530	0.424983	0.343994	-959.640201	-
48	-1788.987286	0.780111	0.651690	-1789.274432	-
49-ts	-1788.958798	0.779263	0.652514	-1789.248192	-177.4
50	-1788.972116	0.780209	0.6530330	-1789.259810	-
51-ts	-1788.944095	0.774491	0.6491530	-1789.243237	-891.7
52	-1789.017757	0.781205	0.655473	-1789.312735	-
53	-1500.735741	0.688397	0.569716	-1500.829074	-
55-ts	-1897.368475	0.710853	0.593019	-1897.670697	-81.9
56-ts	-1897.364387	0.711297	0.593740	-1897.663672	-73.6
57	-1372.079911	0.538089	0.446123	-1372.355256	-
58	-1897.407981	0.713023	0.595408	-1897.716189	-

¹The electronic energy calculated by B3-LYP in gas phase. ²The thermal correction to enthalpy calculated by B3-LYP in gas phase. ³The thermal correction to Gibbs free energy calculated by B3-LYP

in gas phase. ⁴The electronic energy calculated by M11-L in acetone solvent. ⁵The B3-LYP calculated imaginary frequencies for the transition states.

8. B3-LYP geometries for all the optimized compounds and transition states.

1				H	-4.69796300	-1.29388500	0.79635600
Ru	0.24642500	-0.31451600	-0.06317400	C	-2.88648400	1.55465100	-0.12443200
C	2.37630900	-0.84793300	-0.39857600	H	-3.68123900	2.23796900	0.18960400
C	1.77038200	-0.51754700	-1.64382500	H	-1.97506000	1.81166500	0.42984600
C	1.68295800	-1.99966300	0.13521100	C	-2.26392700	-0.93110500	-0.33512600
H	2.05770000	0.30368500	-2.28829200	H	-2.67169700	-1.93598900	-0.17124000
C	0.68724300	-1.42869300	-1.88398700	H	-2.04620200	-0.82765300	-1.40328600
H	1.89557000	-2.49175400	1.07529900	N	-0.97815200	-0.81392100	0.33831100
C	0.66554900	-2.36054600	-0.78054400	H	-0.92892400	-0.93557800	1.33983100
H	0.05949800	-1.46015000	-2.76410000	C	0.15266100	-0.38318300	-0.29843000
H	-0.03864800	-3.17250000	-0.65257900	O	0.22067700	-0.12291000	-1.48999900
H	3.23802700	-0.36219500	0.03875400	O	1.16544500	-0.30575400	0.60252800
N	-0.31902400	1.60470000	-0.58239500	C	2.51373500	0.10778000	0.18992700
C	-0.65713900	2.65592900	-0.93366600	C	3.08045500	-0.88477400	-0.83183800
N	-1.77837500	-0.70137100	0.18957100	C	2.48294000	1.54198900	-0.35085500
C	-2.88788800	-0.95676400	0.39346200	C	3.29844700	0.04004500	1.50345000
N	0.02518100	0.08273700	2.21431400	H	3.04862500	-1.90360900	-0.42969300
C	0.92924000	0.81390900	2.01904800	H	2.51244600	-0.85442000	-1.76287900
C	1.99368400	1.81004100	2.19074100	H	4.12621300	-0.63658800	-1.04644900
H	1.88614100	2.61283400	1.45670300	H	2.03601400	2.21713500	0.38765300
H	1.92823000	2.23223100	3.19927300	H	3.50518100	1.88417200	-0.54881800
H	2.97622300	1.34699900	2.06363600	H	1.90692600	1.59838900	-1.27578500
C	-1.08440900	3.97390400	-1.39094400	H	4.34040200	0.33256600	1.33564200
H	-1.75079500	3.87197300	-2.25371400	H	2.86467400	0.71503000	2.24867300
H	-1.61966900	4.49515800	-0.59089600	H	3.28499400	-0.97663700	1.90994400
H	-0.21627700	4.57234700	-1.68536100	H	-2.66670600	1.73883500	-1.18427200
C	-4.28180000	-1.28988500	0.66364100				
H	-4.64259000	-0.71047300	1.51934000	MeCN			
H	-4.90270200	-1.06274100	-0.20862200	N	1.44098000	0.00030100	0.00012500
H	-4.37266700	-2.35567800	0.89643900	C	0.28069900	-0.00064000	-0.00026900
				C	-1.18114200	0.00015600	0.00006200
2				H	-1.56112900	0.67408900	0.77441800
C	-0.97677600	-0.00150700	-0.00001900	H	-1.56144800	0.33392300	-0.97056700
C	-2.19492000	-0.00113200	0.00023000	H	-1.56162400	-1.00721300	0.19651600
Si	0.86054300	-0.00016400	0.00012200				
C	1.47889500	-1.77721300	0.19777500	4			
H	1.12716000	-2.41469400	-0.62155300	Ru	1.08775600	-0.78164100	-0.20037400
H	2.57566700	-1.81077400	0.20069300	C	1.72181100	-0.72497700	-2.42109100
H	1.12821200	-2.21879400	1.13769800	C	0.44792900	-1.31735700	-2.35276200
C	1.47607200	0.71803000	-1.63840600	C	2.62486100	-1.52778500	-1.63354600
H	1.12424200	1.74651600	-1.77923500	H	-0.45639100	-0.91604300	-2.79115200
H	2.57284000	0.73188600	-1.67117800	C	0.52934100	-2.50185600	-1.53443100
H	1.12350700	0.12551100	-2.49046800	H	3.69055000	-1.37856900	-1.53253000
C	1.47670200	1.06087500	1.44020100	C	1.88754400	-2.64563900	-1.13207100
H	1.12495300	0.67039200	2.40206200	H	-0.27628500	-3.19305600	-1.32836300
H	2.57346600	1.08140000	1.46806500	H	2.29803300	-3.45775800	-0.54698700
H	1.12505200	2.09526300	1.35180700	H	1.97052900	0.19390500	-2.93500100
C	-3.65457500	0.00001300	0.00019800	C	2.62407600	0.94117100	0.22185200
H	-4.05071500	1.01647000	-0.11491300	C	1.48752200	1.45440600	0.14978700
H	-4.05211300	-0.40798100	0.93766300	Si	0.50578100	3.05805200	0.04193900
H	-4.05226400	-0.60729300	-0.82222800	C	-0.10994500	3.25693800	-1.72937400
				H	-0.76211700	2.43295500	-2.03525000
3				H	-0.67907000	4.18896000	-1.83276500
C	-3.27259200	0.11497400	0.10224400	H	0.72967800	3.30588200	-2.43259200
C	-4.44057600	-0.24841200	0.64136300	C	-0.90791600	3.10171500	1.29176000
H	-5.18755200	0.48356000	0.93864700	H	-0.56303400	2.85700800	2.30332800

H	-1.32038200	4.11773600	1.33052900
H	-1.72889800	2.42665600	1.03357400
C	1.75188600	4.41557000	0.45838800
H	2.60033200	4.41270800	-0.23523500
H	1.27405100	5.40087600	0.39087600
H	2.14536200	4.30926900	1.47586100
C	4.08396500	0.81904500	0.36402800
H	4.56553500	0.61489300	-0.59873400
H	4.36961600	0.02312300	1.05904400
C	0.66800200	-1.65816800	1.85128800
C	2.03104100	-1.37366400	1.73037300
H	2.43403500	-0.49513700	2.22607600
H	2.74832500	-2.17491300	1.57172500
C	0.13066900	-3.07561800	1.82919600
H	-0.85269200	-3.13978100	1.35381400
H	0.80849000	-3.76134900	1.31585200
C	-0.16560700	-0.66725600	2.64994200
H	-0.21401100	-1.00472600	3.69252500
H	0.30697600	0.32070400	2.64314300
N	-1.54682300	-0.57537900	2.19171000
H	-2.30583200	-0.60942700	2.85798900
C	-1.87522400	-0.28331100	0.91997700
O	-1.04241900	-0.17114000	-0.00704700
O	-3.18432100	-0.11140900	0.78099800
C	-3.91909000	-0.12380700	-0.52033300
C	-3.50410300	1.07301800	-1.37411400
C	-3.67604900	-1.46334900	-1.21626500
C	-5.37255500	0.00540000	-0.06271300
H	-3.61547400	2.00604500	-0.81254700
H	-2.47113900	0.98551500	-1.71402000
H	-4.15568900	1.13012100	-2.25253300
H	-3.94883600	-2.29656800	-0.56009700
H	-4.29970400	-1.52433400	-2.11405700
H	-2.63218200	-1.57456500	-1.52021200
H	-6.03532600	0.00207700	-0.93344200
H	-5.65308900	-0.82819900	0.58818600
H	-5.52581700	0.94116600	0.48331500
H	0.01616200	-3.43864300	2.86098900
H	4.48880600	1.76413100	0.74508800

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Ru	0.67755200	-0.81622000	-0.29183200
C	1.58734900	-1.76520400	-2.14194800
C	0.23617800	-1.55717100	-2.48649000
C	1.63554100	-2.70255100	-1.03626500
H	-0.14065200	-0.90565300	-3.26275500
C	-0.55619300	-2.39098700	-1.61435000
H	2.53314500	-3.11709000	-0.59821200
C	0.29652200	-3.13205900	-0.77728900
H	-1.63686100	-2.43612300	-1.60662400
H	-0.00978600	-3.84518500	-0.02536900
H	2.44586200	-1.30932400	-2.61615500
C	2.54338500	-0.13214100	0.54321400
C	1.62958200	0.79589300	-0.01056700
Si	1.57311000	2.67719700	-0.32359900
C	3.05936700	2.97718200	-1.45740700
H	2.97277400	2.43464900	-2.40542700
H	3.11027700	4.04717500	-1.69590300
H	4.00689400	2.69800700	-0.98483100
C	-0.02521100	3.19266500	-1.16484100
H	-0.88670600	3.08039800	-0.50045700
H	0.03295900	4.24564900	-1.46643300
H	-0.21345700	2.59637200	-2.06440200

C	1.80963200	3.55118000	1.33542900
H	2.72057600	3.22233800	1.84776300
H	1.89942500	4.63114100	1.16370500
H	0.96153400	3.40016500	2.01280200
C	3.91302600	-0.38797800	-0.05233500
H	3.97522600	-0.11106400	-1.10788100
H	4.20897500	-1.43732800	0.05444900
C	0.79313900	-1.00114700	1.86844800
C	2.27174600	-0.55937900	1.98591400
H	2.46590000	0.22813800	2.73321700
H	2.92304600	-1.40295900	2.24105200
C	0.54482700	-2.40272700	2.42955000
H	-0.48569300	-2.73567800	2.26575300
C	-0.12588800	0.02032600	2.54188200
H	-0.07084800	-0.09308800	3.63368400
H	0.20341600	1.04161700	2.31065100
N	-1.53868200	-0.12187600	2.19216500
H	-2.23378900	-0.12863200	2.92669100
C	-1.99917400	0.11852700	0.94927600
O	-1.25230700	0.22255600	-0.05713200
O	-3.31685700	0.23886600	0.92583200
C	-4.15069900	0.50641000	-0.28662000
C	-3.80996400	1.89274100	-0.83101600
C	-3.94867100	-0.59889600	-1.32226500
C	-5.56509800	0.46706700	0.29335200
H	-3.90447400	2.64969500	-0.04543800
H	-2.79872700	1.92512800	-1.24138600
H	-4.51257600	2.14955300	-1.63073700
H	-4.09185000	-1.58587300	-0.86863200
H	-4.69444800	-0.48491200	-2.11578000
H	-2.95750100	-0.54425200	-1.77601400
H	-6.29298800	0.67067800	-0.49789500
H	-5.78563200	-0.51596000	0.72077800
H	-5.68596300	1.22248100	1.07554800
H	1.21704100	-3.14693000	1.99268400
H	0.72255400	-2.40925400	3.51727000
H	4.65421100	0.21027900	0.49649400

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Ru	0.74708300	-0.94372900	-0.20709200
C	1.90647100	-1.39482600	-2.12139600
C	0.54036700	-1.49791500	-2.43438000
C	2.19981500	-2.37238300	-1.09132800
H	-0.00461700	-0.89929300	-3.15161400
C	-0.01507700	-2.57036700	-1.62642700
H	3.17667300	-2.57550200	-0.67451900
C	1.01789900	-3.14170400	-0.85501300
H	-1.04994300	-2.88783300	-1.63014800
H	0.92199900	-3.96884900	-0.16457500
H	2.61393300	-0.70134200	-2.55478100
C	2.38207000	-0.01374700	0.86122300
C	1.40717000	0.92513500	0.43072900
Si	1.45126600	2.65156300	-0.39204700
C	2.13038300	2.46653200	-2.14452800
H	1.52635500	1.77306700	-2.73883600
H	2.10966600	3.44316900	-2.64450100
H	3.16897200	2.11816800	-2.15744300
C	-0.32149700	3.30236200	-0.43784300
H	-0.75306800	3.40610100	0.56550100
H	-0.34378400	4.29743700	-0.89820400
H	-0.97408700	2.65025100	-1.02865100
C	2.54255900	3.79521900	0.64176000
H	3.57502100	3.43193300	0.69824100

H	2.57160100	4.79862600	0.19914400
H	2.16928700	3.90192500	1.66732500
C	3.82577900	0.07225500	0.41597400
H	3.93256200	0.44322900	-0.60654900
H	4.32167300	-0.90157300	0.48586000
C	0.57327500	-0.97435500	1.95536500
C	2.06841100	-0.75937500	2.16360500
H	2.36987600	-0.20279400	3.07412100
H	2.60060100	-1.71556400	2.17701000
C	-0.07346300	-2.17588300	2.65414200
H	-1.11734300	-2.31222400	2.35354400
C	-0.08956000	0.31730000	2.29479200
H	0.17414000	0.79381300	3.24797200
H	0.63395700	1.11502800	1.45533600
N	-1.43175600	0.54413300	2.00143800
H	-1.97548800	1.15560100	2.59918200
C	-2.01800300	0.22067700	0.78813000
O	-1.39139000	-0.29359800	-0.14311800
O	-3.28455400	0.56297500	0.78680900
C	-4.22862900	0.30652900	-0.36490300
C	-3.74292200	1.07213400	-1.59426200
C	-4.32823500	-1.20119300	-0.58925000
C	-5.53740700	0.88142300	0.17301400
H	-3.61263300	2.13419100	-1.36257500
H	-2.80373500	0.67105600	-1.98115000
H	-4.49972100	0.99174800	-2.38152000
H	-4.61458400	-1.71267800	0.33548200
H	-5.10413100	-1.39880300	-1.33600600
H	-3.38860700	-1.62046800	-0.95555300
H	-6.32550400	0.75431100	-0.57529300
H	-5.84488100	0.36576100	1.08763500
H	-5.43728500	1.94960100	0.38817000
H	0.46882400	-3.09083700	2.40066400
H	-0.05050300	-2.07386300	3.74985100
H	4.36881700	0.75793000	1.08156700

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Ru	0.46000800	-0.69336200	-0.31655700
C	1.67232400	-0.85171400	-2.18478500
C	0.42766100	-0.26563000	-2.50986100
C	1.41942800	-2.16715200	-1.65907300
H	0.26991400	0.72840400	-2.90619200
C	-0.60151600	-1.25778200	-2.26352000
H	2.17206300	-2.88416300	-1.36093800
C	0.00712400	-2.42466200	-1.77316200
H	-1.66317700	-1.10819300	-2.40827200
H	-0.49996400	-3.33739400	-1.49172400
H	2.63882500	-0.38146400	-2.28386700
C	2.34181500	-0.53110500	0.94950800
C	1.71641000	0.73418500	0.89532700
Si	2.33269500	2.40396200	0.20087900
C	3.04665800	2.39530100	-1.55561700
H	2.31312600	2.09532300	-2.31209600
H	3.35249500	3.42060600	-1.80022800
H	3.93834700	1.76869500	-1.67114200
C	0.83436100	3.55648300	0.23671000
H	0.42314000	3.65148300	1.24921200
H	1.11114400	4.56319500	-0.09850800
H	0.03094300	3.19576200	-0.41638000
C	3.65994700	3.03461400	1.39612600
H	4.55473500	2.40085000	1.38837200
H	3.97363500	4.04905600	1.12055700
H	3.28955500	3.07472400	2.42737800

C	3.69905700	-0.78427500	0.32991900
H	3.94450400	-0.07230900	-0.45884800
H	3.80751900	-1.80115400	-0.06194300
C	0.54939900	-2.08859000	1.57980900
C	1.93680200	-1.59235300	1.99651700
H	1.94131900	-1.18918200	3.01785900
H	2.64750300	-2.42340400	1.97756600
C	0.31103300	-3.55675400	1.36142500
H	-0.68154200	-3.75389800	0.94871700
C	-0.44878500	-1.14194700	1.71953800
H	-0.23264300	-0.25356600	2.30669900
H	1.06205400	0.96364900	1.73987000
N	-1.84527500	-1.28538300	1.42372700
H	-2.47991000	-1.68127700	2.11094400
C	-2.30329500	-0.22063500	0.69027000
O	-1.48635000	0.45598600	0.02055500
O	-3.59747900	-0.03193900	0.76589000
C	-4.33883600	1.04234600	0.00935200
C	-3.85689800	2.40746500	0.49722000
C	-4.13936600	0.83652800	-1.49165500
C	-5.78477400	0.77383700	0.42197800
H	-3.97197000	2.49251200	1.58266200
H	-2.81289500	2.58692300	0.23170400
H	-4.46841600	3.18821100	0.03303900
H	-4.40662600	-0.18545100	-1.78222500
H	-4.80043500	1.51997400	-2.03444900
H	-3.11159100	1.04633000	-1.79553400
H	-6.44241800	1.50735800	-0.05423300
H	-6.10278400	-0.22633200	0.11191200
H	-5.90366900	0.85847700	1.50624400
H	1.06825400	-4.00766000	0.71352300
H	0.38106500	-4.06665400	2.33317200
H	4.45607900	-0.67062000	1.11956000

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C	-2.80268600	-1.34600100	-0.38712800
C	-2.79206400	-0.05418900	-0.00866400
C	-0.36031800	-1.73100200	0.39173500
C	-1.53805800	-2.20841700	-0.42642800
H	-1.24039200	-2.31870900	-1.48017500
H	-1.81301800	-3.22553800	-0.10099200
C	-0.48389300	-1.88286900	1.88880500
H	0.29196600	-1.34946700	2.44942100
C	0.72241800	-1.23875800	-0.23313600
H	0.76785600	-1.15370000	-1.31333200
N	1.89578300	-0.78823100	0.37755500
H	2.00199700	-0.83161600	1.38061600
C	2.95133800	-0.26650700	-0.33647500
O	2.97134600	-0.14914800	-1.54910400
O	3.93114500	0.07841200	0.53285600
C	5.18945500	0.67445500	0.05550300
C	5.92190900	-0.30962500	-0.86360700
C	4.90541100	2.01310400	-0.63461700
C	5.97011000	0.88674300	1.35562400
H	6.05861400	-1.27199100	-0.35791600
H	5.36612700	-0.47198100	-1.78833300
H	6.91277100	0.08754000	-1.11167900
H	4.35238800	2.67869300	0.03752900
H	5.85170100	2.50142800	-0.89371000
H	4.32349800	1.86725000	-1.54606300
H	6.94503500	1.33595400	1.13933700
H	5.42355600	1.55329000	2.03089400
H	6.13420000	-0.06640300	1.86908700

H	-1.45101300	-1.49900400	2.23417800
H	-1.81319200	0.33389200	0.28717900
H	-0.43424500	-2.94047500	2.18591400
Si	-4.19159400	1.20515100	0.06235600
C	-4.03482000	-2.08456400	-0.85474100
H	-4.27305800	-2.91524500	-0.17548100
H	-4.91521900	-1.44135200	-0.92280300
H	-3.86756100	-2.53319500	-1.84423000
C	-3.43755500	2.81134800	0.73168000
H	-3.01387500	2.66732100	1.73335300
H	-2.63223100	3.17612400	0.08221600
H	-4.18990500	3.60634900	0.80289600
C	-5.58542700	0.66320800	1.23343000
H	-6.35502800	1.44249700	1.30352900
H	-6.07860900	-0.25728400	0.90027500
H	-5.20220400	0.48384200	2.24515700
C	-4.91776500	1.55051700	-1.65795700
H	-5.36765500	0.65764200	-2.10743900
H	-5.69678100	2.32178800	-1.60423400
H	-4.14215300	1.90908400	-2.34523100

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Ru	-0.84955400	-0.58513300	0.43567200
C	-1.76801100	-0.56388600	2.47156400
C	-0.79247200	0.46980800	2.48033100
C	-1.08776500	-1.83144800	2.29162800
H	-0.96789900	1.52777900	2.61651500
C	0.47960600	-0.14918500	2.26304100
H	-1.55637900	-2.80672100	2.28890600
C	0.30318100	-1.56410700	2.19797700
H	1.41920400	0.37899000	2.16210700
H	1.08718400	-2.29722200	2.06586800
H	-2.83164800	-0.43979700	2.62286800
C	-2.46880600	-0.97044600	-1.19027300
C	-2.31041600	0.24596900	-0.55257200
C	-0.18766600	-1.71165400	-1.30648100
C	-1.42644800	-1.56799400	-2.16137400
H	-1.30331500	-0.93724500	-3.05192800
H	-1.78117500	-2.54384500	-2.50411000
C	0.34884200	-3.11233800	-1.11276100
H	1.13590100	-3.15987300	-0.35687700
C	0.72015500	-0.54659600	-1.31151400
H	0.57434400	0.12177200	-2.16964000
H	0.38645700	0.31381600	-0.46201600
N	2.09449600	-0.78640000	-0.99924000
H	2.55430800	-1.58570300	-1.41475000
C	2.89749800	0.25522100	-0.55833600
O	2.42213100	1.31820000	-0.18340100
O	4.17486200	-0.11840100	-0.58724800
C	5.27552900	0.79579700	-0.15697300
C	5.28980100	2.03155800	-1.05833500
C	5.09896000	1.14504900	1.32206500
C	6.51689300	-0.06857700	-0.37828400
H	5.36539100	1.73901400	-2.11100200
H	4.39349500	2.63887600	-0.91881400
H	6.16453200	2.64403000	-0.81563600
H	5.02047900	0.23435800	1.92631500
H	5.97572700	1.70199100	1.66893800
H	4.21382100	1.76368900	1.48315900
H	7.41341800	0.49382500	-0.09984600
H	6.47620000	-0.97604900	0.23263600
H	6.60640400	-0.36011800	-1.42944200
H	-0.45381800	-3.79152100	-0.80887300

