Metal-catalyzed rearrangement of allenylsulfides to furan: A theoretical mechanistic approach

Michel Rajzmann, Jianbo Wang, Stéphane Humbel

Metal-Catalysed Rearrangement of Allenylsulfides to Furan: A Theoretical Mechanistic Approach

Michel Rajzmann,[a] Jianbo Wang[b], Stephane Humbel,*[a]*

[a] *Aix Marseille Univ, CNRS, Centrale Marseille, iSm2, Marseille, France*
[b] *Key Laboratory of Bioorganic Chemistry and Molecular Engineering of Ministry of Education, College of Chemistry, Peking University, Beijing 100871, China*

Keywords:
Molecular mechanism
Homogeneous catalysis
Transition metals
Cyclization
Allenes
Density functional calculations

A B S T R A C T

A furan catalytic synthesis from allene is studied with quantum chemistry computations. Both specific and non-specific solvent effect are considered. The complete catalytic cycle is studied for three metals, and compared to experimental data. The mechanism is disclosed and the catalyst regeneration shows clear difference between the three metals. For Pt, the regeneration corresponds to a two-steps mechanism with a stable intermediate. For Au and Ru catalysts the regeneration is a one step mechanism with a low barrier only for Au (3.8 kcal/mol). For Au, the results of the computations contrasts with the experiments, hence a poisoning of the catalyst is most likely. On the contrary, in the Ru case, the regeneration corresponds to the highest transition state of the cycle.

1. Introduction

Allenes have attracted significant attentions as a consequence of their unique structural feature and chemical reactivities.[1–11]The allene moieties can coordinate with transition-metals, thus being activated. The activated allene moieties are prone to be attacked by nucleophiles, and subsequently various transformations that are highly useful in organic synthesis can be triggered. In particular, the transition-metal-catalyzed reaction of allenes bearing α-substituents as internal nucleophililes makes it possible to develop efficient synthetic method for heterocycles. One of such transformations is the transition-metal-catalyzed cyclization of allenyl ketones that affords furans in a straightforward manner (Fig. 1). [12–17] Several metals are found in the literature as useful catalysts for this purpose. The catalyst can be for instance a calcium complex, [18–20] but electron-rich metals such as gold, platinum, and ruthenium are also used. The reaction is a cycloisomerisation with atoms or even groups transpositions.[21–23]

Furans are important heterocycles, which are present as key structure units in many biologically important natural products and pharmaceutical substances.[24] Furans are also widely used as building blacks in organic synthesis.[25] Thus, the development of novel and efficient approach to furan derivatives has been an active research area over the years.[26–34] One of the authors previously studied the transition metal-catalyzed reaction of allenic sulfides. The reaction proceeds through an intriguing 1,4-migration of thio group to afford furan derivatives, as shown in Fig. (1).[35] The reaction presumably involves a metal carbene intermediate, which is trapped intramolecularly by carbonyl group. To gain detailed

* *Corresponding author at* : *Aix Marseille Univ, CNRS, Centrale Marseille, iSm2, Marseille, France*
E-mail addresses: michel.raizmann@univ-amu.fr (M. Raizmann), stephane.humbel@univ-amu.fr (S. Humbel)

insights into the reaction mechanism of this novel transformation, we have launched a computational study on this reaction.

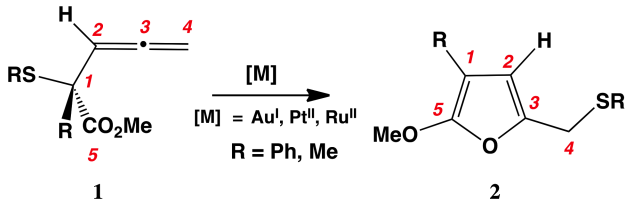


Fig. 1. Cycloisomerisation-transposition at work. Experimentally, Phenyls are used as R substituents. Methyls are used in computations.

Table 1. Main experimental results from ref [35].

Catalyst[a]	T[°C]	t[h]	Yield[%][b]
AuCl	80	17	Trace[c]
$PtCl_2$	80	4.5	73
[{$RuCl_2$(p-cymene)}]	80	1	93
[{$RuCl_2$(p-cymene)}]	25	23	88

[a] Reactions were carried out with 5 mol% catalyst. [b] Yield of isolated product after column chromatography [c] Most of the starting material was recovered.

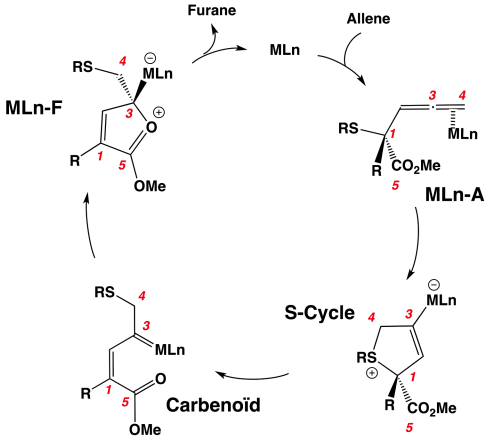


Fig. 2. Catalytic cycle proposed for the cycloisomerisation-transposition; adapted from ref [35]. Experimentally, phenyls are used as R substituents. In computations methyls are used instead.

Indeed, in the present contribution, we address the mechanism of this catalysis by computing the different intermediates and transition states summarized in Fig 2. Three **MLn** catalysts are studied AuCl, $PtCl_2$ and {$RuCl_2$(*p-cymene*)}]. They correspond to the catalysts experimentally studied for this reaction, as reminded in Table 1. We shall thus refer explicitly to experimental results in the discussion.

Moreover, for each catalyst, a special attention will be given to the step that concerns the catalyst regeneration. Notably, the aforementioned $C^1 \rightarrow C^4$ migration involves two ring closures and one ring opening. The postulated cyclic intermediate is named here **S-Cycle**: we use for the name the label of heteroatom that closes the ring. A **Carbenoïd** intermediate is then postulated, and upon the C^3-O bond formation, it connects to the complex formed by the furan (reaction product) and the catalyst. We refer to this complex with the label **MLn-F**. The so-called **MLn** catalyst is then restored upon **Furan** – **Allene** exchange.

2. Methods

The computations were done at the level M06-D3/lanl2dz(d), and we accounted for non specific solvent effects of the toluene with the standard PCM method. Specific effects were handled with one benzene molecule explicitly introduced on the metal: **MLn** refers to the complex with the benzene ligand. The reaction described in Fig 1 is exothermic by -24.4 kcal/mol (when R=Phenyl). In order to alleviate the computations, we modeled the R=Phenyl substituent by R=Methyl throughout. With R= Methyl, the reaction exothermicity is smaller (-16.5 kcal/mol). Such a difference is due to the conjugation of the R=Phenyl with the double bond C^1=C^5 formed in the product (Fig 1). Indeed, the R= Methyl does not conjugate, so the exothermicity is smaller in the model. Hence, the choice of this model will alter the energetics of the reaction mechanism whenever the R substituent conjugates with double bonds: the **Carbenoïd**, and the **MLn-F** intermediates would be about 7 kcal.mol^{-1} lower when R=Phenyl compared to the model computations. We shall be watchful on that. A second simplification concerns the Ru catalyst: the p-cymene was modeled with a phenyl. This was done to limit the number of possible orientations of this ligand and as *a priori* no effect on the energetics. Our computations were done with the Gaussian g09 D01 suite of programs,[36] and the non specific solvent effect was modeled with the IEF-PCM solvation model,[37] as implemented in Gaussian. The M06/lanl2dz(d) level of calculation was used throughout, and this M06 level[38–40] was supplemented with Grimme's long range dispersion correction D3.[41–44] The "(d)" in the lanl2dz(d) acronym corresponds to polarization function that we added to the standard relativistic ECP and basis set lanl2dz[45]. The 3d polarization functions concerned the 3d orbitals of Carbon and Oxygen with exponents ζ_{dC}=0.75 and ζ_{dO}=0.85. These values come from the exponent of the D95(d) (or DZP) basis set, as implement in Gaussian. Our computations used the chain method **(CHAIN)**[46,47] and AMPAC[48] to find the best paths that link **MLn-A** reactive to the product **MLn-F**. More details on the structures can be found in the experimental section. Additionally, several other paths and all the structures are available in the supplementary material (29 pages).

2.1. Metal – Allene complexes: MLn-A Tables

In the first step of the reaction, the metal has to bind to the allene. Upon the formation of the complex, the allene looses its quasi linearity, and bends at the central C^3 atom with an angle of about 160°.[49–54] The stabilization is of 10.1, 34.6 and 12.2 kcal.mol^{-1} for the Au, Pt and Ru catalysts, respectively. Two orientations can be found, with the metal either exo- to the thiolate (a), or endo- (b). These two situations are reminded in Fig 3. It is noteworthy that the (a) situation allows a direct 1,4 migration of the thiolate group. The endo- orientation was also studied, and we showed that this path does not correspond to effective intermediates. A detailed study is included in the supplementary material.

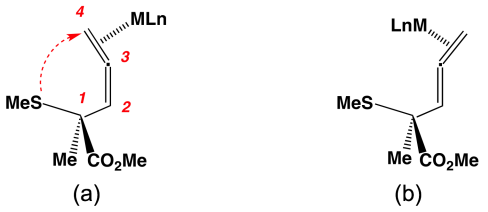


Fig. 3. The interaction with the metal leads to two possible complexes.

2.2. Catalyst regeneration : Furane – Metal – Allene complexes

Once the furane is formed, the catalyst has formed, F-MLn contains a metal–Carbon bond that needs to break in order to renew the catalyst and allow a new allene molecule to come in the cycle. This can be achieved through either a dissociative (Equation 1) or an associative path (Equation 2). However, the dissociation of the furane from the catalyst costs at least 14.6 kcal/mol (for Au, Ru), and up to 38.9 kcal/mol (Pt case). On the other hand, the approach of the allene involves at first stabilizing interactions. Finally, the associative path is always lower in energy than the dissociative.

$$F\text{–}MLn + A \rightarrow F + MLn + A \rightarrow F + MLn\text{–}A \quad (1)$$

$$F\text{–}MLn + A \rightarrow F\ldots MLn\ldots A \rightarrow F + MLn\text{–}A \quad (2)$$

As we shall see, this Furane – Allene exchange that completes the catalytic cycle is of primary importance, and each catalyst behave differently also for this matter. For consistency in the energetics, the second allene molecule is added to our computation since the very first step but does not participate to the reaction until the catalyst regeneration (dispersion terms are thus included). Upon geometry optimization we verified that this additional moieties does not bind to the metal prior to the exchange (see the geometries in the supplementary information).

For the three catalysts of interest, the reaction has been studied and the results are given and discussed in the next section.

3. Results and Discussion

3.1. AuCl•{C_6H_6}

The energy profile for this Gold catalyst is shown on Fig 4. The reaction starts with an easy **S-cycle** formation, and the most energetic step is the actual O–C bond formation that links **S-cycle** to **AuLn–F** via **TS2** (barrier height is 16.0 kcal.mol^{-1}). This step is also the most exothermic (-19.7 kcal.mol^{-1}).

The catalyst's regeneration is a one-step process, where the exchange between the furane (to be released) and the incoming allene (for the next catalytic cycle) is made around the metal in a unique transition state (**TSx**). The furane is easily released when the next allene (noted A in the Figures) strongly binds to the metal (**TSx**, corresponds to a small barrier of only +3.8 kcal.mol^{-1}).

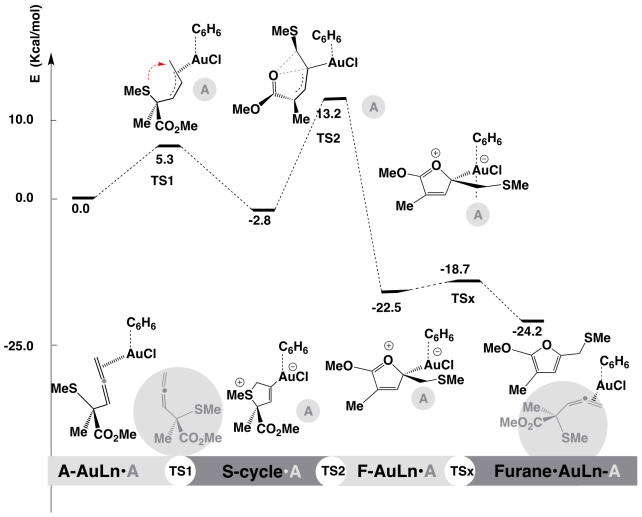


Fig. 4. Energy profile (in kcal.mol^{-1}) for the AuCl•{C_6H_6} catalyst, at the M06-D3/lanl2dz(d) level. A represents the additional allene molecule.

The results we obtained show a facile reaction that should occur, and this is consistent with several cases where gold catalysts are efficiently used with similar reagents.[49,55–60] However it is in contrast with the experimental results: at 80°C during 17h, only traces of furane are obtained, and starting materials are recovered. At this temperature the highest barrier (16 kcal/mol) should be overpassed. The best hypothesis is that allene somehow reacts also stoichiometrically with the catalyst complex and modifies it (poisoning). Sulfur has indeed a strong affinity for gold clusters. Hence, we envisage that a poisoning of the catalyst could produce gold clusters that are stabilized by thiolates.[61] This hypothesis is consistent with the fact that traces of the furane product are found: the reaction is possible but the catalyst is consumed by poisoning. In the end most of the starting materials are indeed recovered.

3.2. $PtCl_2$•{C_6H_6}

The energy profile for the Platinium catalyst is shown on Fig 5. It differs from that of the Gold catalyst only in the catalyst's regeneration steps. The reaction also starts with an easy **S-cycle** formation, and the most energetic step is the actual O–C bond formation that links **S-cycle** to **F-PtLn** via **TS2** (barrier height is 14.2 kcal.mol^{-1}). This step is also the most exothermic (-19.9 kcal.mol^{-1}). For the catalyst regeneration, two steps (hence two Transition States - **TSx'** and **TSx''**) are necessary. They release the furane and prepare the catalyst for the next cycle.

In order to complete the catalytic cycle, the system goes through the very stable complex **F-PtLn-A** (-36.6 kcal/mol) where both the furane and the next allene are firmly attached to the Pt, and the solvent, represented by the benzene, moves away, at more than 4.5 Å from the metal. The release of the furane from this intermediate involves a barrier of 17.2 kcalmol^{-1}. This is the bottle-neck for this catalyst.