H	0.75561500	-3.50379800	-2.05904700
Si	-3.37025000	1.83398600	-0.37745000
C	-4.14772500	1.91553700	1.34333300
H	-3.40337300	2.00616000	2.14054800
H	-4.78932800	2.80413000	1.39499900
H	-4.78165000	1.04702500	1.55570000
C	-2.15977600	3.25294800	-0.65776200
H	-1.34168400	3.23743400	0.07063500
H	-1.71705500	3.21847300	-1.65988800
H	-2.68078000	4.21353900	-0.56291800
C	-4.71112500	1.80885900	-1.70518700
H	-5.42788900	0.99331600	-1.55785800
H	-5.27719500	2.74820100	-1.68172100
H	-4.28705200	1.70950500	-2.71125300
C	-3.78233600	-1.72769400	-1.10226300
H	-4.25820300	-1.74655200	-2.09257200
H	-3.60516000	-2.76840200	-0.80531400
H	-4.47993100	-1.28352100	-0.38801600

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Ru	0.90197400	-0.67330100	-0.34288700
C	1.79988600	-1.46165200	-2.27140800
C	0.78111200	-0.52495600	-2.59590000
C	1.18265000	-2.59586300	-1.63335400
H	0.91419100	0.41264900	-3.11633400
C	-0.47120300	-1.06928700	-2.13455400
H	1.69208700	-3.48674300	-1.28981100
C	-0.21351600	-2.35442500	-1.57881600
H	-1.44149000	-0.60539600	-2.24777700
H	-0.95244000	-3.02277900	-1.15661400
H	2.85311400	-1.36063200	-2.49813200
C	2.45630800	-0.62557100	1.27906600
C	2.31817700	0.42095000	0.36005700
C	0.19976800	-1.22012100	1.80269700
C	1.48022000	-0.71743200	2.45649100
H	1.35072800	0.24856000	2.95852800
H	1.84594400	-1.42720500	3.20515000
C	-0.12578300	-2.68503100	2.00285500
H	-0.93380700	-3.04478500	1.35922100
C	-0.75590800	-0.27248200	1.43471700
H	-0.59699100	0.77894600	1.63650700
H	0.24888800	0.77401700	-0.46139000
N	-2.06277100	-0.54628000	1.09494300
H	-2.41671800	-1.49320100	1.07720700
C	-2.91657300	0.46956800	0.64109800
O	-2.56030700	1.62848800	0.56127100
O	-4.09464500	-0.07205500	0.33501700
C	-5.24358600	0.76639900	-0.12758300
C	-5.60660700	1.77566600	0.96326900
C	-4.87941100	1.43478400	-1.45460500
C	-6.34911400	-0.27253300	-0.31318200
H	-5.79984800	1.26409500	1.91215200
H	-4.81499200	2.51304100	1.10951300
H	-6.52120200	2.30368300	0.67359900
H	-4.58879500	0.68357000	-2.19795100
H	-5.75486500	1.96595600	-1.84276900
H	-4.06720500	2.15355700	-1.33068100
H	-7.26279900	0.21972400	-0.66028100
H	-6.06008700	-1.02320100	-1.05579800
H	-6.56947300	-0.78099400	0.63057100
H	0.74680200	-3.31690100	1.81133600
H	-0.42916000	-2.85411300	3.04603600
Si	3.23665100	2.03266900	-0.09108400

C	5.09215700	1.73239100	0.08994400
H	5.63130000	2.66522600	-0.11689400
H	5.36122400	1.41576400	1.10361300
H	5.46524100	0.98008800	-0.61423900
C	2.78541200	2.56891600	-1.83667300
H	3.13777500	1.85539900	-2.59043700
H	1.70286200	2.69018000	-1.95286500
H	3.25163200	3.53587800	-2.06175500
C	2.60736600	3.26460300	1.19834400
H	2.85141900	2.95233900	2.21986500
H	3.08435600	4.23798500	1.02815000
H	1.52385700	3.41248300	1.13036300
C	3.71245500	-1.47183500	1.33646100
H	4.31685100	-1.17866900	2.20653400
H	3.46057100	-2.53186600	1.46042300
H	4.32720200	-1.36881000	0.43868800

11-ts

Ru	-0.59274300	-0.87621200	0.36023900
C	-0.61235800	0.03188100	2.39638200
C	0.43264600	-0.94974100	2.37363400
C	-1.84952000	-0.65578200	2.17390200
H	1.48924500	-0.75108700	2.49540600
C	-0.15086000	-2.22500900	2.16512500
H	-2.83294800	-0.20848800	2.14019000
C	-1.56174200	-2.04825500	2.00741500
H	0.38664100	-3.15989900	2.10014600
H	-2.29309300	-2.83075000	1.85187800
H	-0.48364200	1.08917400	2.57697500
C	-2.11800700	-0.19547800	-1.39072900
C	-1.71903300	0.66556900	-0.50632100
Si	-2.08821500	2.47944200	-0.11304300
C	-2.98781300	3.26434700	-1.57999100
H	-4.00468300	2.87688100	-1.70864300
H	-3.07608300	4.34466000	-1.40844000
H	-2.44629100	3.12701200	-2.52269100
C	-3.19947400	2.58467200	1.41600000
H	-2.69948600	2.27615500	2.34074900
H	-3.51604400	3.62579400	1.55626800
H	-4.10946900	1.98361100	1.30174700
C	-0.47438800	3.40930400	0.18435900
H	0.15019300	3.41037200	-0.71526800
H	-0.68889400	4.45406700	0.44100900
H	0.11691400	2.98125700	1.00045400
C	-3.14615500	-0.20990800	-2.48528800
H	-3.69566100	0.73346800	-2.47842900
H	-3.86474400	-1.02677500	-2.34953100
C	-0.13815400	-2.45206600	-0.97857300
C	-1.41525300	-1.94812100	-1.53889000
H	-1.32266600	-1.77256800	-2.61027600
H	-2.28866000	-2.55798900	-1.31331100
C	-0.14269800	-3.89629700	-0.48855400
H	0.78527600	-4.14709800	0.03687200
H	-0.98579200	-4.11585400	0.17136100
C	1.06368000	-2.15513000	-1.89032900
H	1.34771600	-3.06521900	-2.43010300
H	0.78132700	-1.40246700	-2.63681500
N	2.25839900	-1.69514400	-1.18879800
H	3.16067100	-2.06909500	-1.45343000
C	2.25514200	-0.43363000	-0.69809800
O	1.18808500	0.18834600	-0.48464500
O	3.47686400	0.03050900	-0.49346400
C	3.80152000	1.41187600	-0.01922400

C	3.30890700	2.41735200	-1.05951100
C	3.20175500	1.64066500	1.36762800
C	5.32877300	1.37602100	0.04081900
H	3.73385700	2.19162900	-2.04297700
H	2.21965100	2.41733300	-1.13200900
H	3.63520000	3.42289700	-0.77425300
H	3.53346600	0.86230800	2.06404400
H	3.55074900	2.60339900	1.75542300
H	2.11119800	1.66054000	1.33343500
H	5.70700100	2.35066300	0.36417800
H	5.67542600	0.61868400	0.75080100
H	5.75207900	1.15170300	-0.94279700
H	-0.21771900	-4.57725200	-1.34910200
H	-2.68520900	-0.33438700	-3.47285400

12

Ru	0.37928800	-0.63178600	-0.13189500
C	1.20458600	-1.09137200	-2.23854500
C	-0.17681300	-1.35203400	-2.23864400
C	1.81998600	-1.93517700	-1.24677500
H	-0.91832800	-0.84343800	-2.84067300
C	-0.44223000	-2.38998500	-1.26462600
H	2.87775300	-2.00432400	-1.03703400
C	0.79830000	-2.77398600	-0.69611700
H	-1.40634000	-2.83315100	-1.05405700
H	0.95012200	-3.55294900	0.03878200
H	1.71020400	-0.34237400	-2.83296200
C	2.01122300	1.05135200	-0.05885800
C	0.89242500	1.60355500	-0.11309400
Si	3.89269200	1.05339200	-0.07906700
C	4.38627500	2.79885900	0.44092200
H	4.04226400	3.03381500	1.45446100
H	5.47853500	2.90000400	0.42886600
H	3.97739100	3.55464700	-0.23910800
C	4.60691200	-0.22143300	1.11395400
H	4.29284500	-1.24517900	0.88242500
H	5.70174600	-0.19470200	1.05028500
H	4.33872500	-0.01223300	2.15540700
C	4.47905600	0.70792600	-1.84187500
H	4.02954600	1.40508400	-2.55847400
H	5.56687900	0.83947000	-1.89755600
H	4.26141500	-0.31227600	-2.17701100
C	-0.06239400	2.72484600	-0.18739300
H	-0.67809300	2.79632400	0.71582600
H	-0.73816800	2.61879400	-1.04071500
C	-0.11580900	-0.99841600	2.05030100
C	1.27094700	-0.99634000	1.87880200
H	1.85222000	-0.12659900	2.16628500
H	1.82367800	-1.93174000	1.87672800
C	-0.89583700	-2.27630100	2.29650000
H	-1.89098300	-2.25537200	1.84122100
H	-0.36578700	-3.15406900	1.92106600
C	-0.74335600	0.25421000	2.63963800
H	-0.84092800	0.12464400	3.72458200
H	-0.09545800	1.12114000	2.47223000
N	-2.09448400	0.51887700	2.14753000
H	-2.82066100	0.78577000	2.79802400
C	-2.43909200	0.49802900	0.84587000
O	-1.65490600	0.20272300	-0.08395600
O	-3.70904800	0.83342800	0.66829400
C	-4.42757100	0.78410900	-0.64248400
C	-3.78803500	1.76677900	-1.62425000
C	-4.43932400	-0.65475500	-1.15919600

C	-5.83264000	1.23975300	-0.24647400
H	-3.72290400	2.76609000	-1.18129500
H	-2.79041900	1.44408800	-1.92885700
H	-4.41496500	1.83789200	-2.51922400
H	-4.85901400	-1.33197500	-0.40793100
H	-5.07000900	-0.71207900	-2.05247100
H	-3.43645700	-0.99452800	-1.42729400
H	-6.48067800	1.24667000	-1.12817500
H	-6.26721200	0.56364400	0.49599900
H	-5.81057400	2.25028600	0.17271600
H	-1.03907700	-2.41501900	3.37806400
H	0.48976400	3.66568400	-0.29315000

13-ts

Ru	-0.14785900	0.96623500	-0.26039000
C	0.67663600	1.82009200	-2.14754100
C	1.41310500	2.39486000	-1.05622200
C	-0.68505800	2.23574000	-2.00819400
H	2.47131800	2.26683800	-0.86977900
C	0.52199600	3.17130600	-0.27373500
H	-1.50341700	1.98483500	-2.67010600
C	-0.78813800	3.04768700	-0.83268000
H	0.78542400	3.72471200	0.61587700
H	-1.68754600	3.53046500	-0.47299700
H	1.08868900	1.21456800	-2.94268900
C	-2.00452400	-0.61489400	-0.24848200
C	-1.13601500	-0.56778500	-1.20889900
Si	-3.66002300	-1.51135200	0.03906900
C	-3.48353500	-2.71437900	1.48693600
H	-3.30868800	-2.22241200	2.45084100
H	-4.41230800	-3.28943100	1.59146400
H	-2.67131800	-3.43056000	1.31742400
C	-5.00202900	-0.22991300	0.39144200
H	-5.06770700	0.51564300	-0.40965200
H	-5.97684600	-0.72922500	0.45497600
H	-4.85163200	0.30027700	1.33838500
C	-4.06880900	-2.45972000	-1.53965900
H	-3.35125700	-3.26165500	-1.74522400
H	-5.05422400	-2.92925500	-1.42772300
H	-4.11786600	-1.80583700	-2.41729800
C	-0.83064400	-1.23869500	-2.50101200
H	-0.89453400	-0.53500400	-3.33912100
H	-1.51901300	-2.06617100	-2.69833100
C	-0.44878800	0.98014400	1.84179000
C	-1.74117200	0.43283200	1.38676300
H	-2.01348700	-0.47010400	1.92763800
H	-2.56415300	1.14165900	1.34393100
C	-0.50424900	2.31817300	2.57422300
H	0.49503800	2.74303500	2.71926200
H	-1.12274600	3.05570300	2.05581200
C	0.40500500	-0.05778900	2.58652200
H	0.34972400	0.12649900	3.66515400
H	0.00493300	-1.06256800	2.40173300
N	1.82697700	-0.05055400	2.23830100
H	2.51134000	-0.14921000	2.97740900
C	2.18562100	-0.53709400	1.02876000
O	1.37487900	-0.59990200	0.07422400
O	3.44538900	-0.93503100	0.98532400
C	4.10474400	-1.52736600	-0.22114200
C	3.40756400	-2.84131900	-0.57524400
C	4.09280900	-0.51811800	-1.36947000
C	5.52701200	-1.77118100	0.28383800
H	3.39475900	-3.51481000	0.28787300

H	2.38183800	-2.67562700	-0.91188100
H	3.95981900	-3.33703700	-1.38043800
H	4.52864100	0.43517500	-1.05059800
H	4.70403500	-0.90438600	-2.19184700
H	3.08164000	-0.34856700	-1.74486500
H	6.12731300	-2.22358200	-0.51139300
H	6.00249600	-0.83204800	0.58329000
H	5.52453900	-2.44990400	1.14193400
H	-0.94009700	2.17455000	3.57417100
H	0.19124900	-1.63412600	-2.48552300

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Ru	0.24840000	0.46160900	-0.16535500
C	0.88909600	2.63898600	0.44846100
C	-0.49867300	2.64914400	0.26418800
C	1.49180600	2.24961200	-0.80682700
H	-1.24108800	2.85527100	1.02342200
C	-0.77336700	2.32919600	-1.12781600
H	2.55204000	2.19499100	-1.00787500
C	0.45489300	2.15225400	-1.78967400
H	-1.75488400	2.28614300	-1.58118000
H	0.59402600	1.92638700	-2.83712900
H	1.41564300	2.83680800	1.37173400
C	2.03889600	-0.75971900	0.19896100
C	1.00008900	-0.69435200	1.12905200
Si	3.85761300	-0.27954700	0.62824400
C	4.57898900	-1.84178200	1.41520200
H	4.50162000	-2.71020300	0.75077300
H	5.64369300	-1.69288700	1.63444200
H	4.08420600	-2.09621900	2.35989800
C	4.80788600	0.12819600	-0.95256800
H	4.39201000	0.97551200	-1.50931500
H	5.84228500	0.38728600	-0.69390400
H	4.85380600	-0.72855800	-1.63434800
C	3.93837800	1.15488900	1.85532000
H	3.27531400	1.01398100	2.71729500
H	4.95979600	1.23488600	2.24722100
H	3.69656400	2.11877600	1.39526500
C	0.64050800	-1.28486500	2.43297200
H	-0.39957100	-1.09110200	2.70477300
H	1.28661300	-0.83031500	3.20028400
C	0.40458700	-1.27421500	-1.45210000
C	1.80527500	-1.72952300	-0.98170400
H	1.88271400	-2.79331500	-0.70075700
H	2.55714100	-1.55184300	-1.75586300
C	0.34573300	-0.98276600	-2.95263500
H	-0.61825000	-0.55833800	-3.25349700
C	-0.63398900	-2.33085400	-1.06303000
H	-0.56616900	-3.18637400	-1.74884900
H	-0.42943400	-2.71917800	-0.05578100
N	-2.02231000	-1.87087000	-1.12343300
H	-2.71832400	-2.45179500	-1.57237400
C	-2.48909800	-0.95880200	-0.25125900
O	-1.73456800	-0.22287100	0.43727400
O	-3.80882700	-0.93994000	-0.19060500
C	-4.61685100	-0.02582500	0.67787500
C	-4.29762600	-0.31272400	2.14541400
C	-4.35524400	1.42669600	0.28209600
C	-6.04557000	-0.44330000	0.32859200
H	-4.43531500	-1.37589200	2.36825700
H	-3.27636300	-0.02230400	2.40142600
H	-4.98567600	0.25482000	2.78065700
H	-4.51484500	1.56968700	-0.79205000

H	-5.05833800	2.07602000	0.81400100
H	-3.34160400	1.73683100	0.54196500
H	-6.75486800	0.15099500	0.91256500
H	-6.25155600	-0.28074100	-0.73379000
H	-6.21013300	-1.50023800	0.55824900
H	1.13495100	-0.29360700	-3.26631000
H	0.48644800	-1.91305500	-3.52692500
H	0.85036000	-2.36248500	2.45548700

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Ru	0.36259000	-0.68178300	-0.11794700
C	1.49663300	-1.72419200	-1.75440100
C	0.15426400	-1.53079500	-2.19450700
C	1.47997700	-2.55753900	-0.59668100
H	-0.16347000	-0.96242900	-3.05770600
C	-0.68727600	-2.28924000	-1.31276700
H	2.35190600	-2.89924500	-0.05657900
C	0.11271700	-2.93064400	-0.33329200
H	-1.76777300	-2.33347200	-1.36782700
H	-0.23445300	-3.60763600	0.43584800
H	2.37631500	-1.28935500	-2.20709900
C	2.01128000	0.92921600	-0.38609300
C	0.91588500	1.42780600	-0.72665500
Si	3.87631400	1.00765200	-0.14650500
C	4.22723400	1.99034900	1.42842300
H	3.86223600	1.48757600	2.33176800
H	5.30884500	2.12980000	1.54802400
H	3.76884900	2.98507000	1.38961000
C	4.64009600	-0.71394600	-0.01548700
H	4.47499000	-1.32004900	-0.91332900
H	5.72567800	-0.61465500	0.10755800
H	4.26839500	-1.27358800	0.85012200
C	4.54408700	1.91578600	-1.66024000
H	4.10687000	2.91620700	-1.75395200
H	5.63161700	2.03583900	-1.58109700
H	4.33702200	1.37068300	-2.58822600
C	-0.01174700	2.46188300	-1.21524800
H	-0.65334900	2.82659000	-0.40732600
H	-0.66131100	2.07566400	-2.00656400
C	0.12177300	-0.22326600	2.14324500
C	1.32075100	-0.89143200	1.92240100
H	2.25714800	-0.34923500	1.98003700
H	1.39603100	-1.96053200	2.10177700
C	0.09241700	1.25061700	2.49187300
H	0.98351100	1.76647200	2.13196200
H	-0.78726300	1.75948100	2.08722200
C	-1.07429000	-1.02870400	2.60706800
H	-0.91706700	-2.09456300	2.41038000
H	-1.17764600	-0.90632400	3.69411300
N	-2.34845800	-0.59296400	2.03466000
H	-3.18686300	-0.72636300	2.58450500
C	-2.54454100	-0.02465600	0.82827500
O	-1.64357000	0.23149600	-0.00662000
O	-3.82927100	0.25285600	0.64573300
C	-4.42428200	0.87164800	-0.57745000
C	-3.92940200	2.31165300	-0.70075200
C	-4.10349500	0.02054700	-1.80687500
C	-5.91870800	0.82773600	-0.25463000
H	-4.13232600	2.86921900	0.21942000
H	-2.86031100	2.35071200	-0.91407500
H	-4.46029900	2.80881700	-1.51929800
H	-4.40227800	-1.02084300	-1.64367100
H	-4.67301200	0.39894400	-2.66208400

H	-3.04201700	0.05725300	-2.05964000
H	-6.48592200	1.27457700	-1.07685900
H	-6.26012400	-0.20325500	-0.12028000
H	-6.13633800	1.38910600	0.65894800
H	0.05458600	1.35920500	3.58499100
H	0.55718000	3.31060100	-1.61271100

16-ts

Ru	0.21498200	0.61832900	-0.03926200
C	0.82736100	2.49913300	1.12356000
C	-0.57942800	2.43392400	1.02910400
C	1.33819300	2.57548400	-0.21250400
H	-1.27167400	2.34860800	1.85591400
C	-0.94587200	2.57309800	-0.37506400
H	2.38516000	2.61671400	-0.48272900
C	0.23585800	2.69526500	-1.12660900
H	-1.95549900	2.60883500	-0.76259600
H	0.31115300	2.83086100	-2.19739600
H	1.41645500	2.43794200	2.02856300
C	2.15843100	-0.63765300	0.23193100
C	1.23774000	-0.66411400	1.16775700
Si	4.06158000	-0.69442700	0.26698900
C	4.67122900	-2.00751200	-0.94891700
H	4.52725100	-1.72970000	-1.99923000
H	5.74977200	-2.14936500	-0.80456700
H	4.19391900	-2.98075800	-0.78341200
C	4.75989800	0.99512800	-0.21689100
H	4.49124200	1.77245700	0.50784200
H	5.85549900	0.94563500	-0.24761800
H	4.42588700	1.31733600	-1.21054400
C	4.58928100	-1.14790300	2.02081900
H	4.23463800	-2.14279600	2.31267700
H	5.68484500	-1.16526800	2.07613800
H	4.23558600	-0.42640900	2.76567700
C	1.02417900	-1.13189600	2.55933200
H	0.89614400	-0.27758200	3.23546400
H	1.84665300	-1.75575400	2.92450900
C	0.14168600	-0.94682100	-1.55961600
C	1.56948600	-0.68445500	-1.57649300
H	2.20372800	-1.55235200	-1.75286700
H	1.91949600	0.17123600	-2.15382200
C	-0.20119700	-2.37086000	-1.13619700
H	0.29868000	-2.64327400	-0.20264500
H	-1.27238900	-2.53984000	-1.00780300
C	-0.80437800	-0.39106300	-2.59734900
H	-0.45609300	0.56248000	-3.00475800
H	-0.90364700	-1.09448100	-3.43825800
N	-2.16831500	-0.23804700	-2.04433800
H	-2.93894700	-0.35922900	-2.68998600
C	-2.52627100	-0.33693200	-0.74288900
O	-1.74099400	-0.25366600	0.23747100
O	-3.82910300	-0.52913300	-0.61247900
C	-4.54741600	-0.63947800	0.69999500
C	-4.05633900	-1.88600600	1.43610600
C	-4.35787500	0.64544000	1.50642300
C	-5.99899500	-0.79731200	0.24665700
H	-4.16279700	-2.77388600	0.80418000
H	-3.01330300	-1.78828800	1.74448200
H	-4.66707500	-2.03729200	2.33230700
H	-4.63382500	1.52144000	0.90940800
H	-5.01625600	0.61817200	2.38094500
H	-3.32979800	0.75431800	1.85724700
H	-6.64680900	-0.90782700	1.12156700

H	-6.33006800	0.07905300	-0.31901200
H	-6.11666100	-1.68443500	-0.38288600
H	0.14736500	-3.07140700	-1.90922800
H	0.09560400	-1.71372300	2.61762900

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Ru	0.20758100	0.42844400	-0.02252000
C	1.00421300	2.60379600	0.23209800
C	-0.38750900	2.70947700	0.28916000
C	1.33956700	2.04261400	-1.06151100
H	-0.97420400	3.05124800	1.13129100
C	-0.91820700	2.32097500	-1.01136200
H	2.34063300	1.87885000	-1.43595000
C	0.13978900	1.97069400	-1.85307200
H	-1.96865200	2.30965400	-1.27142000
H	0.07699000	1.65852400	-2.88652100
H	1.70366800	2.83802700	1.02252700
C	2.14752800	-0.72443100	0.20041600
C	1.34116100	-0.37077300	1.28312100
Si	4.04077200	-0.30906800	0.18151900
C	4.85778000	-1.73931000	1.11116600
H	4.61841300	-2.70879500	0.65931600
H	5.94880000	-1.62608300	1.08428600
H	4.55883600	-1.77877800	2.16490200
C	4.63674100	-0.27942700	-1.61175000
H	4.12584300	0.47270600	-2.22490000
H	5.70717500	-0.04037800	-1.63497300
H	4.51207400	-1.25155500	-2.10164400
C	4.43586500	1.33741500	1.02201900
H	4.03976300	1.40641300	2.04103900
H	5.52507900	1.44762000	1.09430900
H	4.06662900	2.19880400	0.45422400
C	1.54938500	-0.25302700	2.74689500
H	2.60450800	-0.31480200	3.03769700
H	1.03552000	-1.10037100	3.22537600
C	0.15229600	-1.60118700	-0.74206400
C	1.65768400	-1.70388600	-0.89610800
H	2.08183700	-2.71552400	-0.76886500
H	1.98863200	-1.33557700	-1.87324900
C	-0.31860700	-2.64674200	0.27722600
H	0.30923100	-2.64177400	1.17462000
H	-1.35270400	-2.53200900	0.60660400
C	-0.69825700	-1.62666900	-1.99535200
H	-0.29041500	-0.96894300	-2.77127200
H	-0.75254900	-2.64180300	-2.41857900
N	-2.09386800	-1.23998400	-1.70199800
H	-2.81810400	-1.61937500	-2.29897600
C	-2.55745600	-0.64761400	-0.58341400
O	-1.85004600	-0.10612300	0.31071800
O	-3.87833300	-0.69300700	-0.51763500
C	-4.69686200	-0.10414700	0.59345600
C	-4.35418500	-0.81000300	1.90552500
C	-4.47642100	1.40769200	0.65230300
C	-6.11866700	-0.43642300	0.13980100
H	-4.46413700	-1.89430000	1.79941100
H	-3.33861400	-0.58245700	2.23613400
H	-5.05091700	-0.47752000	2.68223400
H	-4.65044400	1.86201400	-0.32930500
H	-5.19438200	1.84620300	1.35313700
H	-3.47037200	1.65611800	0.99631000
H	-6.83569200	-0.06333400	0.87736900
H	-6.34136300	0.03065200	-0.82452200
H	-6.25453400	-1.51783900	0.04383000

H	-0.21893300	-3.64876000	-0.16863900
H	1.09710600	0.65738600	3.15181200

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Ru	1.05398200	-0.82100700	-0.23045600
C	2.23019100	-0.99766600	-2.13766400
C	0.85706000	-0.85621100	-2.47620000
C	2.38915300	-2.19154500	-1.36631000
H	0.41744400	-0.05699600	-3.05618300
C	0.17366900	-2.00767000	-1.94635300
H	3.32570300	-2.58043900	-0.98948700
C	1.10399700	-2.83996300	-1.28180400
H	-0.89042300	-2.19069200	-2.02240100
H	0.89445700	-3.79461900	-0.81800000
H	3.01600000	-0.29942100	-2.39228400
C	2.61957600	0.80274900	0.19014300
C	1.51626000	1.38840600	0.11561100
Si	0.58813700	3.01873200	0.00745700
C	1.92253900	4.35646300	0.04087400
H	2.62406600	4.25075100	-0.79442300
H	1.46427200	5.35034800	-0.03718700
H	2.49784300	4.33205200	0.97343900
C	-0.33038900	3.07345000	-1.64099600
H	-1.02671000	2.23731500	-1.75887700
H	-0.90365900	4.00418100	-1.73148100
H	0.37870900	3.04459900	-2.47709700
C	-0.55677700	3.23526600	1.49108000
H	0.01760200	3.27195400	2.42385600
H	-1.10249700	4.18317500	1.40622100
H	-1.29418900	2.43243900	1.57783900
C	4.08002500	0.64809300	0.32423700
H	4.51618200	0.09744400	-0.51648500
H	4.36289600	0.12360700	1.24305800
C	0.74607400	-1.31248900	2.02404100
C	2.00599500	-1.73194700	1.61574700
H	2.88266700	-1.18005800	1.93299400
H	2.18707000	-2.77298600	1.36281900
C	0.56649400	-0.10407000	2.91675200
H	1.42190000	0.57071800	2.85798500
H	-0.33241900	0.46645400	2.67111900
C	-0.36443800	-2.34078500	2.08306600
H	-0.09616000	-3.22774600	1.49820100
H	-0.48264200	-2.66092100	3.12741200
N	-1.67416900	-1.84270200	1.66785800
H	-2.49392500	-2.28625500	2.06067400
C	-1.93179200	-0.89933900	0.73816800
O	-1.06676800	-0.23582100	0.11934500
O	-3.24341900	-0.75011600	0.58899600
C	-3.92478300	0.11358600	-0.42097600
C	-3.68889900	1.57983000	-0.06844600
C	-3.44848600	-0.24811900	-1.82839200
C	-5.39181100	-0.27222400	-0.22388400
H	-3.99131400	1.78002900	0.96448700
H	-2.64225400	1.85854800	-0.19369300
H	-4.29337000	2.21390100	-0.72565300
H	-3.57506200	-1.32060300	-2.01505400
H	-4.05803900	0.28996600	-2.56163600
H	-2.40392900	0.02734100	-1.98630400
H	-6.01997800	0.31007800	-0.90492200
H	-5.54904900	-1.33484300	-0.43292600
H	-5.71328300	-0.06650600	0.80154600
H	0.46864100	-0.44061000	3.95869500
H	4.54303900	1.64138100	0.35550900

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Ru	0.60373800	-0.90725400	-0.27338700
C	1.30109700	-0.99889800	-2.48453600
C	-0.10780800	-1.04220300	-2.41981200
C	1.78536200	-2.12079900	-1.74592300
H	-0.78089700	-0.30383300	-2.83441900
C	-0.51228900	-2.26109500	-1.73594900
H	2.82738200	-2.36717500	-1.58536800
C	0.66204900	-2.92917300	-1.33546600
H	-1.52815500	-2.60391800	-1.59280700
H	0.72222300	-3.87737300	-0.81681400
H	1.90006600	-0.21882100	-2.93226100
C	2.52994100	-0.36138300	0.84246400
C	1.87891200	0.64893500	0.31810700
Si	2.08694900	2.47477300	-0.10275000
C	1.11746200	3.47218200	1.17692500
H	1.50902700	3.32404100	2.18989000
H	1.19246100	4.54259900	0.94877900
H	0.05409700	3.20770500	1.18167600
C	3.92236600	2.92513100	-0.03229000
H	4.51349500	2.36350200	-0.76513700
H	4.05252600	3.99103900	-0.25762600
H	4.35094700	2.74649400	0.96048400
C	1.39646900	2.78826400	-1.83232600
H	0.34829700	2.47763200	-1.90804900
H	1.44463300	3.85796000	-2.07025800
H	1.96646200	2.25973800	-2.60542200
C	3.98055200	-0.72863900	0.98957800
H	4.61466100	0.07187300	0.60089100
H	4.21900700	-1.64938100	0.44346900
C	0.19284700	-1.24636000	1.84961900
C	1.59311000	-1.62779600	1.80044500
H	2.17674300	-1.37675100	2.69242500
H	1.82772500	-2.64300000	1.47885200
C	-0.07953500	-0.04417700	2.74039100
H	0.52857400	0.81579800	2.44534500
H	-1.12685400	0.26526900	2.73966900
C	-0.92868300	-2.25743900	1.82858700
H	-0.65275000	-3.16283900	1.28011500
H	-1.19134300	-2.55726800	2.85451200
N	-2.15896800	-1.67277400	1.25734000
H	-3.04114100	-1.99998200	1.63107700
C	-2.25092300	-0.51253100	0.56678500
O	-1.28530100	0.10205900	0.04410900
O	-3.50279900	-0.08854900	0.50005800
C	-3.94733600	1.15478500	-0.21164300
C	-3.31535400	2.37203800	0.46306400
C	-3.60675900	1.05269700	-1.69835900
C	-5.45928100	1.11625600	0.01269400
H	-3.53912300	2.37909500	1.53482700
H	-2.23251800	2.39325700	0.32248800
H	-3.73665000	3.28342400	0.02609700
H	-3.98620500	0.11541900	-2.11948900
H	-4.08905000	1.87784400	-2.23258500
H	-2.53059900	1.11925600	-1.86995800
H	-5.92205400	1.99269400	-0.45099100
H	-5.89866600	0.21837400	-0.43269100
H	-5.69545200	1.12726700	1.08100600
H	0.18555400	-0.29147000	3.77869300
H	4.24021300	-0.90355900	2.04228300

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Ru	0.48642900	-0.67780000	-0.28242100
C	1.43876500	-1.00439900	-2.41290900
C	0.12953300	-0.60719400	-2.67464900
C	1.37269000	-2.21193100	-1.60801700
H	-0.18259700	0.28474600	-3.20089200
C	-0.76238600	-1.62606500	-2.13683200
H	2.22216300	-2.80241200	-1.29206700
C	-0.00208000	-2.63679100	-1.54519500
H	-1.84253100	-1.59102800	-2.19125000
H	-0.36704500	-3.54237900	-1.08035600
H	2.34271600	-0.47890700	-2.68918200
C	2.34599200	-0.83751100	0.95420300
C	1.91636900	0.38159600	0.39544300
Si	2.63575500	2.09236200	-0.04229600
C	2.80863900	3.01865900	1.59600400
H	3.46558300	2.49224400	2.29749900
H	3.24573200	4.00818100	1.41301700
H	1.84074700	3.17366000	2.08561400
C	4.32601600	1.87894200	-0.86696600
H	4.27415500	1.28849700	-1.78911600
H	4.71601000	2.86815000	-1.13798200
H	5.05665000	1.40940000	-0.19987900
C	1.43047400	2.96596900	-1.19608900
H	0.43354200	3.04138400	-0.74738700
H	1.77795500	3.98305600	-1.41432400
H	1.32885700	2.43891900	-2.15142200
C	3.71108900	-1.40558900	0.61147000
H	4.14023100	-0.98458100	-0.30072000
H	3.67915900	-2.49679700	0.51530000
C	0.16941600	-1.04331100	1.81989000
C	1.57801800	-1.55161300	2.07152000
H	1.99104900	-1.35118700	3.07599900
H	1.65734700	-2.63283700	1.90103200
C	-0.07081400	0.21194600	2.66702900
H	0.77299600	0.90629400	2.59466200
H	-0.97316400	0.77126000	2.41284800
C	-0.96943300	-2.03494500	1.95158700
H	-0.74391100	-2.97268400	1.43088100
H	-1.15656900	-2.28185000	3.00800800
N	-2.23569900	-1.47570200	1.43999700
H	-3.09637100	-1.81362000	1.85202500
C	-2.38863400	-0.39529900	0.64929600
O	-1.46216000	0.19927800	0.03190500
O	-3.65331300	-0.01185200	0.58517500
C	-4.15002300	1.16150900	-0.20662500
C	-3.51289700	2.44209600	0.33308600
C	-3.87447800	0.93592000	-1.69345000
C	-5.64973800	1.12096300	0.08831200
H	-3.68265300	2.53150900	1.41118000
H	-2.43953500	2.47560000	0.13489500
H	-3.97938200	3.30576100	-0.15227100
H	-4.27214900	-0.03215300	-2.01731700
H	-4.38243000	1.71415400	-2.27250500
H	-2.80741600	0.98592400	-1.91977700
H	-6.14881300	1.94410000	-0.43198800
H	-6.09036600	0.17942300	-0.25366100
H	-5.83887300	1.22606500	1.16077800
H	-0.14614300	-0.08264000	3.72567700
H	4.39617900	-1.18232900	1.44208700

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Ru	0.67387300	0.08143300	0.45000400
C	1.64804600	-1.00790000	2.14341700

C	0.59044700	-1.80760100	1.65489300	H	0.61115800	-0.73106500	3.04228900
C	1.09151000	0.25811100	2.55703200	C	0.57307600	-2.26969800	1.43802200
H	0.68578000	-2.79322600	1.21789600	H	-2.72583300	-2.87546300	1.19315700
C	-0.64664200	-1.07416800	1.80451400	C	-0.52438900	-2.96815300	0.81415100
H	1.63700900	1.08112800	2.99991300	H	1.62220900	-2.37641500	1.19794400
C	-0.33716700	0.17787100	2.39647000	H	-0.44631200	-3.73513000	0.05796700
H	-1.62467400	-1.42912000	1.51162500	H	-2.09668500	-1.05670500	3.06633700
H	-1.04287500	0.96206200	2.63708200	C	-2.19398300	-0.91062400	-1.55666900
H	2.69382800	-1.27854000	2.16809600	C	-2.70028300	0.11879700	-0.78470300
C	2.30846500	1.44284100	-0.66160200	Si	-4.47417700	0.31361800	-0.07890600
C	2.46749300	0.09284900	-0.95243700	C	-4.94757500	-0.86949000	1.32335900
C	-0.01797300	2.12777700	-0.49673200	H	-4.29491600	-0.77386700	2.19788600
C	1.22693200	2.26222600	-1.37032600	H	-5.96630600	-0.63162600	1.65418500
H	1.04850000	1.87862900	-2.37986400	H	-4.95421700	-1.92158600	1.01551700
H	1.52147300	3.31270600	-1.46862200	C	-4.62750400	2.10160300	0.51579700
C	-0.35595200	3.27623300	0.42387500	H	-3.96928000	2.33906500	1.35774300
H	-1.09812600	3.00863400	1.18217500	H	-4.39734500	2.80786600	-0.29090500
C	-0.93862300	1.12324900	-0.77787700	H	-5.65678400	2.30156300	0.83744500
H	-0.74977000	0.41099400	-1.58936900	C	-5.68137100	0.07178200	-1.51877400
H	1.81547000	-0.26053700	-1.77275000	H	-5.69671200	-0.95663400	-1.89560600
N	-2.26801300	1.13336400	-0.37346800	H	-6.70054600	0.31546300	-1.19379200
H	-2.71135600	1.99794900	-0.09112000	H	-5.44044100	0.73252300	-2.35992000
C	-3.09436000	0.02627600	-0.58537100	C	-2.93470500	-2.21780500	-1.74138600
O	-2.65460100	-1.04364000	-0.96924700	H	-3.71809800	-2.35783300	-0.99420900
O	-4.34822900	0.35899800	-0.29122500	H	-2.28494400	-3.09605400	-1.71689900
C	-5.47609000	-0.61511000	-0.43352600	C	0.21222600	-1.29568400	-1.86119500
C	-5.59573500	-1.03770900	-1.89849300	C	-1.01512000	-0.65982200	-2.49736200
C	-5.24571800	-1.79830000	0.50839600	H	-0.86639800	0.41540300	-2.62877900
C	-6.67939500	0.21834300	0.00590200	H	-1.20091600	-1.09087200	-3.49121900
H	-5.70883200	-0.16053800	-2.54438500	C	0.50858200	-2.73186600	-2.24714800
H	-4.72599000	-1.61199600	-2.22327400	H	1.15804800	-3.25965600	-1.54165200
H	-6.48711200	-1.66206000	-2.02032200	C	1.21195400	-0.50955200	-1.32422600
H	-5.10002000	-1.44970500	1.53703100	H	1.15361400	0.56389600	-1.32484800
H	-6.12973700	-2.44452400	0.49764900	H	-2.24705400	1.09119600	-0.97363200
H	-4.38330000	-2.39368800	0.20174200	N	2.46325000	-0.98964400	-0.98401200
H	-7.58913300	-0.38641700	-0.05877500	H	2.71102100	-1.95481300	-1.15230100
H	-6.56462800	0.55763600	1.04028500	C	3.46665400	-0.17883900	-0.44955300
H	-6.80244800	1.09465000	-0.63799600	O	3.31230400	1.00772800	-0.22926500
H	0.53094500	3.64908700	0.94460000	O	4.54873400	-0.93146500	-0.24315200
H	-0.75597000	4.11766200	-0.16110200	C	5.82914700	-0.34791400	0.25897800
Si	3.99484500	-1.06300700	-0.85752600	C	6.33276900	0.70052300	-0.73472300
C	5.22413200	-0.67745300	0.52801100	C	5.61100300	0.22163800	1.66192700
H	5.99643800	-1.45706800	0.52940500	C	6.74972000	-1.56800100	0.29203300
H	5.73682100	0.27789000	0.37237300	H	6.42480400	0.26859600	-1.73697000
H	4.78417400	-0.66336000	1.53182100	H	5.66735400	1.56481200	-0.77793700
C	4.84963800	-0.83018300	-2.52888300	H	7.32518100	1.04319900	-0.42361100
H	5.19066500	0.20170700	-2.67295600	H	5.19895300	-0.54408700	2.32857500
H	5.72968000	-1.48127700	-2.59946800	H	6.57320000	0.54269200	2.07472400
H	4.18816200	-1.08366100	-3.36582100	H	4.93840400	1.08098400	1.64420300
C	3.37683000	-2.84391300	-0.71378100	H	7.74086400	-1.27333600	0.65033700
H	3.03625700	-3.09694800	0.29636200	H	6.35598300	-2.33709200	0.96430700
H	2.55358900	-3.04882400	-1.40911500	H	6.85995400	-2.00098300	-0.70713300
H	4.18869900	-3.53840100	-0.96171000	H	-0.39575100	-3.33090800	-2.36382500
C	3.25794100	2.22142800	0.21564800	H	1.01317800	-2.73496300	-3.22465200
H	3.82413600	1.58107400	0.89243100	H	-3.41510200	-2.20813800	-2.72981300
H	3.97251100	2.76069900	-0.42367100	C	-0.23918300	1.55140900	0.45662100
H	2.73764000	2.98079500	0.80831300	C	-0.89401500	1.27637600	1.48599600
				Si	0.40050700	3.13131700	-0.38679700
				C	-1.12167900	4.24792100	-0.51272400
				H	-1.58812000	4.41372200	0.46480900
				H	-0.83378800	5.22833900	-0.91263700
				H	-1.88445500	3.83198400	-1.18165300
				C	1.68804600	3.87040300	0.77183200
22							
Ru	-0.75006500	-0.78724200	0.40760800				
C	-1.40019700	-1.54324300	2.40063100				
C	0.03880900	-1.39712600	2.41062300				
C	-1.72939600	-2.53260600	1.43164400				

H	2.55435400	3.20760300	0.85526800
H	2.03289300	4.83681900	0.38298900
H	1.28139400	4.04152900	1.77493400
C	1.12118600	2.90509300	-2.11754600
H	0.45003800	2.38858800	-2.81372700
H	1.29256200	3.90702900	-2.53221000
H	2.08683500	2.39172000	-2.10251900
C	-1.54132300	1.55452900	2.78157000
H	-2.59317800	1.25426300	2.79282400
H	-1.49481300	2.63359400	2.97176400
H	-1.03552200	1.05382500	3.61470900

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Ru	-0.69037200	-0.13556500	-0.00015200
C	-2.63020900	0.48851700	0.67664800
C	-2.40653600	-0.84460500	1.17427100
C	-2.61701500	0.42951200	-0.76054100
H	-2.35046800	-1.13366800	2.21545400
C	-2.28811300	-1.71349600	0.04906300
H	-2.76892900	1.25720900	-1.44057500
C	-2.38739300	-0.93929500	-1.14415400
H	-2.06984600	-2.77356400	0.09427600
H	-2.31130600	-1.31111300	-2.15744700
H	-2.79611200	1.36899500	1.28279200
C	0.13311500	1.79659200	-0.00834900
C	1.08500700	0.95292800	-0.00110600
Si	2.52097900	-0.25236700	0.00032000
C	3.42147800	-0.12547500	1.64188000
H	2.75276800	-0.30162200	2.49174300
H	4.22689800	-0.86904900	1.68728800
H	3.87684100	0.86314600	1.76807600
C	1.55624100	-1.89421900	-0.15841700
H	1.51227600	-2.25464600	-1.19055400
H	2.01683000	-2.67281700	0.46219400
H	0.50383700	-1.88214400	0.22820000
C	3.62361700	0.05407800	-1.48531600
H	4.11756900	1.02971100	-1.41581900
H	4.40854200	-0.71085600	-1.53591600
H	3.06270900	0.02294500	-2.42583500
C	-0.40242700	3.17298900	-0.00004400
H	-0.80468000	3.41194300	0.99147500
H	-1.21086700	3.29617300	-0.72682600
H	0.38999700	3.89221400	-0.22994700

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Ru	-0.27508500	0.66369600	0.17218200
C	-0.98478200	2.45484100	-1.10593000
C	0.35646600	2.65822100	-0.73221200
C	-1.74959800	2.35030000	0.11167500
H	1.19783600	2.73197100	-1.40913300
C	0.43212300	2.73539800	0.71566000
H	-2.82070100	2.22562500	0.17464600
C	-0.88043400	2.58480200	1.22488800
H	1.32640600	2.92138100	1.29554900
H	-1.17637200	2.61725700	2.26511900
H	-1.36737000	2.37469100	-2.11365600
C	-1.94950300	-0.76558500	0.06440600
C	-0.87811100	-1.08891900	-0.78942700
Si	-3.77718700	-0.63264900	-0.52818500
C	-4.31796800	-2.41748300	-0.85229500
H	-4.17346900	-3.05412700	0.02851900
H	-5.38521900	-2.44821500	-1.10405900
H	-3.77216500	-2.87069500	-1.68790600

C	-4.82628900	0.08631400	0.87190800
H	-5.87025500	0.15181100	0.54108700
H	-4.81181300	-0.55193900	1.76272500
H	-4.52296400	1.09364100	1.17934100
C	-4.00745200	0.39599000	-2.09834000
H	-3.45503800	-0.00055300	-2.95697800
H	-5.07053300	0.37866300	-2.37031600
H	-3.72696600	1.44669400	-1.97120300
C	-0.80146900	-1.49586100	-2.23388400
H	0.23121200	-1.48483500	-2.59622100
H	-1.36122400	-0.77103600	-2.83563100
C	-0.25866500	-0.88736200	1.71366600
C	-1.74460000	-1.16162600	1.55156800
H	-2.07666700	-2.19866100	1.75864900
H	-2.32568500	-0.50196600	2.20008500
C	0.25264700	-0.49999700	3.10654400
H	1.31414500	-0.23361900	3.09351900
C	0.46728100	-2.01849000	1.10428700
H	0.14486100	-3.03942700	1.34176500
H	-0.14854500	-1.92233700	-0.14229700
N	1.84067900	-1.98018200	0.87453800
H	2.36693300	-2.84635300	0.88720400
C	2.47039700	-0.91501800	0.25073100
O	1.86968200	0.10679700	-0.09547500
O	3.74244000	-1.17567900	0.06793300
C	4.70824800	-0.23149700	-0.61170600
C	4.25284700	-0.01027900	-2.05305200
C	4.79556600	1.05821900	0.20227500
C	6.01240200	-1.02393100	-0.54907100
H	4.14459900	-0.96560100	-2.57714200
H	3.30853600	0.53617100	-2.10299100
H	5.01477000	0.57437300	-2.57879200
H	5.04535600	0.84158600	1.24595600
H	5.59377700	1.68381800	-0.21041400
H	3.86396000	1.62669400	0.16627200
H	6.81307300	-0.44441700	-1.01845000
H	6.29782100	-1.22824000	0.48719500
H	5.91973700	-1.97513600	-1.08194800
H	-0.30397900	0.36185100	3.48296700
H	0.12203400	-1.31987900	3.82874900
H	-1.22806800	-2.49063600	-2.41520700