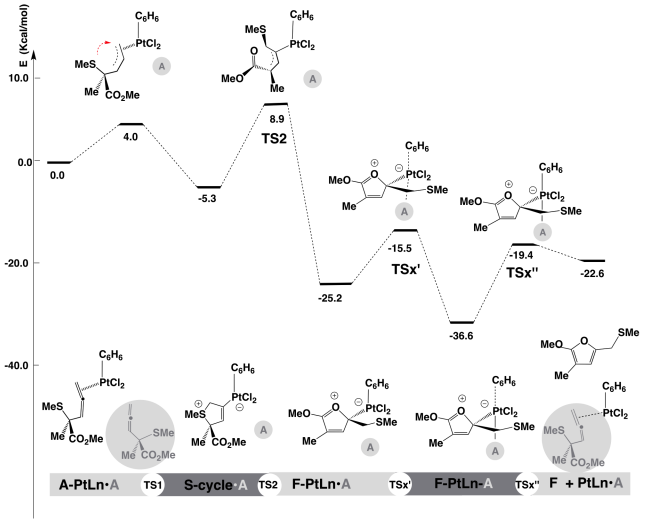


Fig. 5. Energy profile (in kcal.mol^{-1}) for the $PtCl_2$•{C_6H_6} catalyst, at the M06-D3/lanl2dz(d) level. A represents the additional allene molecule.

3.3. $RuCl_2$•{C_6H_6}

The energy profile for this catalyst is shown on Fig 6. It is very similar to that of the Gold catalyst, with an easy furane formation (exothermic and with small barriers - about 10 kcal/mol). Additionally, as it is the case for Gold, the catalyst's regeneration is also a one-step process, where the exchange between the furane (to be released) and the incoming allene (for the next catalytic cycle) is made around the metal in a unique transition state (**TSx**). The release of the furane from the latest intermediate involves a barrier of about a 13.5 kcalmol^{-1}. This is the highest barrier of the catalytic cycle.

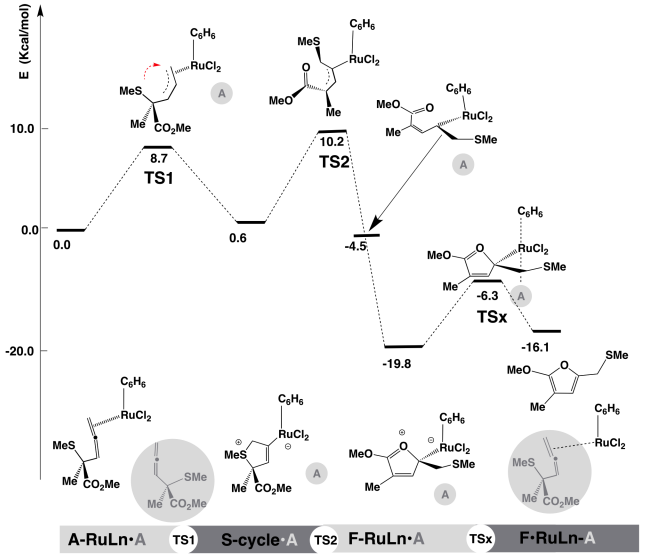


Fig. 6. Energy profile (in kcal.mol^{-1}) for the $RuCl_2$•{C_6H_6} catalyst, at the M06-D3/lanl2dz(d) level. A represents the additional allene molecule.

3.4. Discussion

Fig 7 summarizes our results for the three catalysts studied here. The first step (**S-Cycle** formation, through **TS1**) cannot be a limiting step because the barriere is always small. Gold and Platinium have higher barriers than Ruthenium and it is consistent that their yields are smaller in the experimental results. Our study shows also that the limiting steps are different for Gold and Platinium. In the Gold catalyst the furane formation has a high barrier, but the catalyst regeneration is easy, while the reverse is observed for platinium.

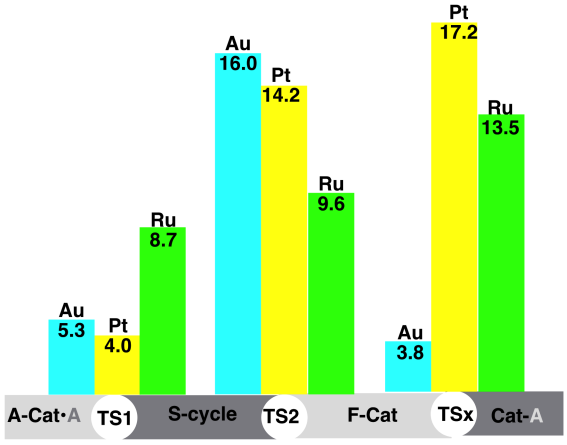


Fig. 7. Barriers of the different steps for the three catalysts (in kcal.mol^{-1}).

It shall be noted that the mechanism initially proposed fits with the computational results, except for the carbenoid intermediate, which could not be found as a minimum. The computations also provide NBO charges[62,63] on the atoms and those can be used to better clarify the way we write mechanisms. For the key intermediates of the Ru catalytic cycle, the sum of charges on fragments are provided below (Fig 8) and details are in Table 2. It is shown that from **RuLn-A** to **RuLn-Cycle-S**, the charge on sulfur atom gets more positive (from +0.14 to +0.65). This charge returns to normal in the product **RuLn-F**. The *modification of the charge* is consistent with the written mechanism.

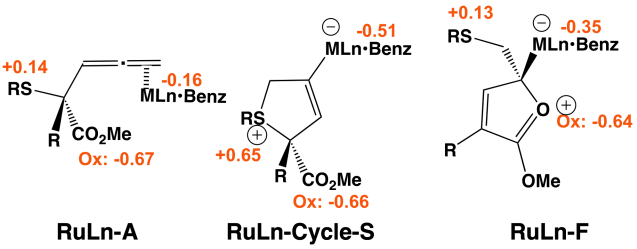


Fig. 8. NBO charges (orange) on S, on the active Oxygen atom (Ox) and on the $RuCl_2$•benzene catalyst (as the sum of the atomic charges per fragment).

On the catalyst fragment **RuLn** (which includes benzene) the *variation* of the charge is also consistent with the charge written in the mechanism: upon the Metal – Carbon bond formation, from **RuLn-A** to **RuLn-Cycle-S**, the charge goes from -0.16 to -0.51, then -0.35 in **RuLn-F**. Such a negative charge on the catalyst does not mean that the metal bears a negative charge: the charge variation is transmitted to the ligands. Hence,

the charge on the metal is fairly constant, and of course positive (+0.20, +0.22, then +0.25) while the two chlorines are negatively charged in the three intermediates (–0.90, –1.08, then –1.06). The total charge on the benzene is also modified along the reaction path (+0.53, +0.35, then +0.46).

Table 2: Details of the NBO charges on the Ru catalyst.

Intermediate	Total	Ru	Benzene	Chlorines
RuLn-A	-0.16	+0.20	+0.53	–0.90
RuLn-Cycle-S	-0.51	+0.22	+0.35	–1.08
RuLn-F -F	-0.35	+0.25	+0.46	–1.06

4. Conclusions

The computations finally confirmed the initially proposed mechanism, with two major clarifications: one is that the gold catalyst in the experiment must be somehow inhibited, for instance through gold clusters. This conclusion is driven by the fact that our computations of the mechanism and the barriers we obtained for the *initial* gold-based catalyst are very similar to that of the other catalysts, while experimentally no reaction occurs.

Second, we showed that the Pt-based catalyst is regenerated through a stable intermediate where both the furane and the allene are in interaction with the catalyst. The rate-determining step for the Ru and for the Pt stands in this catalyst regeneration. However, the key intermediate structure is a stable intermediate in the Pt case, while it is a transition state for the Ru. Hence, we shall anticipate that for bulkier allenes the catalyst regeneration would be easier for Pt because the stable intermediate would be destabilized by the steric hindrance, while for the Ru catalyst the transition state will get higher and the catalyst regeneration would get more difficult.

Acknowledgements

Dr Yoann Coquerel is gratefully acknowledged for its continuous support and careful reading oft he manuscript. Prs Daniel Liotard and Alain Dargelos are acknowledged for the CHAIN program and the coupling between Gaussian 09 and AMPAC 10. The coupling of the two codes helped us to find the different reactions paths.

References

[1] essor N. Krause, essor A.S.K. Hashmi, eds., Modern Allene Chemistry, Wiley-VCH Verlag GmbH, 2004. doi:10.1002/9783527619573.fmatter.

[2] S. Ma, Palladium-Catalyzed Two- or Three-Component Cyclization of Functionalized Allenes, SpringerLink. (n.d.) 183–210. doi:10.1007/b104131.

[3] L. Brandsma, N. Nedolya A., Synthesis. (2004) 735.

[4] S. Ma, Some Typical Advances in the Synthetic Applications of Allenes, Chem. Rev. 105 (2005) 2829–2872. doi:10.1021/cr020024j.

[5] S. Ma, Recent Advances in the chemistry of allenes, Aldrichimica Acta. 40 (2004) 91–102. http://www.sigmaaldrich.com/ifb/acta/v40/acta-vol40-2007.html#111/z (accessed September 12, 2017).

[6] H. Kim, L.J. Williams, Recent developments in allene-based synthetic methods, Curr. Opin. Drug Discov. Devel. 11 (2008) 870–894.

[7] M. Brasholz, H.-U. Reissig, R. Zimmer, Sugars, Alkaloids, and Heteroaromatics: Exploring Heterocyclic Chemistry with Alkoxyallenes, Acc. Chem. Res. 42 (2009) 45–56. doi:10.1021/ar800011h.

[8] S. Ma, Electrophilic Addition and Cyclization Reactions of Allenes, Acc. Chem. Res. 42 (2009) 1679–1688. doi:10.1021/ar900153r.

[9] C. Aubert, L. Fensterbank, P. Garcia, M. Malacria, A. Simonneau, Transition Metal Catalyzed Cycloisomerizations of 1,n-Allenynes and -Allenenes, Chem. Rev. 111 (2011) 1954–1993. doi:10.1021/cr100376w.

[10] S. Yu, S. Ma, Allenes in Catalytic Asymmetric Synthesis and Natural Product Syntheses, Angew. Chem. Int. Ed. 51 (2012) 3074–3112. doi:10.1002/anie.201101460.

[11] J. Ye, S. Ma, Palladium-Catalyzed Cyclization Reactions of Allenes in the Presence of Unsaturated Carbon–Carbon Bonds, Acc. Chem. Res. 47 (2014) 989–1000. doi:10.1021/ar4002069.

[12] J.A. Marshall, X.J. Wang, Synthesis of furans by silver(I)-promoted cyclization of allenyl ketones and aldehydes, J. Org. Chem. 56 (1991) 960–969. doi:10.1021/jo00003a013.

[13] J.A. Marshall, G.S. Bartley, Observations Regarding the Ag(I)-Catalyzed Conversion of Allenones to Furans, J. Org. Chem. 59 (1994) 7169–7171. doi:10.1021/jo00102a056.

[14] A.S.K. Hashmi, Transition Metal Catalyzed Dimerization of Allenyl Ketones, Angew. Chem. Int. Ed. Engl. 34 (1995) 1581–1583. doi:10.1002/anie.199515811.

[15] A.S.K. Hashmi, T.L. Ruppert, T. Knöfel, J.W. Bats, C–C-Bond Formation by the Palladium-Catalyzed Cycloisomerization/Dimerization of Terminal Allenyl Ketones: Selectivity and Mechanistic Aspects, J. Org. Chem. 62 (1997) 7295–7304. doi:10.1021/jo970837l.

[16] A.S.K. Hashmi, L. Schwarz, J.-H. Choi, T.M. Frost, A New Gold-Catalyzed C–C Bond Formation, Angew. Chem. Int. Ed. 39 (2000) 2285–2288. doi:10.1002/1521-3773(20000703)39:13<2285::AID-ANIE2285>3.0.CO;2-F.

[17] S. Ma, J. Zhang, L. Lu, Pd0-Catalyzed Coupling Cyclization Reaction of Aryl or 1Alkenyl Halides with 1,2-Allenyl Ketones: Scope and Mechanism. An Efficient Assembly of 2,3,4-, 2,3,5-Tri- and 2,3,4,5-Tetrasubstituted Furans, Chem. – Eur. J. 9 (2003) 2447–2456. doi:10.1002/chem.200204664.

[18] A.V. Gulevich, A.S. Dudnik, N. Chernyak, V. Gevorgyan, Transition Metal-Mediated Synthesis of Monocyclic Aromatic Heterocycles, Chem. Rev. 113 (2013) 3084–3213. doi:10.1021/cr300333u.

[19] W.J. Moran, A. Rodríguez, Metal-catalyzed Furan Synthesis. A Review, Org. Prep. Proced. Int. 44 (2012) 103–130. doi:10.1080/00304948.2012.657558.

[20] S.P. Morcillo, D. Leboeuf, C. Bour, V. Gandon, Calcium-Catalyzed Synthesis of Polysubstituted 2-Alkenylfurans from β-Keto Esters Tethered to Propargyl Alcohols, Chem. – Eur. J. 22 (2016) 16974–16978. doi:10.1002/chem.201603929.

[21] A.S. Dudnik, A.W. Sromek, M. Rubina, J.T. Kim, A.V. Kel'i, V. Gevorgyan, Metal-Catalyzed 1,2-Shift of Diverse Migrating Groups in Allenyl Systems as a New Paradigm toward Densely Functionalized Heterocycles, J. Am. Chem. Soc. 130 (2008) 1440–1452. doi:10.1021/ja0773507.

[22] C. Bruneau, P.H. Dixneuf, Metal Vinylidenes and Allenylidenes in Catalysis: Applications in Anti-Markovnikov Additions to Terminal Alkynes and Alkene Metathesis, Angew. Chem. Int. Ed. 45 (2006) 2176–2203. doi:10.1002/anie.200501391.

[23] J.T. Kim, A.V. Kel'in, V. Gevorgyan, 1,2-Migration of the thio group in allenyl sulfides: efficient synthesis of 3-thio-substituted furans and pyrroles, Angew. Chem. Int. Ed Engl. 42 (2003) 98–101.
[24] X.-L. Hou, Z. Yang, H.N.C. Wong, Chapter 5.3 Five-membered ring systems: Furans and benzofurans, in: G.W.G. and J.A. Joule (Ed.), Prog. Heterocycl. Chem., Elsevier, 2003: pp. 167–205. http://www.sciencedirect.com/science/article/pii/S0959638003800107 (accessed January 6, 2017).
[25] B.H. Lipshutz, Five-membered heteroaromatic rings as intermediates in organic synthesis, Chem. Rev. 86 (1986) 795–819. doi:10.1021/cr00075a005.
[26] A. Arcadi, Gold-catalyzed synthesis of heterocycles, in: Gold Catal., IMPERIAL COLLEGE PRESS, 2011: pp. 175–224. http://www.worldscientific.com/doi/abs/10.1142/9781848168534_0005 (accessed January 6, 2017).
[27] A. Aponick, C.-Y. Li, J. Malinge, E.F. Marques, An Extremely Facile Synthesis of Furans, Pyrroles, and Thiophenes by the Dehydrative Cyclization of Propargyl Alcohols, Org. Lett. 11 (2009) 4624–4627. doi:10.1021/ol901901m.
[28] Z.-W. Chen, M.-T. Luo, Y.-L. Wen, M. Ye, Z.-G. Zhou, L.-X. Liu, A Highly Efficient Synthesis of 2,5-Disubstituted Furans from Enyne Acetates Catalyzed by Lewis Acid and Palladium, Synlett. 25 (2014) 2341–2344. doi:10.1055/s-0034-1379213.
[29] S. Hosseyni, Y. Su, X. Shi, Gold Catalyzed Synthesis of Substituted Furan by Intermolecular Cascade Reaction of Propargyl Alcohol and Alkyne, Org. Lett. 17 (2015) 6010–6013. doi:10.1021/acs.orglett.5b02980.
[30] Y. Liu, F. Song, Z. Song, M. Liu, B. Yan, Gold-Catalyzed Cyclization of (Z)-2-En-4-yn-1-ols: Highly Efficient Synthesis of Fully Substituted Dihydrofurans and Furans, Org. Lett. 7 (2005) 5409–5412. doi:10.1021/ol052160r.
[31] R.K. Shiroodi, C.I.R. Vera, A.S. Dudnik, V. Gevorgyan, Synthesis of furans and pyrroles via migratory and double migratory cycloisomerization reactions of homopropargylic aldehydes and imines, Tetrahedron Lett. 56 (2015) 3251–3254. doi:10.1016/j.tetlet.2015.01.006.
[32] G. Zhou, F. Liu, J. Zhang, Enantioselective Gold-Catalyzed Functionalization of Unreactive sp3 C-H Bonds through a Redox–Neutral Domino Reaction, Chem. – Eur. J. 17 (2011) 3101–3104. doi:10.1002/chem.201100019.
[33] S.J. Pridmore, P.A. Slatford, J.E. Taylor, M.K. Whittlesey, J.M.J. Williams, Synthesis of furans, pyrroles and pyridazines by a ruthenium-catalysed isomerisation of alkynediols and in situ cyclisation, Tetrahedron. 65 (2009) 8981–8986. doi:10.1016/j.tet.2009.06.108.
[34] V. Cadierno, J. Gimeno, N. Nebra, A Novel Propargylation/Cycloisomerization Tandem Process Catalyzed by a Ruthenium(II)/Trifluoroacetic Acid System: One-Pot Entry to Fully Substituted Furans from Readily Available Secondary Propargylic Alcohols and 1,3-Dicarbonyl Compounds, Adv. Synth. Catal. 349 (2007) 382–394. doi:10.1002/adsc.200600366.
[35] L. Peng, X. Zhang, M. Ma, J. Wang, Transition-Metal-Catalyzed Rearrangement of Allenyl Sulfides: A Route to Furan Derivatives, Angew. Chem. Int. Ed. 46 (2007) 1905–1908. doi:10.1002/anie.200604299.
[36] M. Frisch, G. Trucks, H. Schlegel, G. Scuseria, M. Robb, J. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. Hratchian, A. Izmaylov, J. Bloino, G. Zheng, J. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. Montgomery, J. Peralta, F. Ogliaro, M. Bearpark, J. Heyd, E. Brothers, K. Kudin, V. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. Burant, S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. Millam, M. Klene, J. Knox, J. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. Stratmann, O. Yazyev, A. Austin, R. Cammi, C. Pomelli, J. Ochterski, R. Martin, K. Morokuma, V. Zakrzewski, G. Voth, P. Salvador, J. Dannenberg, S. Dapprich, A. Daniels, Farkas, J. Foresman, J. Ortiz, J. Cioslowski, D. Fox, Gaussian 09, Revision D.01, Gaussian 09 Revis. D01 Gaussian Inc Wallingford CT. (2013).
[37] G. Scalmani, M.J. Frisch, Continuous surface charge polarizable continuum models of solvation. I. General formalism, J. Chem. Phys. 132 (2010) 114110. doi:10.1063/1.3359469.
[38] Y. Zhao, D.G. Truhlar, The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals, Theor. Chem. Acc. 120 (2008) 215–241. doi:10.1007/s00214-007-0310-x.
[39] N. Marom, A. Tkatchenko, M. Rossi, V.V. Gobre, O. Hod, M. Scheffler, L. Kronik, Dispersion Interactions with Density-Functional Theory: Benchmarking Semiempirical and Interatomic Pairwise Corrected Density Functionals, J. Chem. Theory Comput. 7 (2011) 3944–3951. doi:10.1021/ct2005616.
[40] Y. Minenkov, Å. Singstad, G. Occhipinti, V.R. Jensen, The accuracy of DFT-optimized geometries of functional transition metal compounds: a validation study of catalysts for olefin metathesis and other reactions in the homogeneous phase, Dalton Trans. 41 (2012) 5526–5541. doi:10.1039/C2DT12232D.
[41] S. Grimme, J. Antony, S. Ehrlich, H. Krieg, A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu, J. Chem. Phys. 132 (2010) 154104. doi:10.1063/1.3382344.
[42] S. Grimme, Density functional theory with London dispersion corrections, Wiley Interdiscip. Rev. Comput. Mol. Sci. 1 (2011) 211–228. doi:10.1002/wcms.30.
[43] J. Řezáč, P. Hobza, Advanced Corrections of Hydrogen Bonding and Dispersion for Semiempirical Quantum Mechanical Methods, J. Chem. Theory Comput. 8 (2012) 141–151. doi:10.1021/ct200751e.
[44] S. Rösel, H. Quanz, C. Logemann, J. Becker, E. Mossou, L. Cañadillas-Delgado, E. Caldeweyher, S. Grimme, P.R. Schreiner, London Dispersion Enables the Shortest Intermolecular Hydrocarbon H···H Contact, J. Am. Chem. Soc. 139 (2017) 7428–7431. doi:10.1021/jacs.7b01879.
[45] D.J. Gorin, F.D. Toste, Relativistic effects in homogeneous gold catalysis, Nature. 446 (2007) 395–403. doi:10.1038/nature05592.
[46] D. Liotard, J.-P. Penot, Critical Paths and Passes: Application to Quantum Chemistry, in: Numer. Methods Study Crit. Phenom., Springer, Berlin, Heidelberg, 1981: pp. 213–221. doi:10.1007/978-3-642-81703-8_27.
[47] D.A. Liotard, Algorithmic tools in the study of semiempirical potential surfaces, Int. J. Quantum Chem. 44 (1992) 723–741. doi:10.1002/qua.560440505.
[48] M. J. S. Dewar, A. J. Holder, R. D. Dennington, D. A. Liotard, D. G.Truhlar, T. A. Keith, J. M. Millam, C. D. Harris. Holder, Ampac 10, Semichem, Inc., (n.d.).

[49] K. Ando, Mechanistic Study on the Gold-Catalyzed C−S Bond Formation of α-Thioallenes To Form 2,5-Dihydrothiophenes, J. Org. Chem. 75 (2010) 8516–8521. doi:10.1021/jo101883j.
[50] A.S. Dudnik, Y. Xia, Y. Li, V. Gevorgyan, Computation-Guided Development of Au-Catalyzed Cycloisomerizations Proceeding via 1,2-Si or 1,2-H Migrations: Regiodivergent Synthesis of Silylfurans, J. Am. Chem. Soc. 132 (2010) 7645–7655. doi:10.1021/ja910290c.
[51] L. Fensterbank, M. Malacria, Molecular Complexity from Polyunsaturated Substrates: The Gold Catalysis Approach, Acc. Chem. Res. 47 (2014) 953–965. doi:10.1021/ar4002334.
[52] V. Gandon, G. Lemière, A. Hours, L. Fensterbank, M. Malacria, The role of bent acyclic allene gold complexes in axis-to-center chirality transfers, Angew. Chem. Int. Ed Engl. 47 (2008) 7534–7538. doi:10.1002/anie.200802332.
[53] R.S. Paton, F. Maseras, Gold(I)-Catalyzed Intermolecular Hydroalkoxylation of Allenes: A DFT study, Org. Lett. 11 (2009) 2237–2240. doi:10.1021/ol9004646.
[54] W. Yang, A.S.K. Hashmi, Mechanistic insights into the gold chemistry of allenes, Chem. Soc. Rev. 43 (2014) 2941–2955. doi:10.1039/C3CS60441A.
[55] J.E. Bailie, G.J. Hutchings, Promotion by sulfur of gold catalysts for crotyl alcohol formation from crotonaldehyde hydrogenation, Chem. Commun. (1999) 2151–2152. doi:10.1039/A906538E.
[56] W. Debrouwer, R.A.J. Seigneur, T.S.A. Heugebaert, C.V. Stevens, Gold superacid-catalyzed preparation of benzo[c]thiophenes, Chem. Commun. 51 (2014) 729–732. doi:10.1039/C4CC07989B.
[57] Menggenbateer, M. Narsireddy, G. Ferrara, N. Nishina, T. Jin, Y. Yamamoto, Gold-catalyzed regiospecific intermolecular hydrothiolation of allenes, Tetrahedron Lett. 51 (2010) 4627–4629. doi:10.1016/j.tetlet.2010.06.125.
[58] N. Morita, N. Krause, The First Gold-Catalyzed C-S Bond Formation: Cycloisomerization of α-Thioallenes to 2,5-Dihydrothiophenes, Angew. Chem. Int. Ed. 45 (2006) 1897–1899. doi:10.1002/anie.200503846.
[59] I. Nakamura, T. Sato, Y. Yamamoto, Gold-Catalyzed Intramolecular Carbothiolation of Alkynes: Synthesis of 2,3-Disubstituted Benzothiophenes from (α-Alkoxy Alkyl) (ortho-Alkynyl Phenyl) Sulfides, Angew. Chem. Int. Ed. 45 (2006) 4473–4475. doi:10.1002/anie.200601178.
[60] L. Peng, X. Zhang, S. Zhang, J. Wang, Au-Catalyzed Reaction of Propargylic Sulfides and Dithioacetals, J. Org. Chem. 72 (2007) 1192–1197. doi:10.1021/jo0618674.
[61] J.R. Reimers, M.J. Ford, A. Halder, J. Ulstrup, N.S. Hush, Gold surfaces and nanoparticles are protected by Au(0)–thiyl species and are destroyed when Au(I)–thiolates form, Proc. Natl. Acad. Sci. U. S. A. 113 (2016) E1424–E1433. doi:10.1073/pnas.1600472113.
[62] E.D. Glendening, C.R. Landis, F. Weinhold, NBO 6.0: Natural bond orbital analysis program, J. Comput. Chem. 34 (2013) 1429–1437.
[63] E.D. Glendening, C.R. Landis, F. Weinhold, Natural bond orbital methods, Wiley Interdiscip. Rev. Comput. Mol. Sci. 2 (2012) 1–42.

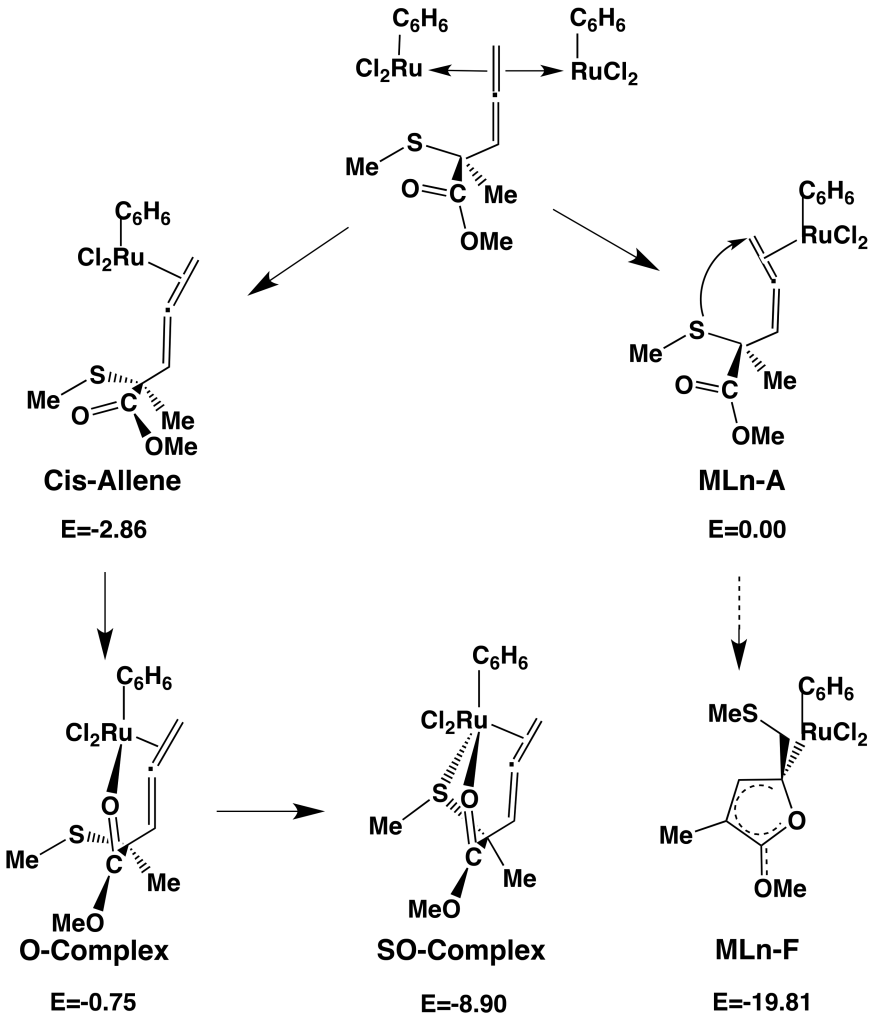
Metal-Catalysed Rearrangement of Allenylsulfides to Furan: A Theoretical Mechanistic Approach

Michel Rajzmann,*[a] Stephane Humbel,*[a] Jianbo Wang[b]

[a] Dr M. Rajzmann, Pr S. Humbel : Aix Marseille Univ, CNRS, Centrale Marseille, iSm2, Marseille, France
[b] Pr J. Wang: Key Laboratory of Bioorganic Chemistry and Molecular Engineering of Ministry of Education, College of Chemistry, Peking University, Beijing 100871, China

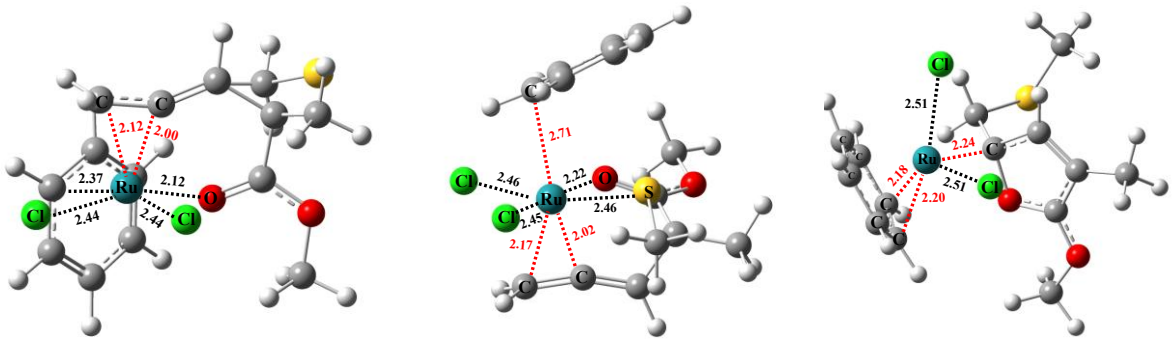
Endo orientation of the MLn-A complex

The metal can bind on either side of the allene bond in a low barrier process (about +3kcal/mol). Only the exo (or Trans) orientation can directly lead to the product.
The endo orientation is slightly higher in energy than the exo when Au or Pt are used as catalysts. Only for Ru, is the first endo (or Cis) intermediate lower in energy than the exo (Trans). But only the exo (Trans) can lead to the formation of the Furane, and this is more exothermic. Bellow are details about the endo coordination and various subsequent intermediates.