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Ru	0.16112600	0.06767700	-0.37990000
C	1.03652300	1.49940200	-1.87721600
C	-0.36835100	1.51927300	-1.98972600
C	1.47332200	0.16138300	-2.19113800
H	-1.00918300	2.36260600	-1.76635100
C	-0.81617900	0.21354100	-2.43923800
H	2.49756400	-0.17632400	-2.24006800
C	0.32469600	-0.59676700	-2.59205100
H	-1.83892700	-0.07427200	-2.64051700
H	0.33072900	-1.63070500	-2.90861500
H	1.66451500	2.32803900	-1.58737700
C	2.01334800	-0.12032800	0.92754900
C	1.09385500	0.78383100	1.51446200
C	0.59952000	-2.08153600	0.42811900
C	1.83067000	-1.63741100	1.22306200
H	1.70759900	-1.83075600	2.29703500
H	2.69939500	-2.21157000	0.89697600
C	0.70854300	-3.19967500	-0.57143700
H	-0.20789100	-3.32485200	-1.15457300
C	-0.58379800	-1.59344500	0.95523400

H	-0.55277400	-1.17252700	1.95679800
H	0.44339400	0.39904300	2.30115100
N	-1.92644200	-1.79956100	0.48900000
H	-2.44925500	-2.62251800	0.77463800
C	-2.60659700	-0.60944000	0.45505600
O	-1.95491900	0.46033300	0.36326500
O	-3.90921200	-0.72603600	0.51542400
C	-4.86581600	0.43998300	0.45789300
C	-4.61792200	1.34017000	1.66722900
C	-4.69852700	1.16504900	-0.87650000
C	-6.21943500	-0.26196300	0.54648000
H	-4.68476600	0.76574000	2.59694100
H	-3.64235300	1.82842900	1.61591500
H	-5.38937100	2.11663600	1.69713900
H	-4.80050500	0.46578600	-1.71339900
H	-5.48785500	1.91764800	-0.97319100
H	-3.73462900	1.67404000	-0.94237400
H	-7.01891100	0.48494800	0.52764500
H	-6.36454600	-0.94342700	-0.29730300
H	-6.30377000	-0.83241300	1.47626500
H	1.55478100	-3.06255000	-1.25069300
H	0.88974600	-4.13565700	-0.02315100
Si	3.85138400	0.31373300	0.50562200
C	4.66856700	-1.10890600	-0.45060000
H	5.67623500	-0.79016900	-0.74550900
H	4.79260400	-2.01104100	0.15891800
H	4.14731500	-1.40093400	-1.37013400
C	4.21477100	1.90547500	-0.45622700
H	3.78802500	2.80965000	-0.01240500
H	5.30489400	2.03592800	-0.44843800
H	3.91579300	1.85973700	-1.50877600
C	4.66782900	0.42911000	2.21013800
H	5.75195500	0.55610000	2.10100700
H	4.29211500	1.28227800	2.78628600
H	4.50376600	-0.47515400	2.80825800
C	1.29426000	2.27771700	1.66150400
H	1.84395300	2.49712900	2.58822000
H	1.84627700	2.72343000	0.83318400
H	0.32763900	2.78743200	1.73530900

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Ru	-0.56657100	0.65273500	-0.06591300
C	-1.42286000	2.51385000	0.80359200
C	-0.22233100	2.84800700	0.13839600
C	-1.11076900	1.54287400	1.82528500
H	-0.12445900	3.51947400	-0.70517600
C	0.86329800	2.12686700	0.77269700
H	-1.81039800	1.10903600	2.52728900
C	0.31800200	1.36339700	1.83314000
H	1.90068000	2.15975300	0.46860200
H	0.86742600	0.70528900	2.49358500
H	-2.40979700	2.87980200	0.55773600
C	-2.43302600	-0.64580100	-0.81407500
C	-2.08811800	0.34653000	-1.72677100
C	-0.36353600	-1.68540500	0.08904200
C	-1.56314500	-1.92085400	-0.83530400
H	-1.22905300	-2.13610200	-1.85717000
H	-2.11881500	-2.80129000	-0.49878700
C	-0.35890200	-2.35543400	1.44239700
H	0.38080900	-1.92442400	2.12461900
C	0.79864700	-1.13357400	-0.43251000
H	0.84042100	-0.80060800	-1.47730500
H	-1.29800900	0.09571000	-2.45299900

N	2.05679800	-1.22993600	0.14346400
H	2.25406900	-1.94577500	0.83083600
C	3.13954700	-0.49719300	-0.35340100
O	2.99997800	0.36646200	-1.20224300
O	4.24999500	-0.90093000	0.25577100
C	5.58998300	-0.32160600	-0.07801000
C	5.91040200	-0.60836100	-1.54564000
C	5.59321700	1.17296300	0.24845700
C	6.51762600	-1.09668700	0.85708300
H	5.84746200	-1.68213600	-1.75121000
H	5.23352200	-0.07475900	-2.21559800
H	6.93430700	-0.28430100	-1.75917200
H	5.29142100	1.34181000	1.28820500
H	6.60870300	1.56440100	0.12812900
H	4.93074500	1.73048600	-0.41669000
H	7.55014200	-0.76632400	0.70775800
H	6.25001000	-0.92619900	1.90472700
H	6.46762300	-2.17091100	0.65385300
H	-1.33499200	-2.29182700	1.92653100
H	-0.12828400	-3.42531800	1.32773500
Si	-4.13168700	-0.76675900	0.10201500
C	-4.00222500	-1.89161900	1.61769100
H	-5.00967600	-2.02039500	2.03292200
H	-3.62326100	-2.89457900	1.39405400
H	-3.38439100	-1.45974300	2.41378700
C	-4.86994400	0.87147800	0.69863800
H	-5.22028800	1.51836900	-0.11139600
H	-5.74589000	0.63462500	1.31593400
H	-4.18550100	1.44832900	1.33052800
C	-5.27543500	-1.56582000	-1.17588100
H	-6.26890000	-1.73036800	-0.74088600
H	-5.40401000	-0.93326100	-2.06159500
H	-4.90056800	-2.53941500	-1.51271100
C	-2.91783500	1.52418100	-2.17731300
H	-3.54752300	1.22396600	-3.02664700
H	-3.57485500	1.90874300	-1.39697700
H	-2.27889600	2.34077800	-2.52809200

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Ru	-0.84175500	-0.03953500	0.82599400
C	-1.13138200	-0.04565900	3.05573400
C	0.20395900	-0.50415500	2.74519200
C	-2.05702300	-0.95868900	2.49077300
H	1.13052000	-0.03166500	3.04197800
C	0.07630800	-1.70175000	2.00093100
H	-3.13282800	-0.88487500	2.55127800
C	-1.32154100	-1.98155900	1.81734200
H	0.90095000	-2.28705200	1.61855000
H	-1.74162800	-2.84455300	1.32245000
H	-1.38938600	0.80537700	3.66636500
C	-2.61635200	-0.13668400	-0.93554300
C	-2.61327500	1.13105900	-0.38262200
C	-0.42929100	-1.21519300	-1.25827400
C	-1.51481200	-0.42036900	-1.97053900
H	-1.10543100	0.52249700	-2.34918600
H	-1.88699300	-0.97952400	-2.83847400
C	-0.60493300	-2.72045000	-1.23503000
H	0.01635200	-3.22921500	-0.49169100
C	0.83071300	-0.66985500	-1.08040400
H	1.06257900	0.33614500	-1.38115300
H	-1.94921300	1.86787500	-0.82804900
N	1.94586100	-1.41615100	-0.75381800
H	1.89302400	-2.42371600	-0.69547300

C	3.20857100	-0.85360900	-0.55191100
O	3.41960500	0.34198300	-0.62444200
O	4.06744800	-1.83705300	-0.28035700
C	5.52040200	-1.57292000	-0.05305600
C	6.12543400	-0.93653200	-1.30575200
C	5.68588800	-0.70224000	1.19398000
C	6.07265700	-2.98000800	0.17573200
H	5.93656600	-1.56163500	-2.18500000
H	5.72198500	0.06189200	-1.48361100
H	7.20999600	-0.85421500	-1.17855100
H	5.19413600	-1.16718500	2.05569700
H	6.75124200	-0.60541100	1.42807400
H	5.27447500	0.29746800	1.04255000
H	7.15026700	-2.92832200	0.35933000
H	5.59864700	-3.45023200	1.04331000
H	5.90287200	-3.61288600	-0.70092600
H	-1.63649300	-3.00616400	-1.03898300
H	-0.34102000	-3.12841800	-2.22187600
C	0.26201800	2.00872200	0.28285400
C	-0.36462600	2.19268000	1.35134400
Si	1.21588300	3.13896500	-0.91591700
C	0.08181100	4.64131300	-1.11863700
H	-0.15304000	5.11271000	-0.15740100
H	0.57157200	5.39848100	-1.74378900
H	-0.86600200	4.37885400	-1.60377600
C	2.82304400	3.62281400	-0.06308500
H	3.46459200	2.74868600	0.07919700
H	3.36851700	4.35053700	-0.67713300
H	2.63801600	4.08437500	0.91348100
C	1.54934500	2.41788400	-2.62908800
H	0.65241100	2.02632300	-3.12374000
H	1.92402800	3.23470300	-3.25968900
H	2.31927200	1.64129000	-2.61515000
C	-0.79770600	2.99577300	2.51388300
H	-1.86403700	2.89078600	2.73380000
H	-0.60147800	4.05312200	2.29880300
H	-0.23571100	2.73680000	3.41880300
Si	-4.23669700	-1.21650400	-0.97961100
C	-5.47305300	-0.12899500	-1.91660200
H	-6.39219300	-0.69799100	-2.10324300
H	-5.75322700	0.77568000	-1.36856400
H	-5.07765400	0.18016200	-2.89161300
C	-4.97287500	-1.74000800	0.68564700
H	-5.91404600	-2.26503300	0.47785200
H	-4.33254500	-2.44522600	1.22693600
H	-5.21709600	-0.90902100	1.35502400
C	-4.04427300	-2.80140700	-2.00062300
H	-3.50541300	-2.66237000	-2.94396000
H	-3.57540600	-3.63034300	-1.45969300
H	-5.05659400	-3.13430300	-2.26354600
C	-3.69757700	1.74921200	0.46462700
H	-3.28297300	2.48902300	1.15372200
H	-4.40363800	2.28914800	-0.18069800
H	-4.26539000	1.01986400	1.04531400

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C	-2.80159000	0.21789400	0.05135800
C	-2.39541100	1.48580000	0.24694500
C	-0.44824500	-0.64478100	0.75614900
C	-1.76635100	-0.92331800	0.06509000
H	-1.57340000	-1.23199800	-0.97297300
H	-2.22106500	-1.80521500	0.54026700
C	-0.48730800	-0.57303200	2.26441300

H	0.41577700	-0.13633500	2.70623500
C	0.67257100	-0.52328700	0.02559000
H	0.65866200	-0.58655800	-1.05695900
N	1.96303400	-0.31678100	0.52355100
H	2.12804700	-0.28010600	1.51888500
C	3.06384900	-0.18825300	-0.29233300
O	3.02829000	-0.22663300	-1.50983800
O	4.15996800	-0.01827000	0.48640100
C	5.49468700	0.14075000	-0.11171600
C	5.86787800	-1.11708500	-0.90418500
C	5.53490600	1.40543700	-0.97666700
C	6.39356600	0.29447700	1.11862300
H	5.78690600	-2.00557600	-0.26808800
H	5.21616200	-1.24154100	-1.77033300
H	6.90496800	-1.03968600	-1.24979200
H	5.22035000	2.27691800	-0.39174300
H	6.55930400	1.58084200	-1.32431500
H	4.88050100	1.30684200	-1.84410900
H	7.43616900	0.42243500	0.80905300
H	6.09769000	1.16857900	1.70818800
H	6.32873200	-0.59151400	1.75888100
H	-1.33440100	0.03800900	2.59675400
H	-1.33121600	1.65950800	0.42676300
H	-0.62043000	-1.57098600	2.70697400
Si	-4.60650400	-0.26913700	-0.31943300
C	-4.71781600	-2.14936600	-0.55808600
H	-4.06501500	-2.50457200	-1.36420500
H	-4.45315400	-2.70249700	0.35093500
H	-5.74554200	-2.42931400	-0.82168300
C	-5.75761600	0.18914900	1.12052700
H	-5.43367600	-0.29615800	2.04926400
H	-5.79153500	1.26779100	1.30879700
H	-6.78277400	-0.14430900	0.91421700
C	-5.22178600	0.54018100	-1.92359100
H	-5.23310300	1.63420600	-1.86993200
H	-4.58406100	0.26021800	-2.77088000
H	-6.24222500	0.20860300	-2.15458800
C	-3.21776500	2.74557100	0.24020300
H	-2.85838700	3.43601500	-0.53567500
H	-4.28216800	2.57197800	0.06445600
H	-3.11878100	3.27820200	1.19638700

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Ru	-1.95946700	-0.87436300	0.07844600
C	-3.61567200	-0.94744300	1.57997200
C	-2.74832700	-2.08073400	1.80402000
C	-4.18520500	-1.10574600	0.28759200
H	-2.16270600	-2.26024700	2.69647200
C	-2.77828700	-2.90889200	0.65839900
H	-4.87920100	-0.41925500	-0.17907900
C	-3.64881000	-2.29010000	-0.30810500
H	-2.24103500	-3.83955100	0.53242200
H	-3.91334000	-2.69199600	-1.27697900
H	-3.82939300	-0.15277400	2.28158300
C	-2.55875500	0.56926900	-1.60273000
C	-1.99368800	1.28712900	-0.74881500
Si	-1.57644800	2.98807400	-0.06505400
C	-2.27537000	3.13233000	1.68333400
H	-1.85075200	2.39239800	2.36979100
H	-2.06729200	4.12842400	2.09294200
H	-3.36394600	3.00198400	1.68098600
C	0.28496000	3.29805400	-0.10598200
H	0.67207800	3.23089600	-1.12934000

H	0.49001700	4.31515300	0.25132600	H	6.23317900	-1.70627700	-0.87929900
H	0.86615500	2.60717400	0.51298900	H	5.02531700	-2.51270600	0.12169100
C	-2.44531000	4.21016800	-1.21302400	C	4.74896700	1.25786700	-1.35932600
H	-3.52956900	4.05188200	-1.22801300	H	4.55373600	2.26712200	-0.97737400
H	-2.26575800	5.23910900	-0.87737200	H	5.75124200	1.26463000	-1.80446900
H	-2.07684000	4.13063600	-2.24214400	H	4.03103100	1.05181400	-2.16150800
C	-3.32105600	0.24427800	-2.82287800	C	5.84055200	0.47148200	1.41754300
H	-4.30983800	-0.16285400	-2.58382700	H	5.90121300	-0.28934900	2.20396200
H	-2.80947000	-0.48806200	-3.45548200	H	6.85104600	0.59158900	1.00694200
C	0.24588400	-1.52058200	-0.93669000	H	5.56211300	1.42377700	1.88295900
C	-0.83622100	-1.87965700	-1.71327100	C	2.71917500	0.11220400	3.24004800
H	-1.06382000	-1.31412200	-2.61009400	H	2.32774100	0.97352300	3.79498700
H	-1.21410500	-2.89784200	-1.69721600	H	3.81012800	0.13349200	3.28446800
C	0.92441000	-2.51173900	-0.01909500	C	-0.67211200	0.10560700	1.08682400
H	1.29697800	-2.04125800	0.89476400	C	0.45919900	0.51178700	1.96002600
H	0.26034400	-3.33710200	0.24813600	H	0.58846200	1.59242700	2.03637200
C	1.03779200	-0.25311500	-1.27989100	H	0.37777500	0.04136800	2.93846700
H	0.62821800	0.20307800	-2.18653500	C	-1.44339900	-1.07937500	1.66478600
H	0.94921600	0.47610800	-0.47706800	H	-2.14768300	-1.51959900	0.95752900
N	2.45818200	-0.48529100	-1.45362300	C	-1.57646400	1.21372800	0.47597300
H	2.81929000	-0.84260500	-2.32697100	H	-1.19055100	2.19983800	0.75211000
C	3.36985900	-0.14085500	-0.48875700	H	-1.55629500	1.14520400	-0.61292300
O	3.05262600	0.32335100	0.60366100	N	-2.97212700	1.15133700	0.86144500
O	4.60876900	-0.39583900	-0.92993200	H	-3.32988800	1.70995300	1.62283100
C	5.81422300	-0.10841200	-0.11432700	C	-3.87440400	0.43675600	0.11362600
C	5.89913600	1.39393600	0.16753400	O	-3.54156800	-0.26966600	-0.83399900
C	5.78718000	-0.94947800	1.16453700	O	-5.11320700	0.63256700	0.58413400
C	6.94771300	-0.55653600	-1.03922800	C	-6.29561100	-0.03227900	-0.01862600
H	5.87077200	1.96036000	-0.76945700	C	-6.45992400	0.42804200	-1.46941900
H	5.08018200	1.72631900	0.80798400	C	-6.15425100	-1.55169200	0.10437100
H	6.84711700	1.61787300	0.66831600	C	-7.44040900	0.48398000	0.85507900
H	5.67488900	-2.01186200	0.92220800	H	-6.50820200	1.52120300	-1.52089200
H	6.73308800	-0.82446400	1.70223200	H	-5.63524100	0.07829700	-2.09312300
H	4.97090000	-0.64661900	1.82268700	H	-7.39669400	0.02986500	-1.87399400
H	7.91379300	-0.39346500	-0.55126900	H	-5.98759800	-1.83755900	1.14881500
H	6.85709200	-1.62089100	-1.27835900	H	-7.07954000	-2.03150400	-0.23225500
H	6.93331400	0.01194900	-1.97443500	H	-5.32894500	-1.92421900	-0.50496200
H	1.79632900	-2.93370100	-0.53405500	H	-8.39069500	0.06545800	0.50901200
H	-3.46583500	1.15645800	-3.41328900	H	-7.29493300	0.19174900	1.90002100
C	0.20022500	0.27316000	2.18163400	H	-7.50572800	1.57551600	0.80574900
N	-0.56179400	-0.08756700	1.38734800	H	-0.76055600	-1.85670900	2.01980500
C	1.19090300	0.73193800	3.14709400	H	-2.02913700	-0.74119700	2.52974300
H	1.24248500	0.04007500	3.99396700	H	2.37479100	-0.79583500	3.75076700
H	2.16072300	0.76809300	2.63988500	C	1.28841200	2.69144100	-1.09033500
H	0.92734800	1.72772400	3.51759300	N	1.13376000	1.61880100	-0.68196000
30-ts				C	1.48578300	4.03742500	-1.61712200
Ru	0.99943300	-0.38622600	-0.17515700	H	0.73735900	4.25455700	-2.38603000
C	1.70138900	-2.37136900	-0.97559900	H	1.39082700	4.77467100	-0.81352300
C	1.67174800	-1.40070600	-2.02640400	H	2.48399700	4.12268000	-2.05877200
C	0.36964400	-2.54973600	-0.50016700	31			
H	2.51317300	-1.05630700	-2.61136400	Ru	-1.91723800	-0.77753600	0.13031900
C	0.30022000	-1.00460800	-2.20816400	C	-3.97234800	-1.65563700	-0.19182200
H	0.06606100	-3.23060600	0.28265600	C	-3.75924400	-1.75332200	1.20061800
C	-0.50230700	-1.72675100	-1.28925800	C	-2.98911300	-2.48361900	-0.86272700
H	-0.06231700	-0.28538000	-2.93136600	H	-4.31703000	-1.24865000	1.97737900
H	-1.57433500	-1.61301300	-1.18474100	C	-2.64944900	-2.65293300	1.39645900
H	2.57917800	-2.87279200	-0.59380800	H	-2.94151800	-2.67261400	-1.92635600
C	2.26842000	0.12518300	1.80576200	C	-2.22160700	-3.14255200	0.14563200
C	2.88514900	-0.04375300	0.67144900	H	-2.21868600	-2.91426500	2.35475200
Si	4.65804700	-0.02559400	0.02879100	H	-1.41315800	-3.83969800	-0.01914000
C	5.16520600	-1.72523700	-0.62843000	H	-4.73979600	-1.07039600	-0.67940500
H	4.62915100	-2.01757900	-1.53798000	C	-1.94690200	0.35318400	-1.70450000

C	-1.87951800	1.03448500	-0.46439600
Si	-1.88265500	2.85971300	0.08850200
C	-3.65296400	3.41341100	-0.29320600
H	-4.39493500	2.84818500	0.28149100
H	-3.75852000	4.47110700	-0.02021400
H	-3.89683400	3.32269100	-1.35691300
C	-1.50442900	3.06611200	1.92097300
H	-0.45840300	2.83561400	2.14903000
H	-1.67860000	4.11027400	2.20880200
H	-2.14577800	2.43743800	2.54741100
C	-0.64275700	3.80383700	-0.97795300
H	-0.83245400	3.66000900	-2.04764200
H	-0.72405000	4.87824000	-0.77111900
H	0.39266500	3.50951700	-0.77304000
C	-3.14811000	0.47077500	-2.62219000
H	-4.05229800	0.79030500	-2.09768400
H	-3.35474700	-0.47216900	-3.14077600
C	-0.00784000	-0.84201700	-1.02532500
C	-0.62895200	-0.16433200	-2.27311100
H	-0.00561000	0.61880900	-2.73803200
H	-0.84801900	-0.89761800	-3.05866200
C	0.52876000	-2.24430000	-1.30539600
H	0.85751200	-2.74680100	-0.38862700
C	1.05501300	0.03772600	-0.34755800
H	0.69001500	1.07751900	-0.30444700
H	1.21978600	-0.28700400	0.67488700
N	2.37989100	-0.00792100	-0.93839400
H	2.53914500	0.27833600	-1.89470400
C	3.48931700	-0.08735500	-0.12574300
O	3.42964100	-0.25965900	1.08730000
O	4.59845800	0.04195400	-0.86927700
C	5.95344600	-0.02288000	-0.27091100
C	6.13298100	1.12371300	0.72799700
C	6.17248700	-1.39730500	0.36689600
C	6.85851200	0.16673100	-1.49002900
H	5.91989400	2.08580300	0.24917900
H	5.47722200	1.00235400	1.59191900
H	7.17093900	1.14374200	1.07724700
H	5.98974600	-2.19218700	-0.36435000
H	7.21125600	-1.48092300	0.70419800
H	5.51406200	-1.54472000	1.22469500
H	7.90873400	0.13964200	-1.18263400
H	6.69334200	-0.62802900	-2.22450200
H	6.66529100	1.13040400	-1.97230400
H	-0.21025400	-2.87817800	-1.80396300
H	1.40441800	-2.18513100	-1.96617200
H	-2.92581900	1.21832600	-3.39703500
C	-0.13274400	-0.06680600	2.74543400
N	-0.87385000	-0.24287400	1.87375300
C	0.89835000	0.14255900	3.75351200
H	1.87544400	0.11049500	3.25330600
H	0.76477300	1.11249500	4.24254200
H	0.85346000	-0.64697500	4.51019700