Scheme S1: Structures & energies for **$RuCl_2(C_6H_6)$-A**. Reference of the energies is that of **$RuCl_2(C_6H_6)$-A** (**MLn-A**) 0.00 kcal.mol^{-1}.

Figure S1 shows the main intermediates and Table S1 collects NBO charges (**NBO** version 6).[1] The Ru-benzene distance increases from 2.20Å (in **MIn-F**) up to 2.71Å in the **SO-complex** (**Figure 1**). The hapticity is also modified $\eta 6$ in **MIn-F,** against $\eta 2$ in the **SO-complex**. The charges (Table 1) shows very well the modification of the role of the benzene moieties: from strongly donating - **MLn-F** shows very positive charges on the benzene up moderate donnor when the benzene is not close to the metal (as in the SO and O complexes).



(a) (b) (c)

Figure S1: Main intermediates (a) **O-Complex**, (b) **SO-Complex,** (c) **MLn-F**.

Table S1: NBO6 Total charge for **Ru**, O (carbonyl), S, and groups of atoms : the 2 Cl atoms, and benzene molecule.

Total Charge	MLn-A	S-Cycle	MLn-F	O-Complex	SO-Complex
Ru	**0.205**	**0.222**	**0.246**	**0.525**	**0.361**
O	**-0.673**	**-0.657**	**-0.639**	**-0.663**	**-0.637**
S	**0.139**	**0.649**	**0.133**	**0.151**	**0.361**
Cl2	**-0.896**	**-1.085**	**-1.057**	**-0.908**	**-1.001**
Benzene	**0.534**	**0.351**	**0.463**	**0.147**	**0.137**

To make the Trans complex from the Cis can be achieved with a new Allene molecule. The barriere is 12.8 kcal.mol^{-1} (**Figure S2)**. This is much easier than rotating around the double bond (3 step process with the highest at 34.6 kcal.mol^{-1}.

The complete path from the **SO-complex** to **MLn-F** is given in Figure S2 bellow. The equilibrium constant between the **SO complex** and the **RuLn-F** product corresponds at 80°C, gives a ratio **SO complex/RuLn-F** of about 10^{-7}, and is smaller at 25°C (k_c/k_f ~10^{-8}). Hence, under thermodynamic conditions, the Cis-Allene, readily transforms to the furane product.

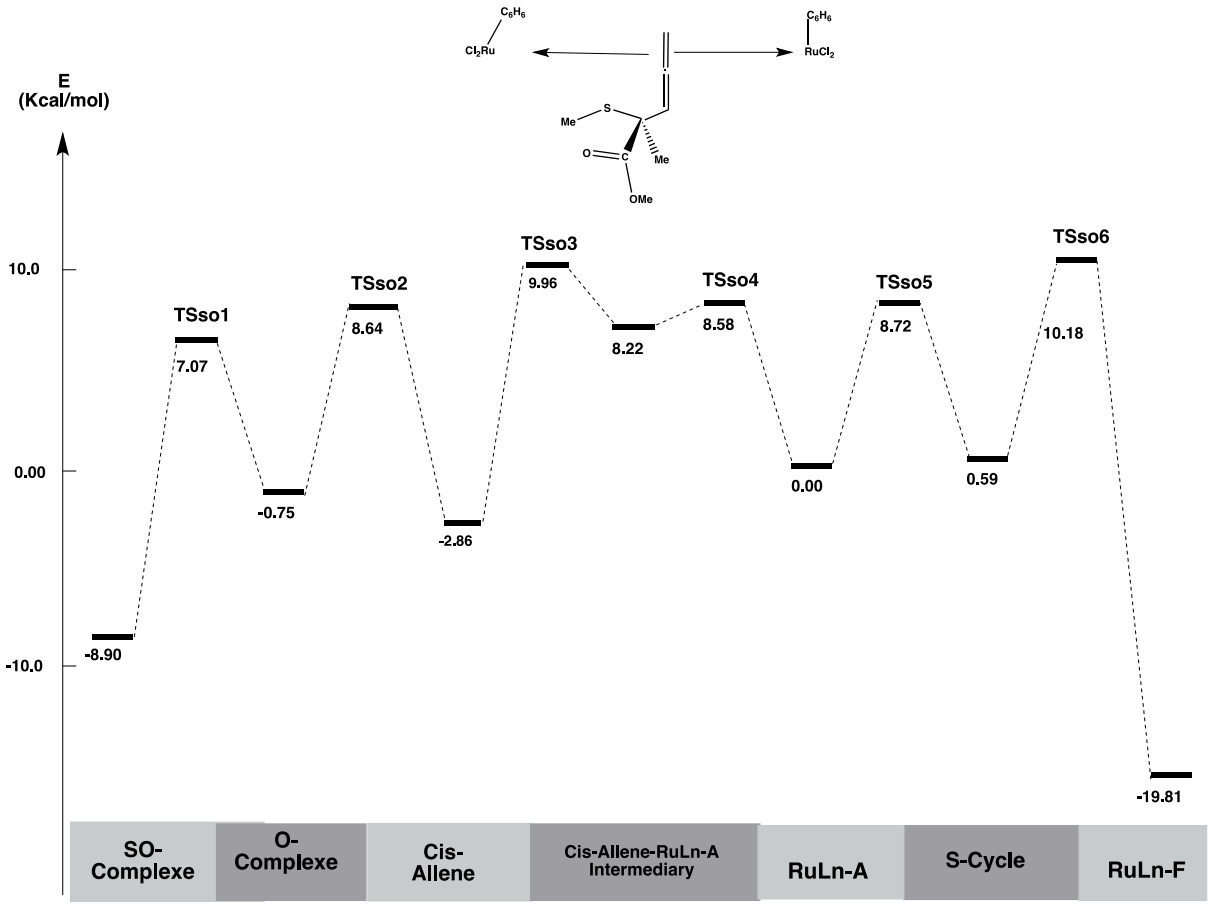


Figure S2: Energy profile for **O-Complex** & **SO-Complex** formation.

Table S2: Energies for **O-Complex, SO-Complex** etc… paths (**Energy** in ua**, ΔE** in kcal.mol^{-1}).

	Energy	**ΔE**
SO-Complexe	-1300.52943	-8.90
TSso1	-1300.50397	7.07
O-Complexe	-1300.51643	-0.75
TSso2	-1300.50147	8.64
Cis-Allene	-1300.51980	-2.86
TSso3	-1300.49936	9.96
Cis-Allene-MLn-A-Intermediary	-1300.50213	8.22
TSso4	-1300.50156	8.58
RuLn-A	-1300.51524	0.00
TSso5	-1300.50134	8.72
S-Cycle	-1300.51430	0.59
TSso6	-1300.49902	10.18
RuLn-F	-1300.54681	-19.81

(1) Glendening, E. D.; Landis, C. R.; Weinhold, F. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* 2012, *2* (1), 1–42.

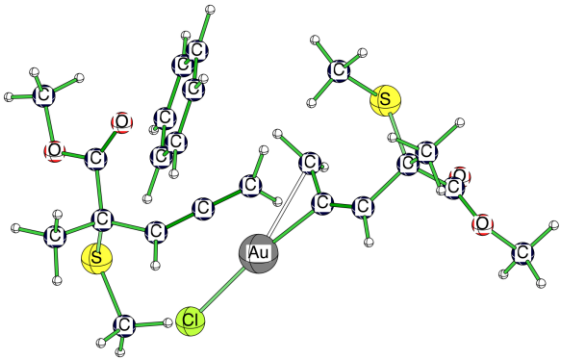
Structures

In the following, energies and xyz coordinates (in Å) are provided for all structures. Additionally for transition states the negative frequency is provided (LOWEST FREQUENCY).

1 Au CATALYST

1.1 AU- CATALYST TS1

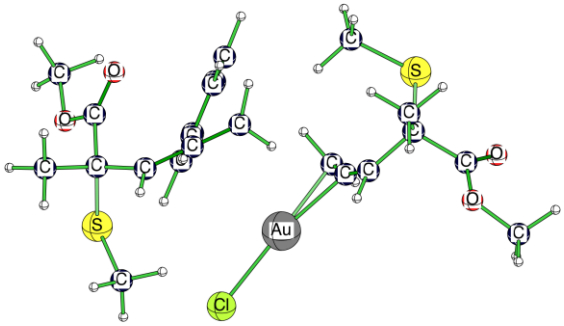
ENERGY=-1327.11544 LOWEST FREQUENCY=-209.63



C	3.80002000	1.00712800	1.07177600
C	2.70722500	-0.06194300	1.01941500
C	1.97456100	-0.20580000	-0.07969100
C	5.07740500	0.26909800	0.66156100
S	3.54270300	2.29279600	-0.29096700
C	1.94330600	0.52672800	-1.26915200
O	5.53412000	0.25323900	-0.45948600
O	5.56845400	-0.42449700	1.68894200
C	6.68955000	-1.26152000	1.38060000
C	2.13967000	3.25848600	0.45138700
H	2.64517500	-0.72305600	1.88545300
H	1.14694600	1.25471600	-1.45601300
H	2.52875600	0.20496900	-2.13252800
C	3.88453100	1.63789600	2.45505200
H	2.50656100	3.90581500	1.25101000
H	1.72606700	3.86398500	-0.35936500
H	1.37002300	2.57163600	0.82224600
H	7.54141300	-0.65320700	1.06003900
H	6.92736600	-1.79605600	2.30184200
H	6.42903900	-1.96502500	0.58352600
H	2.93409500	2.11466900	2.72351500
H	4.08201400	0.85666300	3.19746200
H	4.68702100	2.38199300	2.51361100
Cl	-0.96628600	-3.36290800	-1.26916400
C	-0.77880200	3.23533000	-2.11990100
C	-0.78949800	2.57055100	-3.35135200
C	-1.18467800	1.22959500	-3.42170200
C	-1.56097800	0.55028700	-2.25884700
C	-1.53178100	1.21183500	-1.02668900
C	-1.14981400	2.55436000	-0.95419300
H	-0.49069500	4.28549400	-2.07213600
H	-0.49940700	3.10146800	-4.25722700
H	-1.20259000	0.71572500	-4.38168700
H	-1.87536300	-0.49398700	-2.29866400
H	-1.80753100	0.66239300	-0.12335000
H	-1.16745200	3.06928400	0.00773600
Au	0.55817800	-1.57098900	-0.70498200
C	-4.07695300	0.01494200	1.72528800
C	-2.98316500	-0.08359800	2.75381800
C	-1.78387300	0.44985700	2.66763100
C	-4.10550100	1.37966200	1.03415700
S	-3.81898500	-1.29857000	0.34666500
C	-0.58381700	0.97498200	2.59610500
O	-3.58699100	2.38946800	1.45741100
O	-4.85376600	1.33512700	-0.07129600
C	-4.98350300	2.56656200	-0.78276000
C	-3.34750500	-2.75847600	1.39279400
H	-3.21416800	-0.69311700	3.63263300
H	0.23985000	0.43564400	2.11970800
H	-0.38556600	1.97131000	2.99392700
C	-5.44098600	-0.19917600	2.38477500
H	-2.38310800	-2.58882900	1.88110100
H	-4.12755200	-2.98088400	2.12886600
H	-3.24863100	-3.58985000	0.69029000
H	-5.64134900	2.35560500	-1.62789200
H	-5.41862000	3.33828300	-0.13850700
H	-4.00294000	2.90369300	-1.14033900
H	-5.48222400	-1.18808200	2.85916700
H	-5.60802500	0.55826600	3.16412000
H	-6.24479400	-0.13696400	1.64461800

1.2 AU- CATALYST Allene MLn-A

ENERGY=-1327.12239

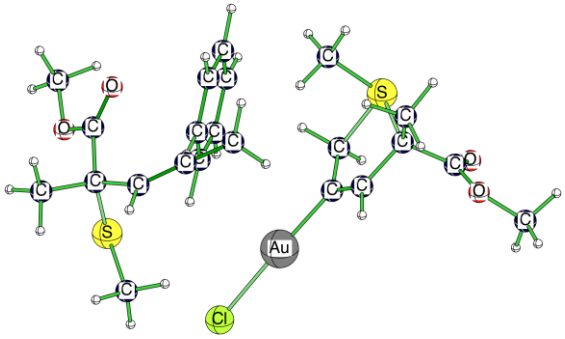


C	3.85196300	1.01284500	1.06728400
C	2.73189400	0.03661000	0.74017500
C	2.16151700	-0.05107700	-0.44605300
C	5.15629100	0.24581800	0.81954300
S	3.90791000	2.48807700	-0.10908400
C	1.82180300	0.19827300	-1.74140200
O	5.91449800	0.42746500	-0.10391900
O	5.31541000	-0.69660400	1.75361900
C	6.46385800	-1.53533700	1.58941900
C	2.29763200	3.29964600	0.34536200
H	2.44238300	-0.64666100	1.54319100
H	1.11948900	1.00179900	-1.98717100
H	2.39633900	-0.24660200	-2.55446700
C	3.73821200	1.45553300	2.52390400
H	2.35403100	3.78395400	1.32417200
H	2.12033800	4.05578200	-0.42408300
H	1.47878900	2.56992400	0.32071000
H	7.37878700	-0.93410300	1.59273100
H	6.45554100	-2.22420400	2.43598100
H	6.39987200	-2.08717100	0.64569700
H	2.79825200	1.99416400	2.69430800
H	3.75145500	0.58371600	3.18850200
H	4.57078100	2.11543300	2.79224000
Cl	-0.92187700	-3.32609300	-0.65122200
C	-0.84407600	2.85769200	-2.18577000
C	-1.09061200	2.24786000	-3.42185600
C	-1.63724900	0.96016900	-3.47450400
C	-1.92561200	0.27632000	-2.28935700
C	-1.66120400	0.88150200	-1.05631700
C	-1.13190200	2.17317100	-0.99997500
H	-0.43759700	3.86810200	-2.14862100
H	-0.86518600	2.78151000	-4.34435600
H	-1.83686000	0.49209000	-4.43737500
H	-2.35683300	-0.72507100	-2.30886100
H	-1.87719200	0.32674300	-0.13945400