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Ru	-2.09308100	-0.56571700	-0.04578800
C	-4.35290000	-0.01182100	-0.24760200
C	-4.19595700	-0.67783200	0.97463100
C	-3.93256600	-0.91935100	-1.29704900
H	-4.39432500	-0.26976300	1.95692100
C	-3.70460600	-2.01907700	0.69767500
H	-3.99189100	-0.72356200	-2.35866800
C	-3.61049100	-2.17693300	-0.70280000

H	-3.50217300	-2.78168300	1.43820800
H	-3.30406400	-3.07048400	-1.22900400
H	-4.70260600	1.00187500	-0.38780600
C	-1.31488000	0.55642600	-1.72728500
C	-0.95076600	1.05849900	-0.44978500
Si	-0.59297300	2.78016700	0.30817400
C	0.50331400	3.73712000	-0.89481900
H	0.02499900	3.87140400	-1.87163900
H	0.72073900	4.73586900	-0.49649800
H	1.46433000	3.23453300	-1.05622600
C	-2.26386400	3.62928100	0.54760400
H	-2.92112500	3.03960600	1.19597700
H	-2.11223000	4.60691200	1.02225500
H	-2.78254000	3.80412900	-0.40126800
C	0.29233900	2.54930200	1.95703600
H	1.19357500	1.93197400	1.86185400
H	0.60391100	3.52753700	2.34315200
H	-0.36367900	2.09435800	2.70705000
C	-2.10879300	1.41400500	-2.69425000
H	-2.80996200	2.08524400	-2.19147600
H	-2.66489700	0.80016400	-3.40971800
C	-0.28018200	-1.36826700	-0.95267000
C	-0.52526400	-0.63150500	-2.27605700
H	0.36227900	-0.34711900	-2.87631700
H	-1.17040200	-1.21696200	-2.94027900
C	-0.06370200	-2.87661600	-1.02986700
H	-0.02093800	-3.32822600	-0.03216900
C	0.85938700	-0.65364400	-0.24363400
H	0.41041000	0.48331500	-0.23389400
H	0.94525800	-0.83615300	0.82496500
N	2.14298900	-0.68789300	-0.80395500
H	2.27611700	-0.75283300	-1.80526900
C	3.27727100	-0.45448800	-0.02086500
O	3.20894500	-0.24828700	1.17858400
O	4.35749700	-0.50374200	-0.79818700
C	5.73206000	-0.31788700	-0.24654800
C	5.85464200	1.08727800	0.34617000
C	6.02265200	-1.41892600	0.77528300
C	6.60466500	-0.47395800	-1.49216000
H	5.58596700	1.84416800	-0.39875400
H	5.21741500	1.20690300	1.22441900
H	6.89346800	1.26352200	0.64465800
H	5.86879700	-2.40748900	0.32956300
H	7.06915900	-1.35090900	1.09078000
H	5.38834500	-1.32186000	1.65831100
H	7.65872000	-0.35767000	-1.22165400
H	6.47142500	-1.46369300	-1.94020900
H	6.35562300	0.28422400	-2.24141000
H	-0.87110400	-3.36357000	-1.58487900
H	0.87929100	-3.12376300	-1.54067500
H	-1.40981600	2.03083100	-3.27645800
C	-0.77987200	-0.81859000	2.90000900
N	-1.21193500	-0.70918500	1.83053800
C	-0.20558600	-0.94907700	4.23413000
H	0.87391700	-0.77066100	4.18422400
H	-0.65539700	-0.22132000	4.91707800
H	-0.37972900	-1.95749400	4.62292500

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Ru	-1.31244600	-0.84227200	0.34261100
C	-3.49062000	-0.94964200	0.88628500
C	-2.72597000	-0.80011500	2.07225400
C	-3.11678300	-2.18269000	0.26046000

H	-2.77948300	0.02604800	2.76819500
C	-1.88734700	-1.97126800	2.20139600
H	-3.55947200	-2.59956500	-0.63322000
C	-2.14672300	-2.82230500	1.10189300
H	-1.18657800	-2.16801900	3.00212900
H	-1.67988700	-3.78116900	0.92280100
H	-4.22028500	-0.24557500	0.51501500
C	-1.70159300	0.16763100	-1.75622100
C	-1.24507400	1.13780500	-0.85964400
Si	-2.09228300	2.74282000	-0.25759800
C	-3.80757900	2.57516400	0.52811500
H	-3.79245100	1.98334900	1.44971900
H	-4.15677900	3.57972700	0.79900800
H	-4.56291800	2.15186800	-0.14345300
C	-0.93122600	3.52516200	1.01614600
H	0.09089500	3.62149300	0.62952900
H	-1.27682700	4.53242600	1.27738600
H	-0.89147200	2.94048700	1.94248500
C	-2.21415600	3.87357400	-1.77222900
H	-2.89060800	3.46915500	-2.53444100
H	-2.59657100	4.86093300	-1.48540600
H	-1.23567400	4.02505600	-2.24339400
C	-3.12006600	0.11866600	-2.27712300
H	-3.83483600	0.60952100	-1.61505300
H	-3.46024500	-0.90374000	-2.46786200
C	-0.26311300	-1.75363600	-1.57025800
C	-0.69484200	-0.67140700	-2.54968700
H	0.13224100	-0.05576500	-2.92733300
H	-1.16549000	-1.12366600	-3.42777400
C	-0.72600400	-3.16494600	-1.86997100
H	-0.45814700	-3.86586000	-1.07456000
C	0.83985900	-1.57836900	-0.74411500
H	-0.16352300	1.29467400	-0.88262200
N	1.79531300	-0.58598700	-0.90498800
H	1.76742200	0.01008700	-1.72175900
C	2.98196300	-0.56184800	-0.17501000
O	3.18003300	-1.25872700	0.80415700
O	3.80077300	0.33602500	-0.73549400
C	5.23465000	0.45055300	-0.34251100
C	5.34545400	0.89317800	1.11800500
C	5.93319300	-0.88541000	-0.60288500
C	5.74397700	1.53938800	-1.28743000
H	4.75764500	1.80196300	1.28991200
H	5.01232800	0.10662800	1.79794200
H	6.39114800	1.12474800	1.34621200
H	5.80725100	-1.18842900	-1.64771900
H	7.00574900	-0.77746300	-0.41039200
H	5.54547000	-1.67262400	0.04739800
H	6.80928600	1.71554400	-1.10947400
H	5.61456400	1.23988700	-2.33203400
H	5.20772000	2.48012900	-1.12580500
H	-1.80242500	-3.22958300	-2.04946200
H	-0.22564500	-3.50685700	-2.78736400
H	-3.14673000	0.64369600	-3.24330600
H	1.17113200	-2.38070900	-0.09315300
C	0.91132000	0.54055400	2.19466400
N	0.13634700	0.10972500	1.45074200
C	1.90713100	1.04497400	3.13117300
H	2.07583600	2.11434500	2.97034200
H	1.56607500	0.89277400	4.16026200
H	2.84411100	0.50036300	2.97934900

C	-2.17825800	0.93865000	1.00351000
C	-2.23805900	0.16633700	-0.09804700
C	-0.63636300	2.68891800	-0.16506700
C	-1.33481000	2.21441400	1.09060300
H	-0.59537800	2.06829800	1.89611500
H	-1.98578500	3.02064400	1.46171500
C	-1.31351500	3.77085000	-0.96657300
H	-0.72632800	4.05353800	-1.84663900
C	0.53947600	2.17778400	-0.56566600
N	1.20433600	1.12441600	0.07185600
H	0.69767400	0.53193800	0.71542000
C	2.45968900	0.70337100	-0.30617900
O	3.14559000	1.25500200	-1.14887500
O	2.77983700	-0.40005400	0.41113800
C	4.07629800	-1.07115600	0.22821400
C	4.19623300	-1.59740700	-1.20630600
C	5.21849800	-0.11694900	0.59493100
C	3.99372500	-2.22882500	1.22701700
H	3.34391700	-2.24252800	-1.44718200
H	4.23206500	-0.77601500	-1.92366500
H	5.11123200	-2.19256900	-1.30463000
H	5.07820200	0.27217200	1.60956600
H	6.17189200	-0.65677100	0.56684400
H	5.26902000	0.72173200	-0.10127300
H	4.91331700	-2.82239500	1.19235600
H	3.86294800	-1.85152700	2.24656400
H	3.14898500	-2.88399200	0.99017500
H	1.07353800	2.55044600	-1.43298000
H	-1.64842200	0.52134600	-0.94751500
H	-2.30391600	3.44527800	-1.31529800
H	-1.47469600	4.67576200	-0.36332700
Si	-3.19153700	-1.43052500	-0.41158400
C	-2.83152200	-1.93141900	-2.20389700
H	-1.75894600	-2.09376500	-2.36701400
H	-3.35008000	-2.86067500	-2.46977500
H	-3.15865100	-1.15760700	-2.90927500
C	-5.06440300	-1.18928400	-0.21526300
H	-5.60206500	-2.11071800	-0.47283900
H	-5.34749600	-0.91793000	0.80824800
H	-5.42934300	-0.39642100	-0.87908800
C	-2.61147400	-2.82886600	0.73524100
H	-1.53833800	-3.01830000	0.61162700
H	-2.78585300	-2.60137900	1.79327400
H	-3.14067400	-3.76280600	0.50695600
C	-2.92070100	0.64519500	2.28718500
H	-3.46948800	-0.29848000	2.25292100
H	-2.22919900	0.60380200	3.14041700
H	-3.63927000	1.44611200	2.51115700

35-ts

Ru	-0.71697500	-0.59522300	0.37604400
C	-1.16115900	-0.24689900	2.66134000
C	0.20412300	-0.00285400	2.49239500
C	-1.41697600	-1.59206200	2.18727900
H	0.71889200	0.93310100	2.66175100
C	0.83092200	-1.21931200	2.00677200
H	-2.37135700	-2.10148700	2.21773000
C	-0.15189000	-2.21642700	1.88064000
H	1.88535300	-1.32796500	1.79438300
H	-0.00675200	-3.24362200	1.57502600
H	-1.90574600	0.45206400	3.01695200
C	-2.50419500	-0.99291700	-0.87962000
C	-2.27842500	0.27012000	-0.32674200

C	-0.36814800	-1.45406300	-1.55694500
C	-1.75395400	-1.32850400	-2.17735900
H	-1.84537200	-0.54444200	-2.94220900
H	-2.12181400	-2.26277900	-2.61362200
C	0.24021200	-2.84177600	-1.61826100
H	1.17691400	-2.90695200	-1.05931600
C	0.54842700	-0.27038300	-1.91425800
H	0.35722100	0.03219400	-2.95623000
H	0.25359900	0.63852600	-1.33307700
N	1.96497100	-0.44389800	-1.70196000
H	2.52668000	-0.86581100	-2.42890600
C	2.63081500	0.26044100	-0.72858200
O	2.03895400	0.89530300	0.14391200
O	3.94771500	0.11542800	-0.87734400
C	4.93688800	0.80380600	-0.00079200
C	4.76810500	2.31842400	-0.13538700
C	4.77678800	0.31738100	1.44101600
C	6.26890700	0.34062300	-0.59227200
H	4.84242400	2.62086600	-1.18534400
H	3.80871800	2.65211400	0.26511900
H	5.56803400	2.82220500	0.41736600
H	4.82770500	-0.77640900	1.48611400
H	5.59521100	0.71461700	2.05054700
H	3.83271900	0.65506800	1.87302500
H	7.09738800	0.78954900	-0.03565600
H	6.36435600	-0.74831300	-0.53433000
H	6.35474300	0.64221700	-1.64074800
H	-0.45301100	-3.58837500	-1.21792400
H	0.44996800	-3.12516700	-2.66235400
Si	-3.14461600	1.96628500	-0.20312400
C	-3.38103100	2.52409300	-1.99352300
H	-2.42640600	2.66169000	-2.51379500
H	-3.98770100	1.81504100	-2.56762700
H	-3.90045600	3.49036300	-2.00621900
C	-2.06420400	3.16438600	0.76219500
H	-1.07136800	3.26941700	0.31030000
H	-2.52794400	4.15825600	0.78104500
H	-1.92715700	2.84722100	1.80181200
C	-4.80552900	1.66578400	0.65012100
H	-4.68918800	1.27143200	1.66588800
H	-5.34380400	2.61867600	0.72998800
H	-5.43845500	0.97456100	0.08332100
C	-3.63802300	-1.90782100	-0.46204200
H	-4.42438800	-1.86688700	-1.22882300
H	-3.30491900	-2.94956900	-0.39581800
H	-4.08061600	-1.62037500	0.49475900

36-ts

Ru	-0.87915300	-0.65711400	0.38281700
C	-1.83633000	-0.82939700	2.40825200
C	-0.71904800	0.03107300	2.56358000
C	-1.34966000	-2.13945200	2.02613800
H	-0.73767600	1.06908500	2.86241900
C	0.45443300	-0.73841000	2.25536400
H	-1.95809300	-3.02034700	1.86844200
C	0.06866200	-2.07990700	1.97779500
H	1.46774700	-0.35711600	2.26164700
H	0.73108000	-2.89969400	1.73422200
H	-2.87232600	-0.57241600	2.58499200
C	-2.44068900	-0.76586400	-1.30000200
C	-2.30312700	0.34298400	-0.47456500
C	-0.17602100	-1.46523600	-1.54211700
C	-1.39331700	-1.11938300	-2.37457500

H	-1.24027300	-0.29463300	-3.08168200
H	-1.74026200	-1.98150500	-2.95099000
C	0.29468600	-2.90266300	-1.58109200
H	1.02474000	-3.13571200	-0.80115200
C	0.74958100	-0.36473200	-1.30411500
H	0.62944000	0.50101700	-1.95958300
H	0.33901300	0.36858100	-0.23785700
N	2.10243300	-0.64642300	-1.01365200
H	2.49500100	-1.55626100	-1.20899500
C	2.93422800	0.35904100	-0.53955500
O	2.49531300	1.46197700	-0.25432200
O	4.18259900	-0.09525600	-0.45084800
C	5.30992800	0.78660200	-0.02081300
C	5.44423000	1.95049700	-1.00442400
C	5.07243900	1.25029600	1.41755200
C	6.50951600	-0.15662800	-0.10941700
H	5.55986900	1.57769900	-2.02778500
H	4.57881700	2.61470100	-0.96143100
H	6.33827900	2.53171200	-0.75518800
H	4.92594900	0.38919800	2.07938300
H	5.95333600	1.79661700	1.77086800
H	4.20645700	1.91141100	1.48717500
H	7.42006100	0.37496200	0.18361600
H	6.38204000	-1.01471500	0.55821700
H	6.64037300	-0.52593600	-1.13133400
H	-0.54894900	-3.58752400	-1.45190700
H	0.74782700	-3.13165400	-2.55828300
Si	-3.32801600	1.92079800	-0.14734900
C	-5.17127500	1.50346200	-0.14302000
H	-5.74492900	2.42940700	-0.01046900
H	-5.49766300	1.04707100	-1.08353100
H	-5.44741500	0.83196600	0.67807800
C	-2.81826600	2.74472200	1.46644700
H	-3.05935200	2.13678500	2.34552600
H	-1.74661700	2.97130800	1.48330300
H	-3.35670200	3.69437600	1.57408400
C	-2.87845300	3.01281700	-1.62523200
H	-3.16359200	2.55431900	-2.57867700
H	-3.41317100	3.96746800	-1.54432400
H	-1.80677600	3.23949100	-1.65764700
C	-3.72277300	-1.57678000	-1.33430900
H	-4.24116000	-1.40017000	-2.28756900
H	-3.50045300	-2.64898900	-1.28169400
H	-4.40247400	-1.32571400	-0.51736500

37-ts

Ru	0.84031900	-0.18654000	0.48938900
C	1.46325000	-2.12561500	1.47575800
C	0.62858200	-2.40749500	0.36396000
C	0.67149000	-1.40690000	2.44565900
H	0.90577700	-2.95396600	-0.52641700
C	-0.65766400	-1.81152500	0.60797200
H	1.02689000	-1.04359200	3.40239800
C	-0.62798200	-1.23225000	1.92393800
H	-1.50817200	-1.85766000	-0.05835800
H	-1.44966600	-0.73357900	2.41959200
H	2.49022400	-2.43781400	1.60382900
C	2.43251000	1.76903800	-0.11823800
C	2.53495200	0.42454700	-0.37492000
C	0.01461700	1.97121100	0.33064600
C	1.16573600	2.55803300	-0.45530400
H	0.99199200	2.50805300	-1.53677000
H	1.30335100	3.61499600	-0.20117700

C	-0.23234700	2.58546600	1.69729800
H	-0.88612200	1.97721900	2.32950200
C	-0.98391700	1.27948100	-0.35191800
H	-0.90498800	1.07037900	-1.41147400
H	0.98615400	-0.25507000	-1.12172700
N	-2.25185000	1.06370200	0.14200900
H	-2.55669300	1.50575400	0.99928700
C	-3.20777100	0.33180400	-0.57825800
O	-2.92996700	-0.26256200	-1.60235200
O	-4.37347700	0.41438400	0.05706900
C	-5.61507700	-0.21616000	-0.49499400
C	-5.93416700	0.41311100	-1.85183000
C	-5.42463400	-1.73176800	-0.57403600
C	-6.66075800	0.15913000	0.55438600
H	-6.01516300	1.50164200	-1.76258700
H	-5.17270400	0.17009500	-2.59548900
H	-6.89739900	0.03246000	-2.20748800
H	-5.13226800	-2.13579800	0.40159400
H	-6.37424700	-2.19779100	-0.85728700
H	-4.67332800	-2.00389100	-1.31772900
H	-7.63576000	-0.24305200	0.26245000
H	-6.39849700	-0.25349500	1.53392000
H	-6.75047100	1.24609900	0.64543000
H	0.70361600	2.72122800	2.24860900
H	-0.69125600	3.57945100	1.58960200
Si	4.08176700	-0.55618200	-0.97863900
C	5.20098700	-0.93931200	0.49898200
H	6.04589500	-1.55182700	0.15978300
H	5.61872300	-0.03613500	0.95689000
H	4.68220700	-1.50105800	1.28346800
C	4.97832000	0.52940200	-2.23714900
H	5.33091500	1.47242800	-1.80524200
H	5.85676100	0.00178600	-2.62847800
H	4.33545700	0.76993100	-3.09220300
C	3.51309500	-2.14925400	-1.81273100
H	3.17249800	-2.90422400	-1.09663200
H	2.70958600	-1.97281600	-2.53699500
H	4.35663800	-2.58432400	-2.36241700
C	3.57809000	2.57002000	0.45387200
H	4.46374300	1.97006700	0.66708800
H	3.84763700	3.36948400	-0.25080200
H	3.26651600	3.06304600	1.38332300

38-ts

Ru	0.87333100	-0.79988800	-0.25929000
C	2.08642500	-1.65233000	-1.95424500
C	0.74448300	-1.83943500	-2.35825300
C	2.32074500	-2.44910400	-0.76618800
H	0.25386500	-1.38184400	-3.20603400
C	0.15245600	-2.76523300	-1.42943800
H	3.27107100	-2.57038800	-0.26421900
C	1.12314300	-3.17886400	-0.49636400
H	-0.88401400	-3.07736800	-1.43612000
H	0.96759600	-3.87344600	0.31670200
H	2.82248900	-1.03554800	-2.45122000
C	2.45277500	0.47860400	0.40913600
C	1.27519800	1.04899100	-0.13974400
C	1.02848400	-0.69387500	1.91577600
C	2.36262500	0.10428400	1.88465500
H	2.40613400	0.97008200	2.56645500
H	3.21336000	-0.53864000	2.14169200
C	1.20960200	-2.06446300	2.58347500

H	0.30621100	-2.68042000	2.50666700
C	-0.08544200	0.07429000	2.67624300
H	-0.43236600	-0.55414200	3.50665600
H	0.34023800	0.97816400	3.12763400
N	-1.31088800	0.52867900	1.97956800
H	-2.00095500	0.93416700	2.60219700
C	-1.85828900	0.08225800	0.83253100
O	-1.23362500	-0.46094900	-0.10673300
O	-3.15973100	0.34243900	0.77929000
C	-4.09562000	-0.20511600	-0.25686900
C	-3.74994200	0.34088900	-1.64180200
C	-4.05876400	-1.73270400	-0.19461600
C	-5.44292200	0.33395900	0.22487300
H	-3.74347500	1.43477400	-1.63808100
H	-2.78090500	-0.01924600	-1.99221200
H	-4.51742900	0.01294100	-2.35107100
H	-4.26957600	-2.08534000	0.82045400
H	-4.82855100	-2.13961700	-0.85832200
H	-3.09120700	-2.12631800	-0.51525700
H	-6.23599100	-0.00522700	-0.44848300
H	-5.66966500	-0.02448600	1.23340100
H	-5.44389600	1.42815200	0.23397300
H	2.04280500	-2.62582000	2.15250400
H	1.42907900	-1.94096700	3.65618200
C	3.81527700	0.62731000	-0.23552000
H	4.35635300	1.44196300	0.26663100
H	4.42103400	-0.27776200	-0.11496500
H	3.75697500	0.87266700	-1.29893900
Si	0.68445800	2.83205400	-0.47314000
C	1.91682400	3.46747500	-1.76191200
H	1.88636400	2.88078300	-2.68679700
H	1.65366400	4.50117900	-2.01984900
H	2.94607700	3.47169700	-1.38850500
C	0.84274000	3.78723400	1.14940500
H	0.15041500	3.41117700	1.91068200
H	1.85906500	3.74462300	1.55634000
H	0.59953000	4.84329200	0.97824000
C	-1.06799000	2.90506900	-1.14692200
H	-1.81223600	2.62159400	-0.39646500
H	-1.29310600	3.93201300	-1.46094200
H	-1.19568900	2.25553100	-2.01895700