H	-0.97254700	2.64559100	-0.02905200
Au	0.56750700	-1.45895100	-0.91266000
C	-4.02298100	0.14053100	1.85699500
C	-2.81943300	0.08898000	2.75871600
C	-1.64401400	0.63367500	2.53278400
C	-4.07494900	1.42951000	1.03604200
S	-4.00940700	-1.34043600	0.63601000
C	-0.46874800	1.18164000	2.33559600
O	-3.58942000	2.48383000	1.38307300
O	-4.80970500	1.27495500	-0.06744500
C	-4.95087400	2.44022500	-0.88117000
C	-3.40472200	-2.68934100	1.76055900
H	-2.94686200	-0.49572700	3.67478200
H	0.31985600	0.64777500	1.79752200
H	-0.25251300	2.19103700	2.68885200
C	-5.30408600	0.09923700	2.69549400
H	-2.39344800	-2.46991500	2.11470700
H	-4.09419300	-2.85205200	2.59595700
H	-3.36165000	-3.58425200	1.13345100
H	-5.53176900	2.12973300	-1.75171200
H	-5.47372900	3.23115600	-0.33237600
H	-3.96519100	2.80708600	-1.19159200
H	-5.33297700	-0.81523600	3.30145300
H	-5.33610000	0.96187000	3.37646000
H	-6.19100900	0.11389200	2.05305400

1.3 AU-CATALYS TS-Cycle

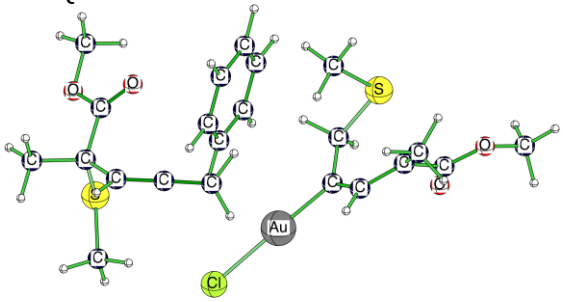
ENERGY=-1327.12689



C	3.70425200	1.00877100	1.11027800
C	2.68245600	-0.10692000	0.99935400
C	1.92706200	-0.21111700	-0.10679800
C	5.02912500	0.44098900	0.60208300
S	3.18821700	2.23199200	-0.26611500
C	2.10124500	0.86182600	-1.12020400
O	5.41984500	0.54522400	-0.54027400
O	5.63268800	-0.25208000	1.56042600
C	6.80327100	-0.97488800	1.15105800
C	1.82062600	3.15974200	0.57396800
H	2.68070300	-0.82755700	1.81875300
H	1.17429200	1.37681100	-1.40734600
H	2.66383800	0.55607600	-2.00905300
C	3.78327600	1.65616700	2.47927200
H	2.26097900	3.82416600	1.31971800
H	1.32529100	3.73628900	-0.21116500
H	1.12205100	2.44153600	1.01670300
H	7.58733900	-0.27843300	0.83827000
H	7.12198600	-1.54517400	2.02451000
H	6.55915700	-1.64420900	0.32066100
H	2.79156300	1.96874400	2.82705000
H	4.15552000	0.90435900	3.18427300
H	4.46911200	2.51132400	2.50231800
Cl	-0.91100500	-3.46638700	-1.27555600
C	-0.82855700	3.30687500	-2.15974900
C	-0.74813900	2.61602900	-3.37386700
C	-1.04912900	1.24966600	-3.42471700
C	-1.42016100	0.57133100	-2.25989800
C	-1.47993500	1.25897000	-1.04408700
C	-1.19386900	2.62537800	-0.99210600
H	-0.61682800	4.37604400	-2.12658800
H	-0.46301200	3.14553800	-4.28222900
H	-0.99722900	0.71477100	-4.37181400
H	-1.66560700	-0.49160600	-2.28068900
H	-1.74459600	0.70721400	-0.13905700
H	-1.27519900	3.15680000	-0.04245600
Au	0.60268900	-1.67741600	-0.60412100
C	-4.04785000	0.01216400	1.65319300
C	-2.96258700	-0.06922900	2.69192800
C	-1.77232300	0.48594800	2.62673700
C	-4.10313100	1.38063800	0.97359900
S	-3.74712800	-1.29116700	0.27363100
C	-0.56976400	1.00900300	2.57566200
O	-3.62151400	2.40098600	1.41595900
O	-4.83433100	1.32703900	-0.14241400
C	-4.99452700	2.56220700	-0.84003800
C	-3.25910700	-2.73984100	1.32729200
H	-3.18703200	-0.69612000	3.56018400
H	0.24976800	0.46074300	2.09947900
H	-0.36714500	1.99436800	2.99974500
C	-5.41334600	-0.23250300	2.30013000
H	-2.29167100	-2.55913300	1.80519400
H	-4.03375000	-2.96111600	2.06973900
H	-3.15808600	-3.57534400	0.63062600
H	-5.64180300	2.34296000	-1.69118200
H	-5.45387000	3.31438800	-0.18953500
H	-4.02216100	2.93021900	-1.18919000
H	-5.43877000	-1.22338400	2.77139600
H	-5.60271900	0.51895100	3.08030300
H	-6.21169300	-0.18460500	1.55303100

1.4 AU-CATALYST TS2

ENERGY=-1327.10129 LOWEST
FREQUENCY=-201.60

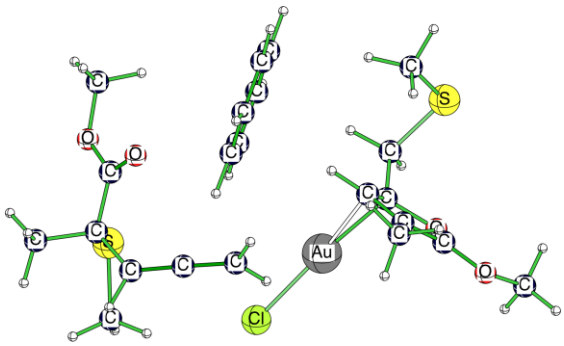


C	4.08239100	0.09545500	1.49438900
C	2.87104600	-0.58752600	1.22987800
C	2.11023300	-0.44638200	0.09065400
C	5.18680600	0.01496700	0.46058500
S	3.39293800	2.10821500	0.12325300
C	2.28028500	0.81301800	-0.70599600

O	5.06540400	-0.50127400	-0.62793700
O	6.30969400	0.57152800	0.91716600
C	7.39988900	0.58297000	-0.01090300
C	2.14251300	2.77693400	1.31669300
H	2.48934900	-1.20775900	2.04676100
H	1.30756000	1.29991800	-0.84849300
H	2.71483000	0.61425900	-1.69385100
C	4.47460700	0.39596000	2.90068500
H	2.66156900	3.44042300	2.01113900
H	1.37679200	3.32093200	0.75621400
H	1.68454200	1.93237800	1.84787600
H	7.13058800	1.16290500	-0.90056800
H	8.23481300	1.05218700	0.51211600
H	7.65657300	-0.43782500	-0.31136100
H	3.59881300	0.42488200	3.55670600
H	5.17219000	-0.37018700	3.26774800
H	5.01264400	1.34887300	2.95797600
Cl	-1.14625800	-3.22155600	-1.09838000
C	-0.30567100	3.32948400	-1.58787100
C	0.00575400	2.86723600	-2.87117400
C	-0.34725100	1.56651200	-3.25039200
C	-1.00781900	0.72824700	-2.34682800
C	-1.30996300	1.18761000	-1.06033600
C	-0.96274800	2.48802100	-0.68073100
H	-0.04341000	4.34790500	-1.29868200
H	0.51673000	3.52170900	-3.57628200
H	-0.10949400	1.20780100	-4.25090500
H	-1.29327900	-0.28499000	-2.63308200
H	-1.81930400	0.52109500	-0.36075300
H	-1.22660900	2.83812400	0.31833100
Au	0.62511900	-1.68445500	-0.47100000
C	-4.67940400	0.20354600	1.26062900
C	-3.83868300	-0.33287600	2.38900600
C	-2.52382500	-0.38224300	2.39457200
C	-4.25993000	1.62803100	0.88478600
S	-4.41166200	-0.78318900	-0.37220000
C	-1.21477500	-0.45631300	2.37607100
O	-3.38046600	2.27528600	1.40956700
O	-5.01829700	2.08896200	-0.11579400
C	-4.68084900	3.39206100	-0.59272200
C	-4.33959400	-2.52108400	0.27568100
H	-4.38269800	-0.70762900	3.26044800
H	-0.70972400	-1.34525400	1.98648900
H	-0.59741400	0.37510800	2.71999400
C	-6.15784100	0.17039100	1.64142400
H	-3.49813800	-2.63955000	0.96332700
H	-5.28610800	-2.80198600	0.74906600
H	-4.15506900	-3.14479900	-0.60341000
H	-5.38244000	3.60638500	-1.40123000
H	-4.78118000	4.13298200	0.20806500
H	-3.65105600	3.40367900	-0.96926500
H	-6.45918600	-0.85808000	1.87779600
H	-6.33666200	0.78654300	2.53471200
H	-6.78536100	0.53784600	0.82510000

1.5 AU-CATALYST Cycle-O F-MLn

ENERGY=-1327.15825

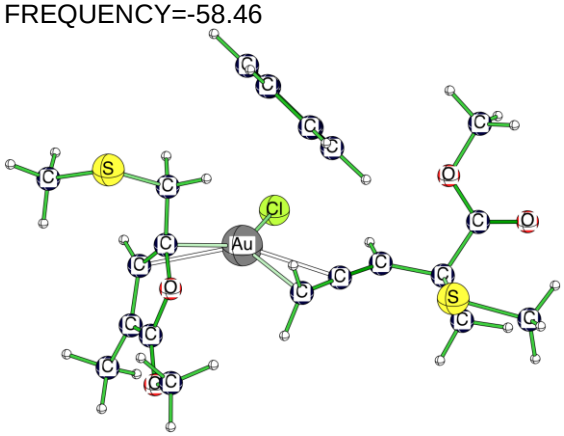


C	2.96060200	-0.34155700	2.03340600
C	2.10388200	0.35836900	1.19150400
C	2.55250500	0.24680600	-0.16682000
C	3.96226000	-0.81365200	1.17252700
S	3.97892700	2.65617100	-0.66978200
C	2.65199800	1.40011800	-1.12000700
O	3.77833600	-0.48837100	-0.08884400
O	4.97819300	-1.56020900	1.51177500
C	5.93284900	-1.87973600	0.48522600
C	3.16528500	3.46052200	0.79652900
H	1.22326100	0.93303000	1.47362600
H	1.68499700	1.91729500	-1.17911200
H	2.92225800	1.05761100	-2.12399700
C	2.86857700	-0.61570000	3.49643800
H	3.71336400	4.38559900	0.99339600
H	2.12381500	3.69778000	0.55159000
H	3.21160500	2.81440000	1.67892600
H	6.37089300	-0.96089900	0.08110500
H	6.69730500	-2.48568300	0.97187700
H	5.44784300	-2.44452400	-0.31693900
H	2.17099600	0.07881200	3.97573400
H	2.51401700	-1.63635200	3.68905400
H	3.84675200	-0.50855400	3.97886200
Cl	-0.61585700	-2.70983800	-1.60823100
C	-0.48211400	3.59583600	0.13584800
C	-0.31409000	3.85108700	-1.23014400
C	-0.60808900	2.85526900	-2.16923500
C	-1.06821500	1.60511600	-1.74318100
C	-1.23181900	1.35057100	-0.37767500
C	-0.94049500	2.34442700	0.56246200
H	-0.27282400	4.37745000	0.86643300
H	0.04295000	4.82487700	-1.56344000
H	-0.47971200	3.05525900	-3.23206300
H	-1.30226000	0.82155900	-2.46441400
H	-1.60457200	0.37535200	-0.05318800
H	-1.10708100	2.14464700	1.62186400
Au	0.98643500	-1.08846900	-0.78657800
C	-4.51937100	-0.56230100	0.86558100
C	-3.68406000	-1.51087400	1.68253800
C	-2.39988400	-1.39795200	1.94621200
C	-4.17940400	0.90092800	1.15023000
S	-4.23182000	-0.83136100	-1.01513800
C	-1.12005100	-1.31930800	2.22280300
O	-3.56209400	1.30398800	2.11162900
O	-4.72713600	1.70006800	0.22978000
C	-4.49411700	3.09824100	0.39968100
C	-4.17255300	-2.68632000	-1.04544500
H	-4.20518700	-2.39712400	2.05705800
H	-0.37832800	-1.76214000	1.54970600

H	-0.76329200	-0.80531600	3.11649000
C	-6.00206400	-0.77246000	1.18067000
H	-3.29203900	-3.03848000	-0.50182500
H	-5.09646000	-3.11404500	-0.64075300
H	-4.07538200	-2.96045800	-2.09946900
H	-5.05079000	3.59425200	-0.39781000
H	-4.84762100	3.43253600	1.38119700
H	-3.42276100	3.31628000	0.30579700
H	-6.29106900	-1.80647600	0.95239500
H	-6.19220900	-0.59567800	2.24922000
H	-6.62912100	-0.10010200	0.58735100

1.6 AU-REGENERATION TSx

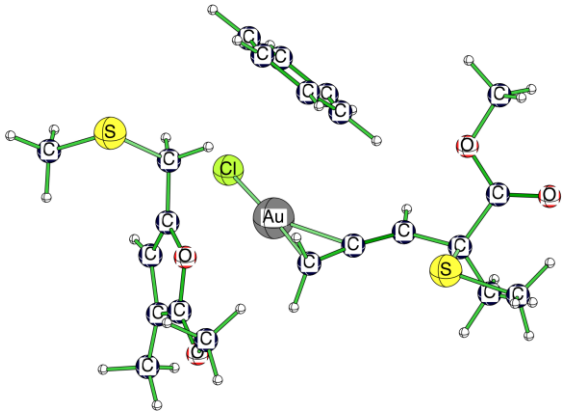
ENERGY=-1327.15227 LOWEST
FREQUENCY=-58.46



C	3.95451000	-1.08964600	0.03150700
C	2.55265800	-0.83598700	-0.46099100
C	1.45739100	-0.98722300	0.24603900
C	4.85479500	0.11630500	-0.22035900
S	3.89548000	-1.26914800	1.92827500
C	0.41000100	-1.14978300	1.06416100
O	6.05930400	0.04368900	-0.35153000
O	4.16644100	1.25895800	-0.23418400
C	4.94751400	2.44815700	-0.36990900
C	5.65021700	-1.77378800	2.29467100
H	2.45612900	-0.52657400	-1.51050100
H	-0.04177100	-2.13381200	1.20539900
H	0.09933100	-0.34293000	1.73272400
C	4.51472900	-2.33475800	-0.63941100
H	5.83917600	-2.79528500	1.95434400
H	6.35267700	-1.07617000	1.82886100
H	5.74687700	-1.72523000	3.38233100
H	5.52266400	2.42507200	-1.30126900
H	4.23602400	3.27664200	-0.38091200
H	5.63617700	2.54831200	0.47599300
H	3.92358900	-3.21004100	-0.34695100
H	4.45478700	-2.22491400	-1.73048800
H	5.56559500	-2.49389600	-0.37877000
Cl	0.45450700	-0.00172800	-3.19281100
H	-3.17837700	-3.71838800	3.61978300
C	-3.07580600	-2.77021100	3.08936100
O	-3.23722600	-3.07832900	1.70452100
H	-3.84577900	-2.06556400	3.42541600
H	-2.08410900	-2.34106000	3.27909500
C	-3.18891200	-2.06693800	0.85161400
C	-3.44757200	-2.07437000	-0.49759400
O	-2.77245000	-0.86717400	1.30181700
C	-3.15863600	-0.73771600	-0.91656900
C	-3.88032200	-3.23978000	-1.32122500
C	-2.70129100	-0.02731100	0.20461900
H	-3.36790700	-0.29624800	-1.88695200
H	-3.08319200	-3.56056900	-2.00418900
H	-4.13707100	-4.09001500	-0.68043500
H	-4.75859000	-2.99619300	-1.93058000
C	-2.68320100	1.42869000	0.48290300
S	-4.23647900	2.06555000	1.33408500
H	-2.56093900	1.97225900	-0.46198600
H	-1.86166300	1.71669800	1.15139200
C	-5.46277000	1.64379200	0.00094200
H	-6.41667800	2.08956500	0.29334900
H	-5.13638400	2.07117500	-0.95339900
H	-5.57901600	0.55859100	-0.08863900
Au	-0.67959300	-0.36732800	-0.98466800
C	-0.04249000	3.49744200	-0.66736200
C	-0.72292300	4.22472700	0.31466900
C	-0.45910400	3.98844600	1.66784700
C	0.49077700	3.02942900	2.03835100
C	1.17590200	2.30673600	1.05625300
C	0.90611400	2.53826200	-0.29756800
H	-0.25048000	3.66956800	-1.72316600
H	-1.46574100	4.96844500	0.02861600
H	-0.99302900	4.55113100	2.43273200
H	0.70103700	2.84955400	3.09218800
H	1.92941800	1.56681500	1.33492300
H	1.43642900	1.97485600	-1.06681700

1.7 AU-REGENERATION Furane

ENERGY=-1327.16098



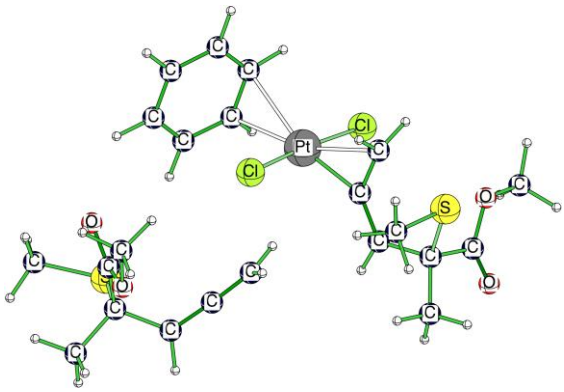
C	3.95955300	-0.89350800	-0.21405100
C	2.64012600	-0.54192600	-0.85675500
C	1.45350200	-0.85569400	-0.37865900
C	4.84724800	0.34134900	-0.08324700
S	3.62669600	-1.44639500	1.57847600
C	0.42309200	-1.27552400	0.41088000
O	6.05739500	0.29559800	-0.01525500
O	4.13247800	1.46660300	-0.01220000
C	4.88593100	2.66177600	0.21701800
C	5.31664800	-2.03359300	2.09363300
H	2.71093700	-0.00581900	-1.80607200
H	0.05840900	-2.30436900	0.35977500
H	0.11807700	-0.67439300	1.27163100

C	4.65315400	-1.97770300	-1.02601800
H	5.57449000	-2.96558400	1.58446700
H	6.06584300	-1.26201400	1.89356000
H	5.24545500	-2.21051100	3.16984900
H	5.62943600	2.80354300	-0.57381900
H	4.16266000	3.47990700	0.21411200
H	5.39474300	2.60697900	1.18517800
H	4.05176200	-2.89360000	-1.01081700
H	4.76058200	-1.64899700	-2.06864400
H	5.65572900	-2.18673800	-0.64057900
Cl	-1.47913600	0.90918900	-3.21906900
H	-1.72718900	-4.00451300	3.68809300
C	-2.00039900	-3.07005900	3.19340200
O	-2.19733000	-3.39207800	1.82116600
H	-2.91854500	-2.66643100	3.63892000
H	-1.19100000	-2.33788700	3.31580300
C	-2.62321900	-2.40311400	1.03042400
C	-3.12402600	-2.46647800	-0.24091000
O	-2.48831400	-1.12997300	1.46754700
C	-3.30534000	-1.09062700	-0.61654200
C	-3.37177500	-3.69677800	-1.04770100
C	-2.90361500	-0.31550800	0.43899000
H	-3.67951500	-0.71047400	-1.56230000
H	-2.74126000	-3.71827000	-1.94674300
H	-3.15059800	-4.59462200	-0.45993300
H	-4.41531200	-3.75876900	-1.38017900
C	-2.87145400	1.13590800	0.67168800
S	-4.24784500	1.77489500	1.79710400
H	-2.94497000	1.66377900	-0.28765300
H	-1.94746500	1.45513200	1.17320500
C	-5.68172600	1.35474600	0.69005300
H	-6.58762700	1.71535700	1.18375700
H	-5.56421100	1.85417600	-0.27755000
H	-5.74457300	0.27096400	0.54860400
Au	-0.41438600	-0.21824500	-1.35052600
C	-0.24822800	3.53296000	-0.24359800
C	-0.99875200	3.99821800	0.84031400
C	-0.67728800	3.59447800	2.14024200
C	0.39750800	2.72553300	2.35766900
C	1.15354100	2.26410500	1.27552500
C	0.82842600	2.66715800	-0.02465200
H	-0.50475900	3.83398600	-1.25833500
H	-1.84518900	4.66303900	0.67259900
H	-1.27011800	3.95065500	2.98191100
H	0.64799000	2.41150000	3.37027800
H	2.00077500	1.59499600	1.43912300
H	1.42435200	2.31260000	-0.86808600

2 Pt CATALYST

2.1 PT-CATALYST TS1

ENERGY=-1325.76793 LOWEST
FREQUENCY=-260.70

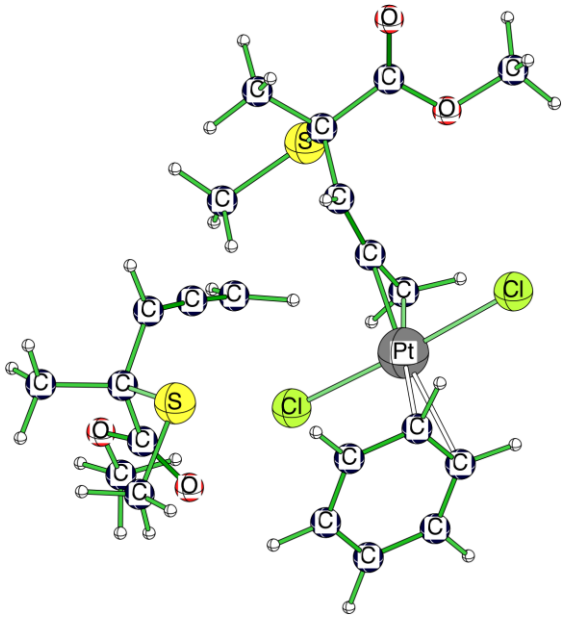


C	-4.76879800	-2.04459300	-0.31996500
C	-3.52148000	-2.81124500	-0.69389100
C	-2.31805700	-2.28324100	-0.63898400
C	-4.47677700	-0.98061400	0.74473000
S	-5.30873800	-1.23840300	-1.94501500
C	-1.14919000	-1.70587200	-0.49879700
O	-4.74267300	0.19959800	0.66509600
O	-3.92204100	-1.54238900	1.82073000
C	-3.52293900	-0.63521000	2.85316600
C	-6.97472300	-0.53376600	-1.50399000
H	-3.67270600	-3.82713600	-1.06713500
H	-0.69422300	-1.12762000	-1.30813400
H	-0.60780300	-1.76588500	0.44796800
C	-5.83727300	-2.99676300	0.21599600
H	-6.87552600	0.12424400	-0.63744600
H	-7.29050600	0.04961700	-2.37315600
H	-7.70365200	-1.32819500	-1.31936600
H	-4.36709900	-0.01233400	3.16871000
H	-3.17683700	-1.25733900	3.68096600
H	-2.70323200	0.00332700	2.49571500
H	-6.09673100	-3.73383100	-0.55367500
H	-5.45563300	-3.52362400	1.09916200
H	-6.74895400	-2.45967700	0.50562900
Cl	1.88361200	1.48068800	-2.30991600
Cl	-0.04328000	0.79608000	2.10264100
C	-2.30572100	1.87504800	-0.40353800
C	-2.67910400	2.57065300	0.73700600
C	-1.91875900	3.66724700	1.18104800
C	-0.78114500	4.06453200	0.48945500
C	-0.38843100	3.36914500	-0.66977500
C	-1.15005600	2.26322800	-1.11864900
H	-2.91447800	1.04113400	-0.75386300
H	-3.57209200	2.25996800	1.27764300
H	-2.22403500	4.20846900	2.07531700
H	-0.19958100	4.92052200	0.82654500
H	0.43512400	3.73679400	-1.27976900
H	-0.94229400	1.82641500	-2.09618400
Pt	0.82088800	1.19818600	-0.13715200
C	3.78682200	-2.05701800	0.33471000
C	2.42775600	-1.45627300	0.00865900
C	2.21479200	-0.17145600	0.25851900
C	4.56750400	-2.01909500	-0.98419500
S	4.70010300	-0.93013800	1.56782700
C	3.03721100	0.81242200	0.85682400
O	4.64598500	-2.96511600	-1.73433900
O	5.05773000	-0.80605100	-1.23307300
C	5.64140200	-0.62632900	-2.52801700
C	3.74148100	-1.29969100	3.11873900

H	1.71818700	-2.10270500	-0.51021300
H	2.84566300	1.15337200	1.87492100
H	3.68817300	1.42349400	0.22998700
C	3.66503400	-3.48053900	0.84783600
H	2.66749600	-1.22320800	2.91378400
H	4.00333800	-2.29069600	3.49532800
H	4.03757900	-0.53725300	3.84335000
H	4.88242300	-0.77643300	-3.30267400
H	6.00721500	0.40141100	-2.55129300
H	6.46380600	-1.33281300	-2.67895000
H	3.01903000	-3.52277000	1.73167600
H	3.20676100	-4.09615600	0.06517300
H	4.64450100	-3.90981000	1.08791700

2.2 PT-CATALYST Allene MLn-A

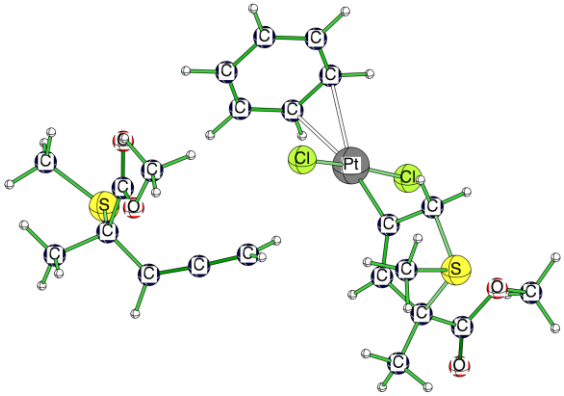
ENERGY=-1325.77428



C	4.74386400	2.05948600	-0.45312600
C	3.43328700	2.68872800	-0.87144300
C	2.26214500	2.16792100	-0.57780400
C	4.46933000	0.93965400	0.55456100
S	5.43981500	1.35409400	-2.06571700
C	1.14331400	1.59123200	-0.21074400
O	4.56508600	-0.24980900	0.34354800
O	4.08426200	1.45353700	1.72481300
C	3.63387500	0.49935300	2.69209100
C	7.05288200	0.63265100	-1.48145700
H	3.51243700	3.59671000	-1.47513500
H	0.68487600	0.81022000	-0.82422100
H	0.64900100	1.84021100	0.73059000
C	5.67341900	3.11763500	0.13810500
H	6.86124300	-0.10107300	-0.69371100
H	7.48893400	0.13066800	-2.34918600
H	7.73696900	1.41403600	-1.13809100
H	4.41318100	-0.24380100	2.89374000
H	3.40781400	1.07025600	3.59470100
H	2.72865200	-0.00783800	2.32855900
H	5.87865500	3.88862700	-0.61399500
H	5.20003600	3.58729000	1.00844700
H	6.62790800	2.68578600	0.46364300
Cl	-2.33084500	-1.95510200	-2.01646200
Cl	0.07979800	-0.94416700	2.06710000
C	2.06851700	-1.96911700	-0.59169400
C	2.60098200	-2.60237100	0.52417000
C	1.95081100	-3.71228100	1.08817200
C	0.76873400	-4.19761900	0.53897000
C	0.22501100	-3.57832000	-0.60050800
C	0.87303400	-2.45056400	-1.16610200
H	2.58904500	-1.11563400	-1.02846900
H	3.52768900	-2.22138400	0.94941900
H	2.37667900	-4.19623900	1.96558300
H	0.27125500	-5.06275800	0.97239000
H	-0.63277000	-4.01598100	-1.10945900
H	0.52588200	-2.05913500	-2.12308500
Pt	-1.07386400	-1.49830500	0.00719800
C	-3.28546000	2.41619000	0.01562600
C	-2.24564300	1.34444600	-0.23217000
C	-2.30773300	0.13525000	0.28651500
C	-4.40381800	2.25755700	-1.02324500
S	-4.13952400	2.20998600	1.70429200
C	-2.88957800	-0.89759400	1.00729100
O	-4.71623100	3.11370500	-1.82012000
O	-4.96459800	1.05043400	-0.95374600
C	-5.97398500	0.78362600	-1.92931500
C	-2.67509900	2.47734600	2.82005100
H	-1.43250500	1.61183800	-0.91094700
H	-2.72607500	-0.98372100	2.08270400
H	-3.72381800	-1.44538000	0.56499200
C	-2.64538400	3.78903300	-0.10987800
H	-1.84223500	1.83627800	2.50470000
H	-2.37419600	3.52811500	2.83473200
H	-3.00177000	2.17572900	3.81863000
H	-5.55291200	0.85286500	-2.93784600
H	-6.31983200	-0.23278100	-1.73272000
H	-6.79920000	1.49708300	-1.83239500
H	-1.81225700	3.88935100	0.59730300
H	-2.24520300	3.92230100	-1.12316300
H	-3.37612000	4.58205400	0.07842800