39

Ru	-0.68054400	-0.76426500	0.41494900
C	-2.13417100	-1.93465900	1.63010300
C	-2.13217200	-0.57517200	2.12447000
C	-0.87325600	-2.52061200	1.96436700
H	-2.97307800	0.10408500	2.09238800
C	-0.85771800	-0.31484800	2.68883500
H	-0.56710300	-3.53661500	1.75446100
C	-0.07899700	-1.51616200	2.56075500
H	-0.52753700	0.60524100	3.14990000
H	0.95093300	-1.62885000	2.87612400
H	-2.97992400	-2.45074800	1.19516600
C	-1.47139500	-0.02690900	-1.67073900
C	-1.30330100	0.79585100	-0.57817300
C	-0.24063500	-2.07246700	-1.26672100
C	-0.39188900	-0.95462700	-2.28359900
H	0.53612400	-0.39663200	-2.43259200
H	-0.73081500	-1.29904300	-3.27152200
C	-1.27664200	-3.18308100	-1.43638700
H	-1.16513800	-3.96480000	-0.67703400
C	1.14160700	-2.72307800	-1.18530400

H	1.18889300	-3.38212500	-0.30824900
H	1.28171200	-3.36281500	-2.06818400
N	2.28018600	-1.80769300	-1.18352500
H	3.14994500	-2.11945800	-1.59574600
C	2.35256600	-0.67342100	-0.46658400
O	1.38375200	-0.16324700	0.14448000
O	3.56297300	-0.14013200	-0.49424400
C	3.91885800	1.18010500	0.11699700
C	3.72460600	1.11161300	1.63211000
C	5.39940100	1.30343300	-0.24445100
C	3.09536800	2.28544100	-0.54498600
H	2.66981900	1.02850000	1.90193100
H	4.27192200	0.26112700	2.05208500
H	4.12500900	2.02422500	2.08611400
H	5.53818500	1.29420700	-1.32979200
H	5.79582100	2.24567200	0.14589600
H	5.97657900	0.48084100	0.18852400
H	3.44888100	3.25827000	-0.18747500
H	3.22191500	2.26233700	-1.63265300
H	2.03333900	2.19716800	-0.30510600
H	-2.30169900	-2.80950800	-1.36926600
H	-1.16649800	-3.66542500	-2.42060900
Si	-1.93028100	2.55526400	-0.15607400
C	-1.03096500	3.17354000	1.38197300
H	0.05429200	3.04852400	1.29835200
H	-1.23179200	4.24277900	1.52183300
H	-1.36355900	2.65897600	2.28991000
C	-3.80070700	2.55403800	0.14404500
H	-4.10068700	3.55517900	0.47910700
H	-4.37272400	2.33166100	-0.76266000
H	-4.10892000	1.84610000	0.92142100
C	-1.49802800	3.62658000	-1.65033500
H	-2.00197500	3.27942900	-2.55957400
H	-1.80846200	4.66409400	-1.47642300
H	-0.41947900	3.63480900	-1.84644600
C	-2.80625700	-0.07007100	-2.39641900
H	-3.57854200	0.53107700	-1.91412800
H	-2.65523200	0.30149800	-3.42012600
H	-3.17505200	-1.09789900	-2.48530600

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Ru	1.29866800	-0.62061700	-0.35867000
C	3.35127000	-0.82233400	-1.10282100
C	2.76035800	0.31551000	-1.79247000
C	2.70730400	-2.00458200	-1.58519800
H	3.08540000	1.34247500	-1.69389600
C	1.70962800	-0.15645200	-2.60576800
H	2.94647600	-3.02086700	-1.30315200
C	1.66252000	-1.58881200	-2.44492200
H	1.05808900	0.43217500	-3.23555500
H	0.94410300	-2.24105300	-2.92815000
H	4.21627700	-0.78860100	-0.45313700
C	1.49594200	0.37914400	1.67764800
C	0.97996300	1.03915200	0.57185700
C	0.89437500	-1.79289900	1.43086500
C	0.64277900	-0.67518400	2.41096800
H	-0.40667900	-0.37867900	2.47993400
H	1.02477400	-0.86604700	3.41945500
C	1.93595400	-2.81238900	1.85721600
H	2.14208300	-3.54546100	1.07097500
C	-0.30965000	-2.39285800	0.67973000
H	-0.20743200	-2.25018400	-0.42652500
H	-0.26816500	-3.48445400	0.78414700

N	-1.63086300	-1.91553400	1.01246800
H	-2.20616000	-2.44656300	1.65218500
C	-2.26743400	-1.01440900	0.19230800
O	-1.66836700	-0.40858800	-0.69721900
O	-3.55206900	-0.91309000	0.52689500
C	-4.52803800	-0.09037700	-0.24409700
C	-4.59115900	-0.59708200	-1.68622600
C	-5.83704300	-0.36486400	0.49713600
C	-4.14277500	1.38671300	-0.15336800
H	-3.65135800	-0.42279300	-2.21433700
H	-4.82106500	-1.66764500	-1.70805500
H	-5.38983900	-0.07105800	-2.21964800
H	-5.76693700	-0.04945300	1.54285500
H	-6.65352800	0.18917500	0.02379200
H	-6.08335800	-1.43078900	0.47080500
H	-4.92873600	1.99461500	-0.61391700
H	-4.05050200	1.69621400	0.89352400
H	-3.20371000	1.58683300	-0.67296000
H	2.88494300	-2.33697600	2.12239400
H	1.58913800	-3.36225500	2.74599700
Si	0.54930300	2.84280700	0.13043100
C	2.10020300	3.89455800	0.40434100
H	1.86838600	4.93924300	0.16057200
H	2.43736500	3.86820400	1.44614500
H	2.93827000	3.59196900	-0.23399900
C	-0.79929300	3.32466400	1.36263400
H	-0.44802800	3.25207700	2.39811300
H	-1.10206700	4.36454700	1.18790500
H	-1.69197000	2.69936800	1.25777500
C	-0.05589300	2.96323000	-1.64609200
H	-0.47520200	3.95984400	-1.83085800
H	0.75297500	2.81409600	-2.37004900
H	-0.83785600	2.22349700	-1.84747400
C	2.82270000	0.74184300	2.31438600
H	2.62652400	1.26628500	3.26036900
H	3.40581800	-0.15221800	2.55958500
H	3.42960700	1.38906700	1.67716500

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Ru	1.44978900	-0.72261000	-0.26649300
C	3.06158000	-0.14802400	-1.71494600
C	1.92575600	-0.46660500	-2.50148300
C	3.47514800	-1.34435300	-1.00719200
H	1.38302200	0.19782800	-3.15806800
C	1.62521200	-1.85134200	-2.26643800
H	4.33761300	-1.43157900	-0.35921300
C	2.60720200	-2.40151500	-1.39524400
H	0.79597000	-2.39126000	-2.70806200
H	2.66233600	-3.42759100	-1.05700700
H	3.56581800	0.80832000	-1.67571800
C	1.65602000	0.44709800	1.69666800
C	1.22675300	1.03893300	0.51649900
C	0.69583000	-1.68615700	1.54658900
C	0.75845500	-0.51467100	2.50036600
H	-0.20744200	-0.05959000	2.74015200
H	1.25212700	-0.78211700	3.43846300
C	1.35126700	-2.97395200	1.99591500
H	1.34636700	-3.73530800	1.21031200
C	-0.45387000	-1.75342800	0.61988200
N	-1.68393400	-1.12880900	1.02572200
H	-2.05453200	-1.35958700	1.93927100
C	-2.59509400	-0.73278400	0.05517500
O	-2.28200100	-0.65817800	-1.12487500

O	-3.76377100	-0.44410600	0.62268200
C	-4.93488600	0.02352900	-0.17739600
C	-4.59530700	1.35899200	-0.84194700
C	-5.32697700	-1.05686800	-1.18734600
C	-6.01093100	0.19630700	0.89461500
H	-4.27453900	2.09101400	-0.09221000
H	-3.81097000	1.24369000	-1.59264800
H	-5.48962600	1.75471600	-1.33487100
H	-5.50423500	-2.01129000	-0.68007600
H	-6.25718700	-0.76349000	-1.68527600
H	-4.55685200	-1.19445500	-1.94873400
H	-6.93935000	0.54600400	0.43258500
H	-6.21412100	-0.75311400	1.39973100
H	-5.70080600	0.93113400	1.64426100
H	-0.27298100	-1.10918600	-0.43637900
H	-0.58655100	-2.75563800	0.19546100
H	2.38853600	-2.80614900	2.30293700
H	0.81900400	-3.38821800	2.86599000
Si	0.95077100	2.83375500	-0.07451200
C	2.35800300	3.92875400	0.55363000
H	2.16826800	4.96468800	0.24567200
H	2.43531000	3.92007900	1.64606900
H	3.33115800	3.64153300	0.13908200
C	0.80868600	2.91675000	-1.94838300
H	0.02516800	2.24840500	-2.32143000
H	0.54310000	3.93783700	-2.24896100
H	1.74865100	2.66763400	-2.45313600
C	-0.68955600	3.29546900	0.74576400
H	-0.62971000	3.25145000	1.83890600
H	-0.95531700	4.32337700	0.46907700
H	-1.50595200	2.64248100	0.41838100
C	2.95275200	0.85440400	2.37204300
H	2.72377400	1.40165400	3.29738700
H	3.53229400	-0.03190300	2.65507100
H	3.57759800	1.48762900	1.73870600

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Ru	1.53302000	-0.63881800	-0.25176800
C	3.05246900	0.04085200	-1.76700100
C	1.93089800	-0.43047800	-2.49425200
C	3.61705800	-1.07392100	-1.03365700
H	1.30073400	0.14338600	-3.15834200
C	1.79055200	-1.83215100	-2.19713700
H	4.50125100	-1.03999800	-0.41019300
C	2.85697500	-2.23222600	-1.34429100
H	1.01758900	-2.47918200	-2.59375800
H	3.03353000	-3.22966400	-0.96432200
H	3.44849900	1.04758200	-1.78084500
C	1.66403700	0.59262200	1.67532100
C	1.11840700	1.09662700	0.49960500
Si	0.55811800	2.81047400	-0.12566300
C	2.90425100	1.20974700	2.29727900
H	3.61919900	0.42789700	2.57973900
H	2.62732500	1.74493000	3.21669000
C	0.84862200	-1.63825100	1.59256700
C	0.94258900	-0.45970800	2.53814600
H	-0.00390600	-0.07878800	2.94540500
H	1.57155100	-0.71037200	3.39649800
C	1.58207600	-2.90008400	1.99805800
H	1.55905600	-3.65923600	1.21060900
C	-0.30561500	-1.74976800	0.71687200
N	-1.54039500	-1.15140700	1.05949600
H	-1.68975800	-0.76197800	1.97970700

C	-2.50796700	-0.95704900	0.08373400
O	-2.31941800	-1.30460900	-1.07137200
O	-3.57067300	-0.35265000	0.61367700
C	-4.82417100	-0.13919000	-0.17351100
C	-4.53894100	0.80258000	-1.34492700
C	-5.37175900	-1.49417200	-0.62519500
C	-5.74409600	0.51710200	0.85576600
H	-4.09696600	1.73938700	-0.98754300
H	-3.86794500	0.34315500	-2.07296300
H	-5.48059200	1.04757500	-1.84752800
H	-5.51518900	-2.15756200	0.23428700
H	-6.34569800	-1.34752600	-1.10367900
H	-4.70545800	-1.97667000	-1.34314600
H	-6.71543100	0.73100600	0.39924500
H	-5.90454800	-0.14375700	1.71321200
H	-5.31872100	1.45928700	1.21616200
H	-0.08213600	-1.07976900	-0.47752400
H	-0.42651900	-2.72951100	0.25227400
H	2.62779600	-2.69122600	2.24510800
H	1.11415200	-3.33642200	2.89345000
H	3.40739800	1.90907700	1.62612200
C	-1.08682800	3.04947700	0.78100300
H	-1.79250200	2.23377600	0.58701800
H	-0.94228900	3.12670300	1.86463300
H	-1.55707100	3.98151000	0.44346200
C	0.31159400	2.78723000	-1.99076500
H	-0.36563900	1.98268900	-2.29754000
H	-0.13067000	3.73626500	-2.31773600
H	1.25648500	2.66865700	-2.53303400
C	1.81085500	4.12970300	0.38497900
H	2.78874900	3.98449800	-0.08833200
H	1.44163700	5.11376200	0.06974500
H	1.95701100	4.16614200	1.46971600

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Ru	1.42383600	-0.64419500	-0.28069600
C	3.09528800	-0.57810000	-1.82562500
C	1.85706100	-0.72787100	-2.50429100
C	3.32607500	-1.76629800	-1.04413400
H	1.41745800	-0.02561600	-3.19812300
C	1.29835600	-2.00068600	-2.11771300
H	4.19840500	-1.96522400	-0.43516100
C	2.23127800	-2.64156400	-1.25186900
H	0.36542400	-2.41778300	-2.47230400
H	2.10758300	-3.61800500	-0.80259900
H	3.76958100	0.26395600	-1.90956900
C	1.91853300	0.63413700	1.53014900
C	1.30001500	1.15602600	0.38724300
C	0.80443800	-1.43079200	1.78287000
C	1.09853300	-0.15549100	2.55595600
H	0.21368400	0.39591600	2.90058900
H	1.70160700	-0.36654400	3.44366200
C	1.59897600	-2.65594600	2.19112000
H	1.41508600	-3.50732900	1.53017100
C	-0.36802200	-1.57870100	1.03339000
H	0.04483000	-0.17004500	-0.89529600
H	-0.55447800	-2.51553100	0.51877500
N	-1.51696400	-0.81922700	1.16946300
H	-1.55678500	-0.04753400	1.82158500
C	-2.57247900	-0.94182400	0.26193000
O	-2.56283100	-1.75542900	-0.64162300
O	-3.50997700	-0.04322600	0.57187900
C	-4.82037600	-0.00522900	-0.14640900

C	-4.58425100	0.34059500	-1.61790200
C	-5.53660100	-1.34454100	0.03797700
C	-5.55551200	1.12157700	0.57911600
H	-4.02196300	1.27681200	-1.70828800
H	-4.04235900	-0.45492400	-2.13249500
H	-5.54998500	0.48048300	-2.11490500
H	-5.63586700	-1.58499400	1.10181000
H	-6.54347200	-1.27551100	-0.38692900
H	-5.00583500	-2.15565500	-0.46414500
H	-6.54972600	1.25517800	0.14178600
H	-5.67550300	0.88894200	1.64184000
H	-5.01062200	2.06689200	0.48817300
H	2.67644100	-2.46258600	2.21798700
H	1.29470100	-2.95580900	3.20418600
Si	0.77295000	2.87476800	-0.25167200
C	-0.87060000	3.17545200	0.64068000
H	-1.28666100	4.13728500	0.31534500
H	-1.61565200	2.40303500	0.41754200
H	-0.73969300	3.22847700	1.72771000
C	0.54401800	2.83630200	-2.11859700
H	0.15826400	3.80226000	-2.46669700
H	1.48890200	2.65613300	-2.64411600
H	-0.17199200	2.06535100	-2.42391800
C	2.07121400	4.14384700	0.26556100
H	3.04170000	3.96440400	-0.21086700
H	1.74123500	5.14513800	-0.03806700
H	2.22125200	4.16252300	1.35060000
C	3.30622200	1.08120800	1.94651600
H	3.23505100	1.74457400	2.82010000
H	3.91826200	0.22075900	2.24307400
H	3.82925600	1.61400900	1.14851000

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Ru	0.99509600	-0.91068000	-0.24405400
C	2.14065400	-1.53765700	-2.08741400
C	1.02997800	-0.75393700	-2.47965900
C	1.64094700	-2.75846300	-1.49024300
H	1.06293600	0.19727400	-2.99258800
C	-0.16486900	-1.44704300	-2.05706000
H	2.24938500	-3.56524100	-1.10076100
C	0.23417200	-2.71215400	-1.50800100
H	-1.18676500	-1.12641400	-2.20476000
H	-0.43598200	-3.47464800	-1.13272200
H	3.18339500	-1.29551600	-2.24105700
C	2.04380400	0.35191700	1.83858600
C	1.93421100	0.68999400	0.51077800
C	0.28815400	-1.34372400	1.88552200
C	0.85820300	-0.17230700	2.65022600
H	0.14566700	0.64697600	2.81131400
H	1.19433200	-0.48794200	3.64301700
C	0.83209300	-2.70849400	2.28065100
H	0.48266200	-3.49767500	1.60964300
C	-0.90754100	-1.27255900	1.16926900
H	0.27718200	0.52650200	-0.26110500
H	-1.31653100	-2.17829200	0.73767100
N	-1.84844100	-0.26133000	1.22548100
H	-1.71324300	0.55255800	1.81050000
C	-2.94090100	-0.24211000	0.35313800
O	-3.11770400	-1.10568000	-0.48773900
O	-3.68039900	0.83225200	0.61743000
C	-4.96367700	1.10134200	-0.10198800
C	-4.67793900	1.31065000	-1.59014600
C	-5.93917400	-0.04771700	0.15840900

C	-5.43905300	2.39477900	0.55946400
H	-3.93003200	2.09873000	-1.73225400
H	-4.32782600	0.39143700	-2.06347500
H	-5.59817100	1.62786100	-2.09200300
H	-6.07364900	-0.20235700	1.23419700
H	-6.91483200	0.20550300	-0.26959300
H	-5.59455800	-0.97831000	-0.29645200
H	-6.38933100	2.70796200	0.11622400
H	-5.59142000	2.25062600	1.63361600
H	-4.71060200	3.19907700	0.41459700
H	1.92737600	-2.73293600	2.29015500
H	0.49086400	-2.96066600	3.29498600
Si	2.75582100	2.15420000	-0.43802600
C	3.34482100	0.47699200	2.59480300
H	3.21140000	1.15363600	3.45074700
H	3.62685900	-0.50002800	3.00729000
H	4.16951900	0.83899700	1.98066800
C	4.01801200	1.54113800	-1.70394000
H	3.55374000	1.03483300	-2.55648400
H	4.57307400	2.39974700	-2.10183400
H	4.75148900	0.85963000	-1.25748200
C	3.59123200	3.34499100	0.76926000
H	4.53804500	2.96681600	1.16843000
H	3.81785900	4.27784400	0.23784400
H	2.94419500	3.60420000	1.61522200
C	1.32073200	3.05425100	-1.27571400
H	0.77768900	2.41828700	-1.98284700
H	0.59948500	3.42990800	-0.54007800
H	1.70081300	3.92015700	-1.83142200

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Ru	-0.60532400	-0.85432200	0.36107300
C	-2.10809500	-1.01519700	1.95419100
C	-1.13599300	-0.04462400	2.39021700
C	-1.44515900	-2.27279100	1.81843900
H	-1.32403700	0.99375300	2.61860700
C	0.11508200	-0.70881300	2.50590900
H	-1.91051700	-3.20621200	1.52953300
C	-0.05999800	-2.08003400	2.14576100
H	1.05522500	-0.24791700	2.78108400
H	0.71461100	-2.83516700	2.14561900
H	-3.16342400	-0.83790400	1.80210500
C	-1.99564500	-0.19351400	-1.41236300
C	-1.43148400	0.94441000	-0.82472600
C	-0.57009500	-2.08096700	-1.66475900
C	-1.22714100	-0.97560000	-2.47792300
H	-0.50191100	-0.34559000	-3.00866200
H	-1.89206700	-1.39827500	-3.23795500
C	-1.13606100	-3.47498200	-1.78050200
H	-0.68433600	-4.16821900	-1.06489900
C	0.65562900	-1.91424400	-1.01801400
H	-0.50971300	1.28825600	-1.30815700
H	1.24515000	-2.73332900	-0.62302400
N	1.23957600	-0.62780700	-0.90608900
H	1.12756100	0.01567500	-1.68704300
C	2.53016800	-0.49913900	-0.26377100
O	2.94754200	-1.34141900	0.49474300
O	3.06323600	0.64008200	-0.66017800
C	4.42324500	1.09291200	-0.17892600
C	4.38191400	1.26372600	1.33880900
C	5.46754000	0.07719000	-0.64022200
C	4.58408500	2.43244600	-0.89364200
H	3.57057100	1.93929000	1.63116900

H	4.26120300	0.30667800	1.85046500
H	5.32451900	1.71127600	1.67061500
H	5.42145100	-0.06071900	-1.72556200
H	6.46447800	0.45616800	-0.39279900
H	5.33804200	-0.88905700	-0.14852600
H	5.55235000	2.87005000	-0.63233200
H	4.54807800	2.30443300	-1.97988300
H	3.79905300	3.13458300	-0.59558900
H	-2.21998000	-3.48200700	-1.62853000
H	-0.95387900	-3.86022800	-2.79337000
Si	-2.26088500	2.49993700	-0.07894700
C	-3.45023900	-0.58216900	-1.27044800
H	-3.99354700	-0.24666400	-2.16615700
H	-3.58663800	-1.66667800	-1.20559800
H	-3.92315000	-0.12518000	-0.40064400
C	-3.71532900	2.22789600	1.10211800
H	-3.47208900	1.63749700	1.99117400
H	-4.05105000	3.21110700	1.45602000
H	-4.57640100	1.76226200	0.61008600
C	-2.88081800	3.47949600	-1.57571800
H	-3.67620800	2.94649400	-2.11001400
H	-3.28980600	4.44635100	-1.25739700
H	-2.07642900	3.68365400	-2.29225800
C	-0.88579700	3.47619300	0.77833300
H	-0.45571500	2.94572000	1.63561800
H	-0.06700500	3.69501500	0.08158000
H	-1.26585800	4.43812100	1.14231400

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C	-2.28826200	-0.18942500	0.00013900
C	-1.16751900	-0.64877200	0.00019600
C	-3.59556700	0.42409100	0.00011400
O	-3.79860300	1.62142100	0.00071700
O	-4.57289500	-0.51027400	-0.00062200
C	-5.91012300	0.01505300	-0.00064300
H	-6.08361800	0.62696100	-0.89007900
H	-6.56356400	-0.85780300	-0.00111600
H	-6.08393000	0.62624600	0.88922000
C	0.19184100	-1.18355100	0.00039000
C	1.28419700	-0.09206200	0.00051200
H	0.31863500	-1.83461500	-0.87655600
H	0.31837900	-1.83452500	0.87744000
C	2.69900700	-0.68318200	0.00023600
H	1.14530400	0.55049500	-0.87808800
H	1.14549900	0.55007500	0.87945200
C	3.80118600	0.38400800	-0.00010000
H	2.82251000	-1.33317500	0.87938900
H	2.82211000	-1.33330200	-0.87887900
H	3.67765000	1.03410100	-0.87887900
H	3.67781800	1.03451800	0.87839500
C	5.21911800	-0.20279200	-0.00009100
C	6.31538200	0.86767000	-0.00059800
H	5.34164200	-0.85285500	-0.87816400
H	5.34187200	-0.85226600	0.87838400
H	6.24084600	1.51171500	-0.88558000
H	6.24101400	1.51239000	0.88390800
H	7.31426100	0.41664100	-0.00052000

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C	0.02684800	2.34467100	-0.11364300
C	-0.84641700	3.16321200	-0.70485500
H	-1.91430600	2.96643900	-0.69492700
H	-0.51799200	4.06093700	-1.22264100