2.3 PT-CATALYST S-Cycle

ENERGY=-1325.78125

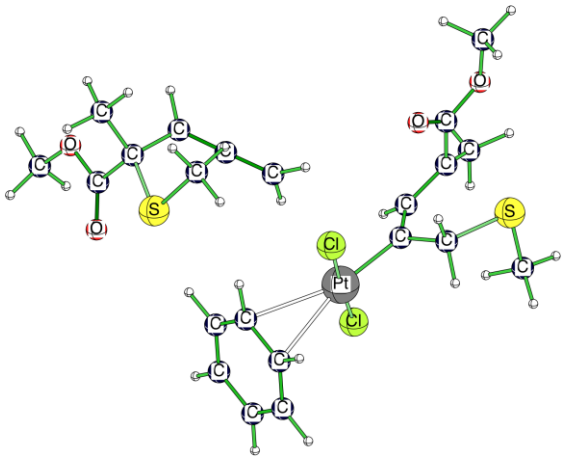


C	-4.79189100	-2.02376000	-0.27612000
C	-3.54068900	-2.77575600	-0.66518000
C	-2.33914000	-2.24143500	-0.62129700
C	-4.50373400	-0.92326100	0.75145000
S	-5.39332000	-1.27685800	-1.90903000

C	-1.17318000	-1.65631800	-0.49177300
O	-4.83758300	0.23858400	0.66020100
O	-3.87296000	-1.42973700	1.81287600
C	-3.46516400	-0.47468300	2.79850900
C	-7.06698000	-0.59925000	-1.45486500
H	-3.69060800	-3.78994700	-1.04422400
H	-0.73444300	-1.06094800	-1.29732200
H	-0.62067000	-1.71130500	0.44915300
C	-5.82366100	-2.98449400	0.31493800
H	-6.96457800	0.09924900	-0.62126800
H	-7.41957800	-0.06415900	-2.34091300
H	-7.76934000	-1.40357600	-1.21771700
H	-4.32124300	0.11800300	3.13938900
H	-3.04785000	-1.05546000	3.62362600
H	-2.69524100	0.18932500	2.38196600
H	-6.08566200	-3.75013600	-0.42561500
H	-5.40537900	-3.47697500	1.20155600
H	-6.73986800	-2.46077000	0.61454300
Cl	1.89610200	1.40713100	-2.34694300
Cl	0.06708300	0.81528600	2.14183600
C	-2.38286400	1.88404300	-0.46002400
C	-2.74530300	2.60389400	0.66934600
C	-1.94808300	3.67440100	1.11568500
C	-0.79258100	4.02126000	0.43057100
C	-0.41497300	3.30220700	-0.72324900
C	-1.21379400	2.22983400	-1.17136500
H	-3.01929400	1.07042200	-0.80928700
H	-3.65449400	2.32932000	1.20277600
H	-2.24020000	4.23255800	2.00417600
H	-0.18061200	4.85656800	0.76707500
H	0.41935500	3.64488800	-1.33343700
H	-0.99888100	1.75859000	-2.13029100
Pt	0.84529100	1.17278300	-0.15224000
C	3.73277000	-2.06385300	0.29247400
C	2.42424700	-1.37901500	-0.01953000
C	2.28941600	-0.08150000	0.28743400
C	4.57259900	-2.01751100	-0.98729500
S	4.55450300	-0.86637900	1.56626400
C	3.41071600	0.57621800	1.01177100
O	4.61606500	-2.93895000	-1.76759300
O	5.13868900	-0.82630800	-1.16332900
C	5.74505300	-0.60933600	-2.44634800
C	3.63664800	-1.31261900	3.11914900
H	1.69306400	-1.95887600	-0.58390600
H	3.10838600	1.09602700	1.92808600
H	4.01830400	1.22267900	0.36892400
C	3.60822900	-3.47093500	0.83452900
H	2.56658000	-1.34837400	2.89118800
H	4.01762800	-2.26883000	3.48103700
H	3.85468300	-0.51840500	3.83634300
H	4.99490700	-0.73259300	-3.23324200
H	6.11573000	0.41633800	-2.43183900
H	6.56507100	-1.31714900	-2.60219800
H	2.90960700	-3.51031000	1.67681500
H	3.20298200	-4.09637800	0.03122200
H	4.57636000	-3.89365400	1.12911700

2.4 PT-CATALYST TS2

ENERGY=-1325.76007 LOWEST FREQUENCY=-241.16

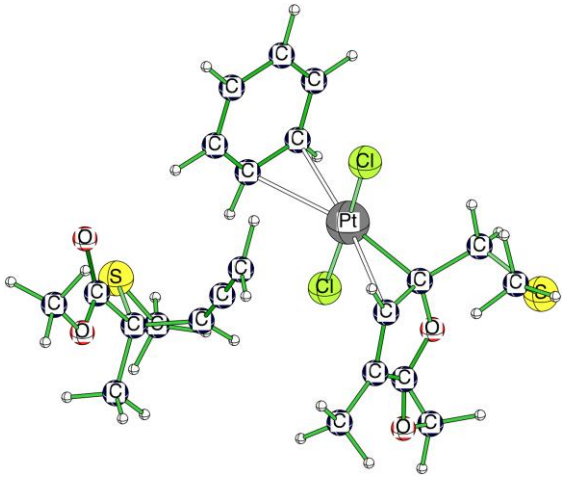


C	-4.41136700	1.93175000	0.31621100
C	-3.25421400	2.56018900	-0.44489200
C	-2.08318700	2.00106200	-0.65877300
C	-5.27629300	1.25528400	-0.74830700
S	-3.87183200	0.54031000	1.47390200
C	-0.90083000	1.46111700	-0.82840400
O	-5.31267000	0.06911600	-0.98590000
O	-5.96184600	2.17232000	-1.44532500
C	-6.72814800	1.65387200	-2.53420700
C	-2.80800000	1.50545100	2.65591600
H	-3.46663100	3.54575100	-0.87170600
H	-0.09353500	1.62675100	-0.10985600
H	-0.69914900	0.79902600	-1.67313900
C	-5.18129800	3.01050600	1.07098500
H	-3.41621000	2.10106100	3.34271300
H	-2.22858100	0.76204500	3.21205000
H	-2.10835400	2.13879800	2.10063500
H	-7.46848000	0.93256000	-2.17257500
H	-7.22343000	2.51277000	-2.99165300
H	-6.07369100	1.15880200	-3.25961800
H	-4.52554700	3.49574000	1.80379800
H	-5.54130600	3.77968200	0.37685800
H	-6.04139300	2.58278800	1.59874200
Cl	0.55227200	-0.33182300	2.53471400
Cl	1.11508500	-2.23919500	-1.92769500
C	-2.33632500	-2.31022900	-0.45182000
C	-2.25240800	-3.48275900	-1.18896500
C	-1.41367500	-4.52973300	-0.76269500
C	-0.66301500	-4.40105600	0.39791500
C	-0.74275200	-3.21669300	1.15929100
C	-1.58384200	-2.17133200	0.73238200
H	-3.00134900	-1.49923000	-0.75007600
H	-2.83809800	-3.59541100	-2.09996600
H	-1.35335700	-5.44526100	-1.34928500
H	-0.02129700	-5.21503500	0.73083300
H	-0.24754400	-3.15206900	2.12758800
H	-1.75113500	-1.30058200	1.36822000
Pt	0.78630100	-1.30763200	0.29164000
C	3.42300400	1.69366100	-1.21341000
C	2.42192300	0.68909000	-1.12785700
C	2.28266300	-0.12908800	-0.03409700
C	3.42010900	2.77395900	-0.14578800
S	5.01154100	0.49084600	0.18358700

C	3.43440400	-0.22562700	0.93675900
O	2.72595200	2.74273700	0.84554400
O	4.26661000	3.75682400	-0.45214800
C	4.33814300	4.81825800	0.50715000
C	5.33423500	-0.89012900	-1.01194500
H	1.85584800	0.46045200	-2.03412400
H	3.64744000	-1.26982600	1.18914000
H	3.22447100	0.33081300	1.85838100
C	3.99400600	2.04509200	-2.54706500
H	4.41500600	-1.07004100	-1.58670100
H	6.15902800	-0.58881500	-1.66046100
H	5.59866400	-1.78446700	-0.44213000
H	4.69946400	4.43577400	1.46761600
H	5.03998000	5.54626400	0.09709500
H	3.35127100	5.27015200	0.64896500
H	4.01677200	1.17175700	-3.20717900
H	3.36059800	2.81346000	-3.01364100
H	4.99551500	2.47652100	-2.45527500

2.5 PT-CATALYST Cycle-O F-MLn

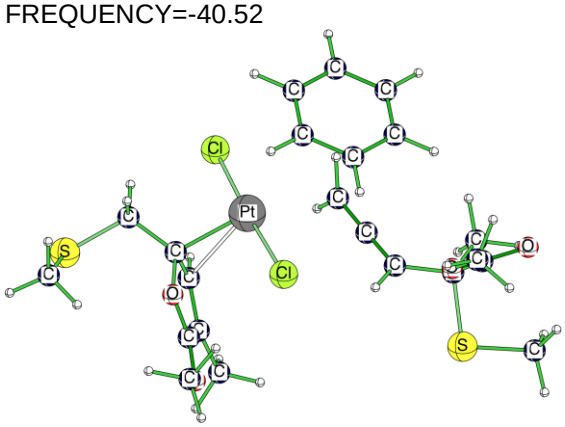
ENERGY=-1325.81441



C	-3.68895900	-1.33291900	-0.04764600
C	-2.22179500	-1.23259700	0.30483900
C	-1.76918600	-0.68620300	1.41289300
C	-4.48070300	-0.63736600	1.05665200
S	-4.06817800	-0.31359700	-1.61611600
C	-1.36803700	-0.12131100	2.52873100
O	-4.74103700	0.54524200	1.08324500
O	-4.79948200	-1.48844800	2.03660100
C	-5.40834000	-0.88503500	3.18038400
C	-3.18376200	-1.32454400	-2.90290000
H	-1.51591600	-1.65382100	-0.42048900
H	-1.08780400	0.93483400	2.54465500
H	-1.26130000	-0.69684500	3.44934500
C	-4.08117700	-2.79277000	-0.24146500
H	-3.68713500	-2.27962900	-3.07712100
H	-3.22232400	-0.72373700	-3.81583000
H	-2.13100700	-1.46985000	-2.63301200
H	-6.34515700	-0.39144300	2.90230400
H	-5.59727700	-1.69678700	3.88555800
H	-4.73084100	-0.14376600	3.61980900
H	-3.45450000	-3.25637800	-1.01301000
H	-3.92722700	-3.34677900	0.69186600
H	-5.13252500	-2.88507000	-0.54009500
Cl	0.44493600	-0.52496800	-2.41212700
Cl	1.31838800	2.19703200	1.56806500
C	-1.93184600	2.56225400	-0.02479700
C	-1.56648900	3.81244100	0.44397500
C	-0.48831600	4.51092500	-0.14231700
C	0.21372600	3.95946700	-1.19835800
C	-0.14385300	2.68035200	-1.69273700
C	-1.22267800	1.98308700	-1.10137600
H	-2.78476000	2.02710100	0.39607100
H	-2.11730200	4.26732600	1.26590900
H	-0.21353300	5.49386300	0.23679300
H	1.03231500	4.50477600	-1.66454800
H	0.27946100	2.32231600	-2.63117000
H	-1.61308100	1.07714200	-1.56701100
Pt	0.94393500	0.89472100	-0.46563000
C	1.53515100	-2.35933000	0.88463000
C	1.77314600	-1.05019300	1.23301900
C	2.50238900	-0.36914500	0.17052600
C	2.16524100	-2.49330000	-0.37704100
S	5.12080400	-0.64944000	1.22126100
C	3.79072600	0.38254000	0.38718500
O	2.77278100	-1.41667700	-0.78700000
O	2.14617600	-3.55902100	-1.11460200
C	2.73025300	-3.45849300	-2.43079300
C	4.57849500	-0.42962200	2.98964500
H	1.45905300	-0.54277000	2.14091200
H	3.62264800	1.27761800	0.99159900
H	4.20363700	0.67926700	-0.58271900
C	0.76563900	-3.43489000	1.57139900
H	3.72451500	-1.07266500	3.22436400
H	5.42711700	-0.70596200	3.62051200
H	4.32039700	0.62028400	3.16439200
H	3.80454400	-3.26873600	-2.34692600
H	2.54626600	-4.42237500	-2.90552800
H	2.23931900	-2.64475000	-2.97758500
H	0.36920000	-3.07311600	2.52484200
H	-0.07742600	-3.77685800	0.95750100
H	1.39996600	-4.30679000	1.77189100

2.6 PT-REGENERATION TSx'

ENERGY=-1325.79899 LOWEST
FREQUENCY=-40.52

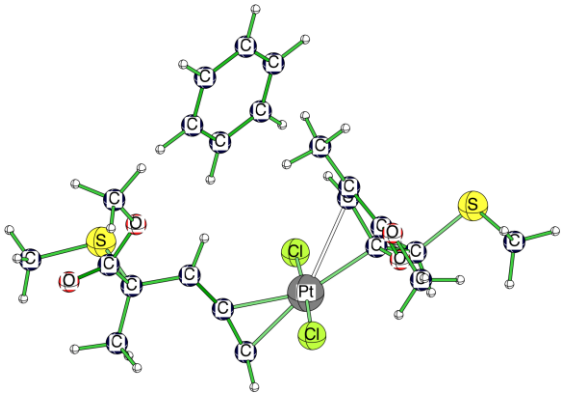


C	4.14953000	-0.77362100	-0.68474700
C	2.66732600	-0.59997400	-0.51787300
C	1.94831500	0.23804500	-1.22759600

C	4.88936100	-0.48360600	0.61787700
S	4.38799100	-2.65603600	-0.97392900
C	1.22023300	1.11142700	-1.89220900
O	6.05209600	-0.13475900	0.67168000
O	4.12380500	-0.67453900	1.69584400
C	4.76210200	-0.45422500	2.95214300
C	6.21873800	-2.75559900	-1.30910800
H	2.17048200	-1.15677100	0.28181000
H	1.17041800	2.15242700	-1.55995300
H	0.69143800	0.84708000	-2.80748800
C	4.73464400	0.03747600	-1.82388700
H	6.45448200	-2.35091500	-2.29679400
H	6.77792800	-2.22530300	-0.53224700
H	6.46935700	-3.81934300	-1.27980900
H	5.16180000	0.56487800	3.00745800
H	3.98996600	-0.60130200	3.71022900
H	5.58041700	-1.16763400	3.09879800
H	4.54066900	1.10669100	-1.65589500
H	4.26763500	-0.25589300	-2.77105900
H	5.81829300	-0.09772700	-1.89298900
Cl	-0.15880500	-0.82523300	1.53868700
Cl	-1.89813900	2.34081700	-1.75658000
H	-2.25278000	-4.46895000	2.59047800
C	-2.55039000	-3.48126000	2.23853700
O	-2.40876100	-3.52584600	0.80350900
H	-3.59282200	-3.27788200	2.50429800
H	-1.88978900	-2.70331000	2.63799300
C	-2.56867500	-2.42306300	0.14713700
C	-2.31994100	-2.25350100	-1.23534700
O	-2.97916300	-1.33989900	0.75936100
C	-2.57222700	-0.91916800	-1.45581900
C	-1.79843700	-3.31435000	-2.14084400
C	-2.90546800	-0.25807500	-0.19326600
H	-2.54779900	-0.38824600	-2.40308100
H	-0.76186800	-3.56658000	-1.88276200
H	-2.39358000	-4.23132900	-2.06274700
H	-1.81748500	-2.97659500	-3.18083600
C	-4.10523900	0.62932500	-0.01864000
S	-5.71753200	-0.27510000	-0.35237700
H	-4.05504100	1.45754400	-0.72997300
H	-4.14024800	1.03698200	0.99856500
C	-6.13041600	-0.84804200	1.36996400
H	-7.12786100	-1.29194200	1.31976300
H	-5.41038500	-1.59389800	1.71836900
H	-6.14780800	0.00836000	2.05070600
Pt	-1.08731000	0.73054000	-0.10726600
C	0.09886700	3.84122100	0.72537800
C	0.32141600	2.71233400	1.52711100
C	1.60571600	2.15392600	1.60788100
C	2.66125200	2.72535700	0.89456800
C	2.43660100	3.85066300	0.09525800
C	1.15451900	4.40612100	0.00670200
H	-0.90002800	4.26794300	0.65529400
H	-0.48667800	2.30140600	2.13422800
H	1.77236800	1.26871500	2.21950200
H	3.66147200	2.29621600	0.96559100
H	3.26060400	4.29311300	-0.46365700
H	0.97692400	5.27528900	-0.62443700