C	-0.36980900	1.07203400	0.61513300
H	-0.02594700	0.19871100	0.05214600
H	0.14995600	1.03745400	1.58290500
C	1.51400000	2.64499500	-0.11107500
H	1.70655500	3.57613200	-0.65573000
H	1.87275300	2.77612200	0.91532800
N	2.33067100	1.58054700	-0.67798300
H	2.24418800	1.35791800	-1.65976100
C	3.01715800	0.69361400	0.10725700
O	3.08677000	0.76408100	1.32577400
O	3.59904100	-0.24098400	-0.68163900
C	4.40330000	-1.32876900	-0.10276000
C	5.62283000	-0.74963700	0.62287300
C	3.53470800	-2.19298000	0.81783500
C	4.83228300	-2.11860000	-1.34272500
H	6.19579800	-0.10409700	-0.05218100
H	5.31877100	-0.16820800	1.49463800
H	6.27802900	-1.56473300	0.95096900
H	2.64910600	-2.55027400	0.28072000
H	4.10688200	-3.06689800	1.14958900
H	3.21315300	-1.62929700	1.69492300
H	5.45218000	-2.97239500	-1.04959300
H	3.95732200	-2.49478500	-1.88297200
H	5.41236800	-1.48615200	-2.02279900
N	-1.79226800	0.89456900	0.80773000
C	-2.50951800	-0.07146800	0.15722600
H	-2.30661900	1.54682700	1.38172300
O	-2.02765300	-0.90908200	-0.58892300
O	-3.82057700	0.05746400	0.48632300
C	-4.82581300	-0.87903100	-0.03441200
C	-4.89434700	-0.78428600	-1.56294700
H	-3.96602200	-1.13285000	-2.01796500
H	-5.72342200	-1.39781300	-1.93379400
H	-5.07383700	0.25156700	-1.87227100
C	-4.51830300	-2.30256000	0.44465100
H	-5.33309600	-2.97460200	0.15174300
H	-3.58655000	-2.66887300	0.01085900
H	-4.43469400	-2.32612200	1.53696300
C	-6.12104400	-0.36261300	0.59924600
H	-6.96730700	-0.98321000	0.28621100
H	-6.05544400	-0.39124800	1.69190500
H	-6.31655900	0.67031400	0.29267700

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Ru	0.01727800	-0.48742300	0.93417600
C	0.48712900	-0.80707900	3.14698400
C	0.04624100	-2.04582300	2.60420300
C	-0.55875000	0.15447700	2.99653900
H	0.65301700	-2.93744400	2.53153900
C	-1.30497100	-1.88256700	2.15886500
H	-0.54590700	1.17986200	3.33994500
C	-1.67645200	-0.53049500	2.40578300
H	-1.93210800	-2.65240500	1.72987600
H	-2.63352900	-0.08134500	2.16440500
H	1.46745100	-0.62760900	3.56454200
C	1.68836700	0.90923800	0.39993800
C	2.15756600	-0.13168200	0.92746300
C	-1.37826000	-0.00546200	-0.80843900
C	-1.19542800	1.14540200	-0.03206600
H	-0.56295800	1.94657100	-0.39186300
H	-1.98290000	1.46154600	0.64227800
C	-2.71483700	-0.76832600	-0.80074200
H	-2.63359900	-1.64527100	-1.44991400

H	-2.97087500	-1.12133800	0.19531000
C	-0.62597500	-0.09407600	-2.12712200
H	-1.28614800	0.26052400	-2.92901200
H	0.25038600	0.56270400	-2.11814100
N	-0.24705700	-1.45586300	-2.49186600
H	-0.31528500	-1.74585900	-3.45800200
C	0.46834800	-2.27061200	-1.68441600
O	0.72688500	-2.02180200	-0.48800700
O	0.84880300	-3.36904500	-2.31694300
C	1.51849300	-4.53745600	-1.66130500
C	2.87874000	-4.11346900	-1.10733000
C	0.59207500	-5.11342400	-0.59024200
C	1.67565400	-5.50342500	-2.83628100
H	3.46140200	-3.59676600	-1.87764700
H	2.78166700	-3.47010600	-0.23145900
H	3.43481200	-5.00970600	-0.81196700
H	-0.38701100	-5.35937500	-1.01529800
H	1.02883400	-6.03685300	-0.19594500
H	0.46017700	-4.41777500	0.24135800
H	2.15299600	-6.42614300	-2.49248900
H	0.70213900	-5.75829200	-3.26632300
H	2.29977100	-5.06446900	-3.62072400
C	3.25182100	-1.00010700	1.36442400
O	3.12364000	-2.03722800	1.98935100
O	4.43193300	-0.48339400	0.98505500
C	5.60080700	-1.22935800	1.39245300
H	5.57982900	-2.23231200	0.96007200
H	6.44819700	-0.66101700	1.01140800
H	5.64178200	-1.30401700	2.48161800
C	1.87353300	2.25465900	-0.18792900
C	3.33710700	2.74101300	-0.13055100
H	1.22399000	2.96990900	0.33572000
H	1.52870800	2.25020800	-1.23237600
C	3.50564700	4.12933000	-0.76159700
H	3.66192000	2.76374700	0.91718400
H	3.97948500	2.01207400	-0.63887100
C	4.94724200	4.65141300	-0.69074500
H	3.18257200	4.09468300	-1.81271000
H	2.83641300	4.84278500	-0.25849800
H	5.26802900	4.68858900	0.36060500
H	5.61809800	3.93674700	-1.18972700
C	5.12232300	6.03860100	-1.32371600
C	6.56189000	6.55706000	-1.24373800
H	4.44799700	6.75032800	-0.82694300
H	4.80395000	5.99948300	-2.37502900
H	6.89707300	6.63822400	-0.20255300
H	7.25561800	5.88562600	-1.76426200
H	6.65287300	7.54837900	-1.70062400
N	-3.82384700	0.05113200	-1.26888700
C	-4.59924600	0.74172000	-0.36812200
H	-4.19631300	-0.06785000	-2.20011200
O	-4.31845000	0.82684100	0.82471300
O	-5.65180700	1.28252300	-0.99122300
C	-6.66570200	2.08991900	-0.26421300
C	-6.00184300	3.33003200	0.33985600
H	-6.77105000	3.97815800	0.77319000
H	-5.29406200	3.05888400	1.12523100
H	-5.47795900	3.90036200	-0.43503800
C	-7.35691200	1.21951600	0.78850400
H	-8.18434700	1.78004500	1.23658800
H	-7.77243400	0.31734500	0.32663700
H	-6.66578200	0.92787900	1.58137300
C	-7.63642100	2.47616800	-1.38156300

H	-8.07011600	1.58505700	-1.84631900
H	-8.45067200	3.08262500	-0.97265500
H	-7.12718400	3.05904800	-2.15577000

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Ru	1.23299000	0.00695100	0.82512000
C	2.61305900	0.74918000	2.38435600
C	2.51595800	-0.67345200	2.54664100
C	1.31270300	1.29752200	2.63079800
H	3.32377400	-1.38492700	2.43430500
C	1.17676800	-0.98797300	2.89636300
H	1.04821000	2.34552400	2.58963400
C	0.41483500	0.22383600	2.91792200
H	0.79774700	-1.97889900	3.09840600
H	-0.63504600	0.31983400	3.16131800
H	3.50048100	1.30924300	2.13295100
C	0.06758700	1.44721300	-0.69630800
C	1.23261100	1.77753800	-0.25315400
C	0.06193000	-1.60655600	0.02392000
C	-0.55237600	-0.44128800	-0.61179400
H	-0.42958500	-0.42557400	-1.69323900
H	-1.55950400	-0.21158900	-0.27915900
C	-0.84965700	-2.36798300	1.00561200
H	-0.27360100	-3.13282400	1.53608600
H	-1.27314700	-1.67926300	1.73873900
C	0.81313000	-2.54620500	-0.93790500
H	0.33579000	-3.52987500	-0.92327700
H	0.72307000	-2.16750600	-1.96345100
N	2.23360000	-2.77315200	-0.64377100
H	2.61777600	-3.68203500	-0.87331600
C	3.08823900	-1.73300400	-0.80368600
O	2.70867600	-0.54253900	-0.70265500
O	4.32287400	-2.11090500	-1.07538100
C	5.46256700	-1.15954500	-1.30114800
C	5.17712300	-0.34150700	-2.56056400
C	5.67350800	-0.29042700	-0.06098900
C	6.63383200	-2.11894200	-1.51042400
H	4.99384000	-1.00078900	-3.41526700
H	4.31708600	0.31819800	-2.42625400
H	6.05120500	0.27543900	-2.79394700
H	5.77032900	-0.91367600	0.83519000
H	6.60815600	0.26858600	-0.17696000
H	4.86090400	0.42544100	0.07645400
H	7.54534800	-1.54742800	-1.71020600
H	6.80067700	-2.73390800	-0.62056600
H	6.44851200	-2.77987800	-2.36235900
N	-1.95605400	-3.04270300	0.33314400
C	-3.19414600	-2.43977200	0.24341500
H	-1.95320000	-4.05075900	0.26158500
O	-3.38258900	-1.25762900	0.50494600
O	-4.09912700	-3.33400300	-0.17370900
C	-5.51492700	-2.95824900	-0.42192700
C	-6.16113700	-2.49390500	0.88570700
H	-5.71661100	-1.56237200	1.24045100
H	-7.23199500	-2.33005200	0.72382500
H	-6.05112300	-3.26034500	1.66048600
C	-6.12406700	-4.27794700	-0.89855100
H	-7.18715800	-4.13854100	-1.11842500
H	-5.62677600	-4.63064000	-1.80776800
H	-6.02990100	-5.05037300	-0.12870700
C	-5.57965300	-1.89472500	-1.52125300
H	-5.13134100	-0.95569900	-1.19162200
H	-5.06282300	-2.24313300	-2.42231400

H	-6.62618300	-1.70758400	-1.78459700
C	2.03749500	2.99884400	-0.43746900
O	1.73518100	3.87680900	-1.22020100
O	3.13559000	3.04018700	0.34618600
C	3.94331300	4.22976600	0.19809600
H	3.36138000	5.11760200	0.45572600
H	4.77733900	4.10101000	0.88735200
H	4.29917100	4.31917100	-0.83059500
C	-1.08951800	2.10729800	-1.37308700
C	-2.19883400	2.56406400	-0.39944800
H	-1.51952800	1.45667600	-2.14414600
H	-0.65809500	2.98154000	-1.87696400
C	-3.33463600	3.29453800	-1.13056800
H	-2.60866800	1.69838700	0.13721700
H	-1.75653000	3.22899900	0.35403300
C	-4.44838700	3.76485800	-0.18551500
H	-2.92305000	4.15852800	-1.67117500
H	-3.76161600	2.62788900	-1.89388600
H	-4.85576400	2.89824800	0.35579700
H	-4.02044400	4.42997500	0.57901700
C	-5.58953400	4.49362200	-0.90858000
C	-6.70195700	4.95518500	0.03848300
H	-6.01232200	3.83040800	-1.67643600
H	-5.18145000	5.36092200	-1.44618900
H	-7.15477200	4.10532200	0.56372000
H	-6.31585700	5.64645500	0.79749100
H	-7.49889500	5.47213900	-0.50699700

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Ru	-1.20648300	-0.32923500	1.00111200
C	-0.80434200	-1.18201500	3.03396400
C	-2.21689800	-1.03715400	3.00682200
C	-0.20632400	0.13302300	2.95675700
H	-2.94811800	-1.83265200	3.04565600
C	-2.48861100	0.36416900	2.90882000
H	0.85052600	0.35428800	3.02410800
C	-1.27130000	1.08449600	2.92009300
H	-3.47325500	0.80437000	2.81591800
H	-1.16945800	2.15962600	2.87963800
H	-0.26200600	-2.11243800	3.12868600
C	0.59000900	-1.18318400	0.12573300
C	-0.70418800	-1.60338200	-0.27193700
C	-0.10810900	1.03746000	-0.30002100
C	1.09638700	0.09021800	-0.54884300
H	1.35826300	-0.04083000	-1.61001000
H	1.99474800	0.44395000	-0.03431000
C	0.30028100	2.35583900	0.38475900
H	-0.58468800	2.98119600	0.54804600
C	-0.87490700	1.29124900	-1.59781500
H	-0.34461400	2.04692600	-2.19142600
H	-0.92255800	0.37952200	-2.20085100
N	-2.23925500	1.80669800	-1.40151300
H	-2.57119600	2.52170700	-2.03687100
C	-3.21286100	1.03392900	-0.87953300
O	-2.99448800	0.02461500	-0.15859700
O	-4.42279700	1.45400100	-1.20121900
C	-5.69924100	0.79137600	-0.78155800
C	-5.75419000	-0.61125000	-1.38747500
C	-5.81073800	0.78696000	0.74310900
C	-6.74844600	1.71030600	-1.40792300
H	-5.61342600	-0.56742100	-2.47224900
H	-4.99502900	-1.26655000	-0.95485300
H	-6.73894600	-1.04864300	-1.19214500

H	-5.65434400	1.79414300	1.14495200
H	-6.81913000	0.46764100	1.02600800
H	-5.09533400	0.09762600	1.19569400
H	-7.74967700	1.32496300	-1.19240500
H	-6.67393700	2.72374400	-1.00156300
H	-6.62429900	1.75949200	-2.49381000
H	0.76364500	2.15664000	1.35105700
N	1.26907900	3.12349300	-0.39474200
C	2.60348500	3.12995100	-0.04710400
H	0.95640700	3.91266700	-0.94282600
O	3.09229600	2.34478400	0.75578400
O	3.23883300	4.09488900	-0.72883300
C	4.70149100	4.30658700	-0.60034000
C	5.04320500	4.69564600	0.84047600
H	4.85394500	3.87134400	1.53014200
H	6.10246500	4.96758900	0.90261600
H	4.45334000	5.56459200	1.15197300
C	5.44700500	3.05176900	-1.06315100
H	5.14337800	2.77902100	-2.07993400
H	6.52382200	3.25187200	-1.07521300
H	5.25783600	2.20933600	-0.39528900
C	4.94780400	5.47470200	-1.55719700
H	6.01062400	5.73653100	-1.55960000
H	4.65540400	5.20988900	-2.57844400
H	4.37615900	6.35615700	-1.24963100
C	-1.30185000	-2.35480600	-1.39619500
O	-1.49636800	-1.84810900	-2.48323600
O	-1.56312500	-3.61421200	-1.05366600
C	-2.10789000	-4.46142000	-2.09952100
H	-2.20589600	-5.44473500	-1.64323200
H	-3.08027200	-4.07974700	-2.41716800
H	-1.42513400	-4.49085900	-2.95090400
C	1.56160900	-2.11182700	0.83238900
C	2.55262000	-2.74082300	-0.17198400
H	1.02264300	-2.91053400	1.35426000
H	2.12500000	-1.54400000	1.58475600
C	3.56017300	-3.68042900	0.50635400
H	1.98968700	-3.29623000	-0.93531300
H	3.09450900	-1.94473200	-0.69896000
C	4.55363100	-4.30449800	-0.48304400
H	4.11290800	-3.12326200	1.27648900
H	3.01766100	-4.47924300	1.03274000
H	3.99896900	-4.85912800	-1.25438800
H	5.09120700	-3.50304000	-1.01074600
C	5.56954300	-5.24271300	0.18281700
C	6.55700300	-5.85992200	-0.81291500
H	5.03207100	-6.04306400	0.71072400
H	6.12359400	-4.68770100	0.95289200
H	6.03606500	-6.45585100	-1.57221000
H	7.13043300	-5.08462000	-1.33550900
H	7.27159400	-6.51785100	-0.30673700

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Ru	-1.05293400	-0.51271900	1.17911200
C	-1.22362900	-2.07223200	2.86165500
C	-2.44473600	-1.38344100	2.78215500
C	-0.19632800	-1.09602100	3.15089200
H	-3.40647800	-1.81528200	2.53890100
C	-2.19326600	0.02174700	3.06768400
H	0.85185800	-1.31233900	3.30373600
C	-0.81759800	0.17946200	3.34687200
H	-2.94050900	0.80432800	3.08870200
H	-0.31110500	1.09808200	3.61179200

H	-1.06676100	-3.12794300	2.68535900
C	0.84088600	-1.15414600	0.28337000
C	-0.32978800	-1.55226700	-0.40733600
C	-0.07833500	0.96591900	-0.08100800
C	1.28500000	0.29254000	0.03224400
H	1.95216900	0.38785400	-0.84438400
H	1.83591300	0.67301700	0.89436000
C	-0.18409500	2.43594700	0.35083500
H	-1.22342900	2.77464400	0.29058500
C	-0.58152000	0.67446200	-1.46047200
H	0.08682400	0.91600800	-2.29511800
H	-0.47872200	-0.60710600	-1.42328000
N	-1.91141300	0.97755100	-1.81359600
H	-2.12539000	1.18005300	-2.78290800
C	-2.99273100	0.61768300	-1.03911500
O	-2.88304800	0.11056300	0.08545100
O	-4.12062000	0.88465000	-1.65669900
C	-5.48548600	0.63222000	-1.06466600
C	-5.65735700	-0.86760500	-0.82907900
C	-5.63998800	1.46724800	0.20559400
C	-6.40490900	1.13295800	-2.17711200
H	-5.48093200	-1.42710700	-1.75352400
H	-4.98493500	-1.23803300	-0.05257600
H	-6.68747000	-1.06055700	-0.51191500
H	-5.43134300	2.52289500	0.00332100
H	-6.67445200	1.39170600	0.55635600
H	-4.98293700	1.11836600	1.00485900
H	-7.44811200	0.99995400	-1.87490700
H	-6.23705500	2.19572400	-2.37584800
H	-6.24112500	0.57248200	-3.10248400
H	0.13643300	2.51196100	1.39224900
N	0.63649800	3.34860200	-0.44175200
C	1.89557600	3.70532000	-0.00389500
H	0.18589800	3.99879600	-1.07074800
O	2.47401200	3.12958200	0.90642100
O	2.34928500	4.73530700	-0.73652800
C	3.69317200	5.31874600	-0.50579300
C	4.76804600	4.25992300	-0.76630500
H	5.75837100	4.72424000	-0.70835300
H	4.71700800	3.45597600	-0.02998100
H	4.65265700	3.83593300	-1.77004100
C	3.75215500	6.43071400	-1.55519500
H	2.95288000	7.16118300	-1.39356800
H	4.71269900	6.95181300	-1.49260800
H	3.64781800	6.01965500	-2.56457900
C	3.77007600	5.89617000	0.91028400
H	2.95510400	6.60886700	1.07753700
H	3.71433300	5.10862700	1.66378400
H	4.71737900	6.43209600	1.03400500
C	-0.76335800	-2.86147500	-0.94393200
O	-0.56428900	-3.89757400	-0.34296400
O	-1.41623000	-2.75353800	-2.11009500
C	-1.88772400	-3.99990500	-2.67977800
H	-1.04940100	-4.68087700	-2.83896600
H	-2.61634700	-4.46494900	-2.01220000
H	-2.34853400	-3.72547600	-3.62751800
C	1.85173600	-2.15835100	0.80478300
C	2.84217300	-2.60729500	-0.29251700
H	1.34160800	-3.03880800	1.20514400
H	2.41697300	-1.68912900	1.62021400
C	3.90754600	-3.57052500	0.24953500
H	2.28437700	-3.09919400	-1.10069400
H	3.33405000	-1.72978600	-0.73339300

C	4.88416600	-4.06045400	-0.82851200
H	4.47054000	-3.07302500	1.05246900
H	3.41018100	-4.43544300	0.71138200
H	4.32015600	-4.56346900	-1.62791500
H	5.37410800	-3.19467900	-1.29826400
C	5.95602900	-5.01564800	-0.28661800
C	6.92372400	-5.50854100	-1.36766700
H	5.46571900	-5.87734600	0.18785900
H	6.52124200	-4.51015100	0.50897200
H	6.39212800	-6.04987300	-2.15979100
H	7.45526000	-4.67162500	-1.83685200
H	7.67536400	-6.18635600	-0.94876200

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Ru	1.35681700	0.27915600	0.70118700
C	0.97444600	1.49053600	2.53763100
C	2.35736000	1.21673000	2.45494200
C	0.28244700	0.23083500	2.63947800
H	3.14390800	1.94930500	2.33118400
C	2.53664500	-0.21826000	2.59213400
H	-0.78536900	0.10134800	2.75126800
C	1.27161500	-0.81110500	2.73783400
H	3.48428000	-0.73972600	2.56623700
H	1.07485800	-1.86772800	2.85752700
H	0.52983000	2.47173300	2.45979900
C	-0.51386100	1.11872300	-0.27401500
C	0.65195000	1.71154900	-0.83206000
C	-0.01407400	-1.26923300	-0.38576500
C	-1.02990000	-0.21770500	-0.83975000
H	-1.13382000	-0.19497200	-1.93203900
H	-2.01005800	-0.44568400	-0.41803900
C	-0.48057800	-2.44116600	0.46412100
H	0.36845500	-3.08013000	0.72727100
C	1.20117400	-1.18581700	-1.03961900
H	1.25949900	-0.56510500	-1.93138000
H	1.01211000	1.36333300	-1.79530700
N	2.36452300	-2.01011000	-0.85979300
H	2.47338700	-2.85499900	-1.41371500
C	3.49027000	-1.24081600	-0.69911800
O	3.37299500	-0.06634100	-0.27460400
O	4.60663600	-1.84911900	-1.01104700
C	5.97468400	-1.22405200	-0.87793500
C	6.05653400	-0.01481400	-1.80795900
C	6.22785300	-0.87414800	0.58756400
C	6.88212900	-2.35940600	-1.34738700
H	5.80748400	-0.29966900	-2.83536800
H	5.39123500	0.78956500	-1.48697000
H	7.08296400	0.36648200	-1.80529600
H	6.06391200	-1.74710700	1.22870200
H	7.27230000	-0.56705800	0.70427500
H	5.59359600	-0.05031500	0.92194700
H	7.92531900	-2.03124400	-1.31081900
H	6.77488800	-3.23917100	-0.70552400
H	6.64811400	-2.64615600	-2.37701400
H	-0.94826400	-2.08035100	1.38182800
N	-1.48634200	-3.21657700	-0.23768900
C	-2.82476100	-3.07328000	0.07308700
H	-1.22047300	-4.01660300	-0.79409400
O	-3.23948800	-2.18868000	0.81017600
O	-3.53438400	-4.01582000	-0.55636000
C	-5.01518300	-4.08848900	-0.43263200
C	-5.39571600	-4.35349600	1.02599400
H	-5.13909000	-3.50687000	1.66527300

H	-6.47522100	-4.52607000	1.09324800
H	-4.88732400	-5.24964800	1.39788400
C	-5.63973000	-2.80306100	-0.98075800
H	-5.30851100	-2.62387600	-2.00963800
H	-6.73018100	-2.90503600	-0.99117700
H	-5.37806100	-1.94100700	-0.36453100
C	-5.35749600	-5.28813900	-1.31741700
H	-4.86808500	-6.19545000	-0.94928400
H	-6.43928000	-5.45472300	-1.31431600
H	-5.03821400	-5.11502900	-2.35011500
C	1.08285100	3.11632800	-0.56516600
O	0.81342600	3.80414900	0.40503300
O	1.86352900	3.54599900	-1.57737100
C	2.36440500	4.89243200	-1.45712200
H	2.99898400	4.98491000	-0.57201300
H	2.94109200	5.06799200	-2.36460700
H	1.53641000	5.60097900	-1.38196700
C	-1.55306400	1.90427700	0.50183800
C	-2.60229600	2.49911500	-0.46932200
H	-1.09736900	2.72408000	1.05464400
H	-2.06953000	1.24395400	1.20873500
C	-3.70298400	3.27239700	0.27133300
H	-2.09518500	3.16964800	-1.17596000
H	-3.06125800	1.70012500	-1.06758400
C	-4.74536600	3.88380400	-0.67448200
H	-4.20420300	2.59917900	0.98183800
H	-3.24291800	4.06982300	0.87218300
H	-4.24130500	4.55294200	-1.38727200
H	-5.20302800	3.08495800	-1.27677700
C	-5.84839200	4.66208400	0.05616600
C	-6.88396900	5.26952300	-0.89578700
H	-5.39016400	5.46008400	0.65715000
H	-6.35153000	3.99369900	0.76895000
H	-6.41430800	5.96769400	-1.59941800
H	-7.38568900	4.49230200	-1.48524400
H	-7.65508800	5.81993900	-0.34592000

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C	-1.11742500	1.42077500	0.38039700
C	-0.40956700	2.33082700	1.08068800
C	0.95308900	-0.05908300	-0.02490900
C	-0.38146400	0.43656900	-0.53440700
H	-0.24849100	0.91061100	-1.51693700
H	-1.04383400	-0.42205500	-0.70702500
C	0.89897300	-0.99483200	1.16616300
H	1.87447800	-1.09050100	1.65893100
C	2.09116900	0.30205600	-0.64381900
H	2.08149800	0.95488600	-1.51043800
H	0.67434400	2.32250500	1.01429200
N	3.38771900	-0.08046200	-0.29839700
H	3.56327200	-0.64081600	0.52316900
C	4.49492000	0.33085000	-1.01473600
O	4.44401700	1.02354500	-2.01449200
O	5.60016400	-0.16766300	-0.41819300
C	6.94316800	0.09984800	-0.96570000
C	7.05946300	-0.49271300	-2.37415900
C	7.22706900	1.60535800	-0.94081900
C	7.85398200	-0.64299000	0.01520800
H	6.80847400	-1.55920500	-2.36092100
H	6.39518900	0.01896400	-3.07248500

H	8.09074800	-0.39145700	-2.73048400
H	7.08986300	2.00194000	0.07117800
H	8.26564500	1.78708800	-1.23936100
H	6.56639400	2.14145000	-1.62387300
H	8.90074300	-0.52785900	-0.28463700
H	7.73843000	-0.24520000	1.02875900
H	7.61465500	-1.71134000	0.03349200
H	0.20359400	-0.60930300	1.91636700
N	0.41997500	-2.33232400	0.82440800
C	-0.86376900	-2.73580500	1.07735300
H	0.94306000	-2.88315500	0.15775500
O	-1.67874300	-2.09210100	1.72212900
O	-1.06290900	-3.95330000	0.51472600
C	-2.34607000	-4.65744800	0.66157700
C	-2.61984400	-4.94950600	2.14093500
H	-2.76843700	-4.02537500	2.70168100
H	-3.52010900	-5.56764900	2.23380600
H	-1.78180400	-5.50148100	2.58100600
C	-3.47151400	-3.84442400	0.01185900
H	-3.21975400	-3.61114900	-1.02888900
H	-4.39753900	-4.43060300	0.01325100
H	-3.64532600	-2.91244400	0.55194600
C	-2.10083200	-5.95632200	-0.11174500
H	-1.26629300	-6.51439200	0.32526100
H	-2.99473200	-6.58809300	-0.08019800
H	-1.86320400	-5.74425300	-1.15942000
C	-0.95294400	3.37880800	1.96679800
O	-2.11801100	3.66150200	2.18684000
O	0.07560100	4.05296600	2.55320500
C	-0.31480200	5.10622600	3.44085300
H	-0.91376900	4.71460300	4.26826400
H	0.61573700	5.53705400	3.81343200
H	-0.90211800	5.86272100	2.91213000
C	-2.62011700	1.29028600	0.39335800
C	-3.27080100	1.65286100	-0.95973400
H	-3.04361500	1.92191100	1.17472500
H	-2.85487900	0.24324900	0.63566200
C	-4.79545900	1.48170600	-0.93802600
H	-3.02249000	2.69415100	-1.20680700
H	-2.84924500	1.03326800	-1.76408700
C	-5.46727200	1.83020400	-2.27243800
H	-5.03918300	0.44353300	-0.66721100
H	-5.21701400	2.11108900	-0.14127100
H	-5.21773400	2.86609200	-2.54670400
H	-5.04776500	1.19653500	-3.06856100
C	-6.99321800	1.66818500	-2.25017900
C	-7.65750000	2.00965800	-3.58820900
H	-7.41250400	2.30646800	-1.45952100
H	-7.24305800	0.63481900	-1.97001100
H	-7.45269700	3.04760300	-3.87884300
H	-7.28513300	1.36265800	-4.39233300
H	-8.74562500	1.88648800	-3.53873200

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Ru	0.47237900	0.50440900	0.30482200
C	0.65083000	2.52077900	1.09891400
C	1.31289400	2.44507200	-0.16399900
C	1.30945600	1.59164900	1.98694800
H	1.05177500	3.01346000	-1.04810900
C	2.37305700	1.47787600	-0.08055100
H	1.03665200	1.39474600	3.01546300
C	2.36329600	0.96173000	1.26631100
H	3.08971800	1.24380800	-0.85605300

H	3.02704900	0.20251100	1.66076300	C	0.06441700	-1.01319900	2.33719700
H	-0.17744900	3.16830900	1.35428700	C	1.50184900	-0.73771500	2.73186400
C	1.43565300	-2.43153100	-0.46385800	H	1.63058100	0.29008400	3.08992200
O	0.73238800	-1.66364400	0.20427900	H	1.82963900	-1.41362200	3.52807000
C	2.33352500	-1.95620200	-1.57255500	C	-0.56241200	-2.30799900	2.78843800
H	2.28788500	-2.63814300	-2.42846600	H	-1.47802700	-2.54640300	2.24591500
H	2.07422600	-0.94138800	-1.87713700	C	-0.68652000	0.07056000	1.89473600
H	3.37328800	-1.96828900	-1.21717800	H	-0.31928900	1.06760600	2.10621900
C	1.41320500	-3.90494100	-0.15586900	H	2.13615000	1.05377800	0.91880800
H	0.97481800	-4.45159100	-1.00105700	N	-2.10632400	-0.01863300	1.74075500
H	2.43428800	-4.28636400	-0.03466800	H	-2.69894000	0.34891900	2.47544600
H	0.83358900	-4.10481200	0.74697300	C	-2.69998100	-0.23393000	0.53126100
C	-1.44078000	0.77483800	-2.22259500	O	-2.05613600	-0.58526700	-0.46302600
O	-0.59518000	0.14546100	-1.57218600	O	-4.01264400	-0.03226900	0.60288900
C	-2.25367300	-0.85935900	1.51503200	C	-4.94022900	-0.26658800	-0.54209800
O	-1.35563500	-0.01594200	1.42211400	C	-4.58331800	0.67496100	-1.69370000
C	-1.86258800	0.26433800	-3.57357700	C	-4.89278800	-1.74142600	-0.94470100
H	-1.79379100	1.06297900	-4.32218400	C	-6.29638700	0.09447400	0.06545400
H	-1.24973600	-0.58550900	-3.87896100	H	-4.58696900	1.71639500	-1.35406100
H	-2.91708200	-0.03983900	-3.54036700	H	-3.60365800	0.44114000	-2.11475400
C	-2.06575000	2.04674400	-1.71868400	H	-5.33484000	0.57802700	-2.48438400
H	-1.59168300	2.90063600	-2.22235300	H	-5.09371400	-2.38304300	-0.07996300
H	-3.13023500	2.08685500	-1.97296100	H	-5.66693700	-1.93665100	-1.69417600
H	-1.92433500	2.15262600	-0.64111200	H	-3.92488800	-2.00921700	-1.37273200
C	-2.43563200	-1.98531900	0.53050400	H	-7.08304000	-0.03045900	-0.68502700
H	-3.49422600	-2.09600800	0.26922700	H	-6.52690700	-0.55215400	0.91774800
H	-1.83446300	-1.83404400	-0.36541100	H	-6.30633000	1.13484700	0.40501300
H	-2.13038000	-2.92613200	1.00676600	H	0.12687500	-3.15256100	2.72078200
C	-3.22326900	-0.77554700	2.66524200	H	-0.81900900	-2.19444400	3.85280800
H	-4.23349600	-0.57152400	2.28721800	H	3.85082600	-2.10557000	2.28431700
H	-3.27501800	-1.73671600	3.19124000	C	-0.01622900	1.61081100	-0.40348400
H	-2.92997900	0.01265300	3.36066900	C	0.35004600	1.08988800	-1.47692200
55-ts				Si	-0.40169100	3.26747300	0.40450800
Ru	0.41887200	-0.74077000	-0.00918400	C	0.93409200	3.68179400	1.67815500
C	0.61229900	-1.93079200	-2.14678100	H	1.93074500	3.71332200	1.22391700
C	-0.74818200	-2.44836800	-2.08577100	H	0.73614700	4.67460700	2.10140900
C	1.34115000	-2.46642200	-1.06695700	H	0.96725000	2.97682400	2.51720900
H	-1.53068000	-2.22976900	-2.80018500	C	-0.35763200	4.50809200	-1.01736400
C	-0.88327500	-3.12698000	-0.90460000	H	-1.13025900	4.29297700	-1.76421500
H	2.41252900	-2.48510300	-0.98019300	H	-0.53770800	5.52146200	-0.63767900
C	0.38317600	-3.04634800	-0.18108800	H	0.61392100	4.51302700	-1.52396800
H	-1.79389500	-3.56385400	-0.51439700	C	-2.10152900	3.30540200	1.22914000
H	0.62453200	-3.64875100	0.68270000	H	-2.12307700	2.78345800	2.19162000
H	1.04984500	-1.43773100	-3.00212600	H	-2.36958300	4.35099200	1.42646600
C	2.28375500	-0.96859200	1.43918600	H	-2.88510400	2.87956500	0.59359300
C	2.47388700	0.08911600	0.53730800	C	0.63190700	1.10762900	-2.92591600
Si	4.00839700	0.39422400	-0.57896600	H	1.62652400	0.72131700	-3.16525000
C	4.30404500	-0.81958900	-2.00208600	H	0.57800800	2.14539600	-3.27672700
H	3.46333000	-0.88928600	-2.70055200	H	-0.10766600	0.52423300	-3.48335600
H	5.17057900	-0.46635200	-2.57528500	56-ts			
H	4.54585300	-1.83361800	-1.66324100	Ru	-0.50411900	-0.23016000	0.35842100
C	3.86114000	2.15089100	-1.26503300	C	-0.77247300	-1.28991500	2.55114000
H	3.02273700	2.28090500	-1.95610600	C	0.30158300	-2.25360500	2.31756800
H	3.74173800	2.88169500	-0.45589900	C	-1.79670800	-1.53833400	1.62013900
H	4.77828200	2.41552100	-1.80530100	H	1.20710400	-2.33229500	2.90505800
C	5.51043100	0.34983800	0.57646000	C	0.01149000	-2.93059300	1.16576500
H	5.70210300	-0.64764100	0.98719600	H	-2.80964500	-1.18299900	1.68661900
H	6.41026500	0.65391500	0.02728800	C	-1.24243400	-2.40458800	0.62847900
H	5.39434900	1.04177100	1.41928300	H	0.64207400	-3.65626100	0.66835300
C	3.13080000	-2.22011100	1.46167300	H	-1.80253400	-2.86745900	-0.16977300
H	3.70670300	-2.38236300	0.55047300	H	-0.88573100	-0.68765700	3.44079800
H	2.55417100	-3.12472100	1.67943300	C	-2.58426700	0.29540000	-0.61382200

C	-2.07086300	1.36063100	0.14723500	H	-4.95243700	0.57060300	-2.70829500
C	-0.73630500	-0.54476300	-1.94196200	H	-6.37892100	0.33163800	-1.69651700
C	-2.06321000	0.18404800	-2.05997400	H	-5.30637700	1.70240500	-1.39334900
H	-1.93839100	1.17785800	-2.51072100				
H	-2.74397300	-0.37646800	-2.70652700	57			
C	-0.64195400	-1.95110000	-2.48167400	Ru	-0.60532400	-0.85432200	0.36107300
H	0.24105000	-2.48400000	-2.12620300	C	-2.10809500	-1.01519700	1.95419100
C	0.39330900	0.24138500	-1.71233500	C	-1.13599300	-0.04462400	2.39021700
H	0.32482100	1.30656300	-1.90572400	C	-1.44515900	-2.27279100	1.81843900
H	-1.51654900	2.12529900	-0.39594400	H	-1.32403700	0.99375300	2.61860700
N	1.71346500	-0.29616300	-1.83748000	C	0.11508200	-0.70881300	2.50590900
H	2.24244100	-0.11516200	-2.68171800	H	-1.91051700	-3.20621200	1.52953300
C	2.40355200	-0.80660900	-0.77989400	C	-0.05999800	-2.08003400	2.14576100
O	1.87686100	-0.99190000	0.32417500	H	1.05522500	-0.24791700	2.78108400
O	3.66451500	-1.06668600	-1.11535800	H	0.71461100	-2.83516700	2.14561900
C	4.64163000	-1.71526500	-0.19348900	H	-3.16342400	-0.83790400	1.80210500
C	4.87727600	-0.81662400	1.02170300	C	-1.99564500	-0.19351400	-1.41236300
C	4.13673800	-3.10804800	0.18777000	C	-1.43148400	0.94441000	-0.82472600
C	5.89461400	-1.80398400	-1.06562600	C	-0.57009500	-2.08096700	-1.66475900
H	5.19752500	0.18215600	0.70563800	C	-1.22714100	-0.97560000	-2.47792300
H	3.97783400	-0.72573700	1.63359300	H	-0.50191100	-0.34559000	-3.00866200
H	5.67522200	-1.24483200	1.63764300	H	-1.89206700	-1.39827500	-3.23795500
H	3.92303000	-3.69866400	-0.70964200	C	-1.13606100	-3.47498200	-1.78050200
H	4.91308000	-3.63089600	0.75611900	H	-0.68433600	-4.16821900	-1.06489900
H	3.23742000	-3.05306900	0.80420400	C	0.65562900	-1.91424400	-1.01801400
H	6.70777700	-2.26762700	-0.49866900	H	-0.50971300	1.28825600	-1.30815700
H	5.70697500	-2.40963400	-1.95763200	H	1.24515000	-2.73332900	-0.62302400
H	6.21980000	-0.80823800	-1.38283800	N	1.23957600	-0.62780700	-0.90608900
H	-1.53046000	-2.54459900	-2.25845700	H	1.12756100	0.01567500	-1.68704300
H	-0.57347800	-1.88008300	-3.57812300	C	2.53016800	-0.49913900	-0.26377100
C	0.85094500	1.78821000	0.61377300	O	2.94754200	-1.34141900	0.49474300
C	0.53748300	1.40397300	1.75749100	O	3.06323600	0.64008200	-0.66017800
Si	1.63574900	3.24415700	-0.29382300	C	4.42324500	1.09291200	-0.17892600
C	0.28657500	4.22867600	-1.17906200	C	4.38191400	1.26372600	1.33880900
H	-0.49209500	4.56269300	-0.48399500	C	5.46754000	0.07719000	-0.64022200
H	0.73003800	5.12600800	-1.62865200	C	4.58408500	2.43244600	-0.89364200
H	-0.19743600	3.67005000	-1.98884200	H	3.57057100	1.93929000	1.63116900
C	2.40273900	4.28241200	1.08435500	H	4.26120300	0.30667800	1.85046500
H	3.18642000	3.73230700	1.61748100	H	5.32451900	1.71127600	1.67061500
H	2.86106400	5.18549500	0.66256200	H	5.42145100	-0.06071900	-1.72556200
H	1.65497700	4.60528900	1.81758200	H	6.46447800	0.45616800	-0.39279900
C	2.97635200	2.73865700	-1.52453600	H	5.33804200	-0.88905700	-0.14852600
H	2.56823000	2.36118400	-2.46809300	H	5.55235000	2.87005000	-0.63233200
H	3.57219200	3.62752300	-1.76729800	H	4.54807800	2.30443300	-1.97988300
H	3.66027500	1.98490500	-1.12102500	H	3.79905300	3.13458300	-0.59558900
C	0.53597600	1.46187700	3.23115300	H	-2.21998000	-3.48200700	-1.62853000
H	-0.47581900	1.49147500	3.64645400	H	-0.95387900	-3.86022800	-2.79337000
H	1.05435500	2.37844600	3.53836200	Si	-2.26088500	2.49993700	-0.07894700
H	1.06527700	0.61041200	3.66944800	C	-3.45023900	-0.58216900	-1.27044800
Si	-4.37267600	-0.43860300	-0.45185500	H	-3.99354700	-0.24666400	-2.16615700
C	-2.68182800	1.90104100	1.42056800	H	-3.58663800	-1.66667800	-1.20559800
H	-1.95326800	2.50863200	1.96405400	H	-3.92315000	-0.12518000	-0.40064400
H	-3.52649400	2.56153100	1.17824300	C	-3.71532900	2.22789600	1.10211800
H	-3.05065600	1.12219200	2.09049800	H	-3.47208900	1.63749700	1.99117400
C	-5.25607600	-0.27880400	1.21642200	H	-4.05105000	3.21110700	1.45602000
H	-4.81162900	-0.84135300	2.04405000	H	-4.57640100	1.76226200	0.61008600
H	-5.36826600	0.76264600	1.53312300	C	-2.88081800	3.47949600	-1.57571800
H	-6.26820100	-0.68064600	1.07535400	H	-3.67620800	2.94649400	-2.11001400
C	-4.45902800	-2.24427800	-1.01078600	H	-3.28980600	4.44635100	-1.25739700
H	-3.93928700	-2.43119000	-1.95719000	H	-2.07642900	3.68365400	-2.29225800
H	-4.06721900	-2.93911700	-0.26043300	C	-0.88579700	3.47619300	0.77833300
H	-5.51235200	-2.50698500	-1.16987700	H	-0.45571500	2.94572000	1.63561800
C	-5.32758600	0.64499000	-1.68188700	H	-0.06700500	3.69501500	0.08158000

H	-1.26585800	4.43812100	1.14231400
58			
Ru	1.38729400	-0.93100900	-0.55147400
C	3.05299000	-2.46767300	-0.70880800
C	3.53945300	-1.16058700	-1.01293500
C	2.05918200	-2.79593300	-1.67987500
H	4.30297800	-0.62709700	-0.46613500
C	2.85209500	-0.66634000	-2.16547900
H	1.49593900	-3.71890500	-1.72704700
C	1.94652300	-1.69981000	-2.58222300
H	3.02057900	0.27999300	-2.65859700
H	1.29711300	-1.65294300	-3.44466800
H	3.40327200	-3.10796000	0.08779700
C	1.84891800	-0.60983500	1.75272200
C	1.90311300	0.64068200	1.12379500
C	-0.09005000	-2.14457900	1.37879700
C	0.52500400	-1.12372100	2.32460400
H	-0.14627500	-0.27485600	2.49028900
H	0.69547500	-1.58286500	3.30925800
C	0.43601900	-3.56848700	1.43337400
H	-0.02290800	-4.19468200	0.66118100
C	-1.33820900	-1.97775800	0.83919600
H	0.95918500	1.18109800	1.16459900
H	-1.78326700	-2.77145200	0.24687200
N	-2.18526100	-0.91659400	0.99961600
H	-1.95081200	-0.15021500	1.61644900
C	-3.48224700	-0.91572200	0.46253600
O	-3.87370900	-1.77456000	-0.30407200
O	-4.13829300	0.14351900	0.93492900
C	-5.60094000	0.34098200	0.67162400
C	-5.83446400	0.52988400	-0.82760800
C	-6.37423400	-0.84817200	1.24446700
C	-5.89913200	1.62297100	1.44832400
H	-5.23585500	1.36303100	-1.21116400
H	-5.59349300	-0.37552300	-1.38726500
H	-6.88925700	0.77081100	-0.99752500
H	-6.13774800	-0.98776700	2.30470200
H	-7.44800800	-0.65001600	1.16274700
H	-6.15355100	-1.77037900	0.70334200
H	-6.95873900	1.87642500	1.34559400
H	-5.67772200	1.49580100	2.51258800
H	-5.30779300	2.46091200	1.06540000
H	1.51832100	-3.63502500	1.31862100
H	0.18961500	-4.01530200	2.40736700
Si	3.35180000	1.91142700	1.05736800
C	3.06090200	-1.32411300	2.31546200
H	3.19621800	-0.99194400	3.35473700
H	2.92108900	-2.40745300	2.35635800
H	3.98664400	-1.10895900	1.78416700
C	4.87875200	1.40206200	2.05811500
H	5.46524000	0.59304800	1.60742900
H	5.54182300	2.27481600	2.11854800
H	4.63630000	1.11119000	3.08568300
C	2.61688300	3.44293700	1.89490100
H	2.32122000	3.22348000	2.92822500
H	3.35934600	4.24925400	1.93247000
H	1.73550400	3.83451300	1.37469100
C	3.95190300	2.35480600	-0.68504600
H	4.63874900	1.60384100	-1.09194300
H	3.14055900	2.49914200	-1.40385600
H	4.51389500	3.29588100	-0.63250600
C	-0.14166500	0.61134700	-1.16932800

C	-0.43072200	-0.49618100	-1.70429800
Si	-0.79861500	2.37766200	-1.10247000
C	0.49922800	3.62542800	-1.66153100
H	0.93983800	3.34434600	-2.62513400
H	0.02014800	4.60362800	-1.79494700
H	1.31123200	3.75571600	-0.94126800
C	-2.24270000	2.41110400	-2.32141300
H	-3.00850100	1.66906600	-2.07037300
H	-2.72062100	3.39872200	-2.31479800
H	-1.90780100	2.21621100	-3.34681200
C	-1.42832200	2.79978500	0.63178500
H	-0.65845300	2.72127100	1.40773000
H	-1.78520000	3.83764700	0.64074900
H	-2.27789300	2.16726900	0.91439800
C	-1.27547300	-1.40329300	-2.51770600
H	-1.47034900	-0.95327200	-3.49908700
H	-2.24085500	-1.56149700	-2.02172800
H	-0.82473200	-2.38607600	-2.67572200