2.7 PT-REGENERATION Complexe F-MLn-A

ENERGY=-1325.83222

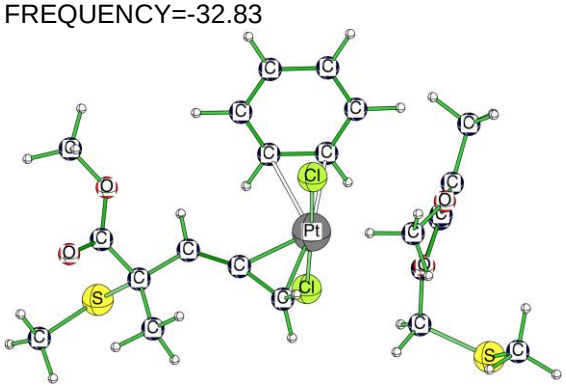


Cl	0.92588500	-2.31967000	1.58147600
Cl	0.50057400	-0.21216300	-2.79080900
C	-1.41902500	2.58909600	-1.25203700
C	-0.38386800	3.37623300	-1.76728400
C	-0.05647700	4.59103000	-1.15672900
C	-0.76704600	5.02112900	-0.03053300
C	-1.80300000	4.23486100	0.48333700
C	-2.12967700	3.01944400	-0.12719200
H	-1.66708900	1.64342000	-1.73848700
H	0.16324000	3.03625300	-2.64687900
H	0.74839400	5.20407900	-1.56034300
H	-0.51617700	5.97001700	0.44235100
H	-2.94689800	2.41010400	0.26147400
H	-2.36034000	4.57167100	1.35724600
C	-3.67394100	-1.05886300	0.09678600
C	-2.19758500	-0.79547800	-0.00727300
C	-1.34869000	-1.64817800	-0.54609700
C	-4.25676400	-0.52525900	1.40018000
S	-4.45205600	0.06274300	-1.25981900
C	-0.76591600	-2.73733400	-1.13812000
O	-5.26998300	-0.95601100	1.91041900
O	-3.56083400	0.50603200	1.89079300
C	-4.11614200	1.12813600	3.04892300
C	-6.25640900	-0.39314600	-1.14013200
H	-1.82205800	0.15676600	0.37488300
H	-0.54643200	-3.62727200	-0.54680500
H	-0.76328700	-2.82395700	-2.22539500
C	-4.04932800	-2.51144000	-0.11906400
H	-6.43375400	-1.38185400	-1.57091200
H	-6.59041800	-0.35947000	-0.09860500
H	-6.78935300	0.36336500	-1.72214700
H	-4.20120700	0.40740200	3.86866500
H	-3.42661100	1.93248500	3.31635500
H	-5.10805200	1.53621000	2.82559000
H	-3.75102700	-2.83226400	-1.12372600
H	-3.53498700	-3.14074300	0.61958500
H	-5.12564900	-2.66380200	0.00124900
Pt	0.76528400	-1.23937900	-0.59960600
H	3.79063900	-0.86199500	4.60338800
C	3.70210600	-0.90552700	3.51776800
O	2.97528600	0.27972300	3.14187000
H	4.69345500	-0.90461000	3.05207400
H	3.13472500	-1.78936800	3.20252700
C	2.69628500	0.43635900	1.88351700

C	1.86968200	1.44829800	1.34420000
O	3.17099400	-0.39331500	0.99027400
C	1.84479400	1.16832900	-0.00440000
C	1.13338300	2.48014100	2.12499000
C	2.56363500	-0.05917600	-0.26916000
H	1.33064800	1.73483700	-0.77788100
H	0.27645000	2.02896600	2.64428100
H	1.77523000	2.94857300	2.87977100
H	0.74449400	3.25801600	1.45686800
C	3.56616400	-0.20210000	-1.37470200
S	5.02361500	0.97511100	-1.22960000
H	3.08754200	0.03744300	-2.32955300
H	3.95730800	-1.22555600	-1.42574900
C	6.07839000	0.06424400	0.00761400
H	7.11750100	0.33635900	-0.19398200
H	5.81529100	0.33997600	1.03270700
H	5.95440600	-1.01422300	-0.13433400

2.8 PT-REGENERATION TSx''

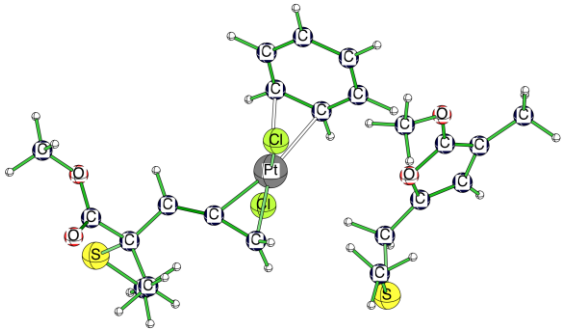
ENERGY=-1325.80524 LOWEST
FREQUENCY=-32.83



Cl	0.34792400	1.38824900	1.50300600
Cl	0.20894100	-1.32683800	-2.51031100
C	-0.71754100	1.94297600	-2.10300000
C	0.69304700	1.96794900	-2.18128900
C	1.40066800	3.03597300	-1.59026400
C	0.71770000	4.04337600	-0.92455800
C	-0.68499900	4.00475900	-0.83869900
C	-1.39994900	2.96401800	-1.42120800
H	-1.26813700	1.17316200	-2.64308000
H	1.20672600	1.26249400	-2.83488200
H	2.48598300	3.07326500	-1.67774700
H	1.26644700	4.86518000	-0.46713700
H	-2.48789200	2.94635000	-1.36671300
H	-1.21432000	4.79831600	-0.31383500
C	-3.87552700	-1.08935300	0.53894600
C	-2.67626400	-0.38714700	-0.02958400
C	-1.43210800	-0.78313700	0.16006500
C	-4.79025500	-0.12670700	1.28982700
S	-4.87945000	-1.59357900	-1.01950900
C	-0.37613200	-1.57378800	0.64533900
O	-5.57602400	-0.48050800	2.14472100
O	-4.66166200	1.13580500	0.87451300
C	-5.54753000	2.07325100	1.48787700
C	-6.30322700	-2.52921000	-0.26208900
H	-2.86180700	0.49933800	-0.63749000
H	-0.04692900	-1.46444200	1.68146000
H	-0.15266100	-2.51711300	0.14254200
C	-3.53906700	-2.29505100	1.39237600
H	-5.97111600	-3.50083300	0.11271000
H	-6.76028600	-1.94150800	0.53982900
H	-7.02401700	-2.67367800	-1.07119000
H	-5.42129200	2.06554100	2.57530600
H	-5.28044200	3.05018500	1.08017600
H	-6.58788500	1.83040200	1.24544900
H	-3.01237900	-3.04814600	0.79492000
H	-2.89939400	-1.99328900	2.23306700
H	-4.44502800	-2.74012000	1.81346100
Pt	0.32300000	0.05528700	-0.51335200
H	2.91860500	0.49528200	4.82738100
C	2.79875000	0.02123700	3.85088400
O	3.56856700	0.79977000	2.93763200
H	3.16557100	-1.01182200	3.89446000
H	1.73970300	0.03016400	3.55571900
C	3.47788300	0.47065100	1.65476500
C	3.75117000	1.23662400	0.54861500
O	3.06962800	-0.77154800	1.33185500
C	3.45082800	0.38010000	-0.55310800
C	4.15557000	2.67259700	0.56218300
C	3.02422000	-0.83297200	-0.04819900
H	3.59700100	0.58585500	-1.61021000
H	3.27527600	3.33192000	0.58818400
H	4.75945200	2.90124100	1.44761800
H	4.74626900	2.93098900	-0.32505400
C	2.96068500	-2.19316400	-0.61745900
S	4.65700800	-2.98043600	-0.90833300
H	2.49285800	-2.18895200	-1.60725400
H	2.39153500	-2.86175100	0.04121900
C	5.34670900	-2.84463000	0.81453900
H	6.28500800	-3.40519500	0.82269100
H	5.54053300	-1.79797000	1.06967900
H	4.64908900	-3.28529700	1.53427600

2.9 PT-REGENERATION Furane

ENERGY=-1325.81022



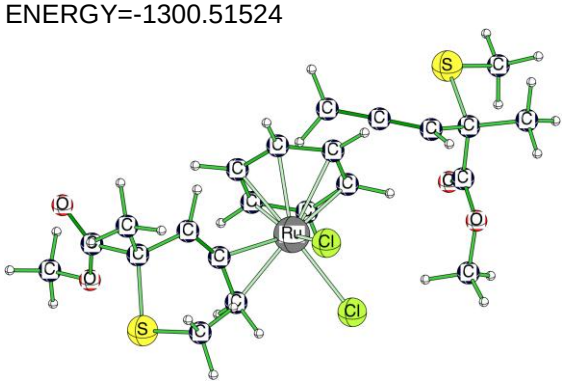
Cl	-0.24359100	-1.31981400	1.59481900
Cl	0.66229200	0.86732500	-2.63672300
C	-0.41496800	-2.30954200	-1.90713500
C	-1.53482000	-1.44014800	-1.89541900
C	-2.65993300	-1.75612400	-1.10427600
C	-2.66351300	-2.91313300	-0.33846500
C	-1.54698600	-3.76795600	-0.34260200
C	-0.43013100	-3.47197600	-1.11475600
H	0.40081700	-2.12578000	-2.60595400

H	-1.58953200	-0.61978200	-2.61102400
H	-3.53192100	-1.10140600	-1.12668100
H	-3.53855000	-3.16325900	0.26106700
H	0.42855100	-4.13980600	-1.12053100
H	-1.55874000	-4.67101800	0.26481900
C	4.39957500	0.63397800	0.61343700
C	3.15378000	-0.05320300	0.12763800
C	1.95910800	0.49849600	0.21336000
C	5.27179800	-0.33109200	1.41759200
S	5.46750600	1.00910600	-0.93944500
C	0.95927800	1.41572400	0.51125500
O	5.82014100	-0.04396800	2.45716200
O	5.36028400	-1.52451500	0.82539500
C	6.17467600	-2.48385900	1.50478100
C	4.39834200	2.29171500	-1.75917400
H	3.27356300	-1.02268000	-0.35662100
H	0.53781000	1.43196700	1.51874100
H	0.81565900	2.30219400	-0.11260300
C	4.14146700	1.89109300	1.41992800
H	3.37248200	1.91815300	-1.86737900
H	4.42158200	3.23521400	-1.20753300
H	4.82921200	2.43905000	-2.75292400
H	5.76157300	-2.69794300	2.49610200
H	6.16371200	-3.38165100	0.88424700
H	7.19650500	-2.10671800	1.61580500
H	3.53259600	2.60462400	0.85322000
H	3.60391600	1.63876500	2.34323600
H	5.08758700	2.36677700	1.69416300
Pt	0.17186700	-0.27507200	-0.54656600
H	-4.16946700	-1.91489900	3.52710600
C	-3.89324500	-1.10922300	2.84336200
O	-4.93308400	-1.04967500	1.86828200
H	-3.82238100	-0.16225600	3.39613000
H	-2.92147200	-1.32474100	2.37681800
C	-4.79765600	-0.12877200	0.91212200
C	-5.68044800	0.25124500	-0.06401100
O	-3.62803200	0.53525600	0.82388700
C	-4.96692600	1.24600000	-0.81806100
C	-7.06334600	-0.27411400	-0.26398600
C	-3.73088900	1.38917300	-0.25302300
H	-5.33124900	1.79189100	-1.68208000
H	-7.18896200	-0.72454300	-1.25699900
H	-7.28966700	-1.04309200	0.48314800
H	-7.81623300	0.51841000	-0.16696900
C	-2.53645100	2.19470700	-0.54557500
S	-2.26616500	3.71184300	0.55401300
H	-2.57904600	2.59700700	-1.56212200
H	-1.62778700	1.57928200	-0.45348000
C	-2.26823100	2.87469500	2.21788100
H	-1.86991500	3.59665000	2.93523600
H	-3.28383000	2.58587300	2.50204900
H	-1.62917600	1.98360400	2.19539600

3 Ru CATALYST

3.1 RU-CATALYST Allene MLn-A

ENERGY=-1300.51524

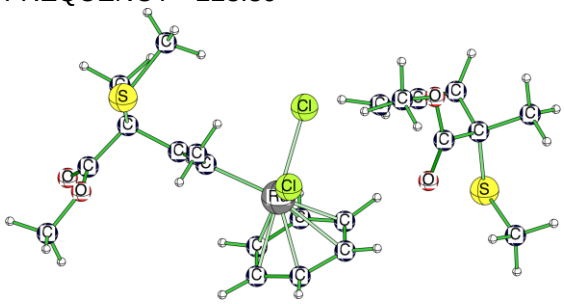


C	4.71954300	1.26117300	-0.24960800
C	3.81874800	2.47859600	-0.33105100
C	2.72175400	2.57141800	-1.05055700
C	4.10269700	0.27125500	0.75128500
S	4.78270900	0.51538700	-1.98333400
C	1.61484100	2.70636800	-1.74378400
O	3.75080800	-0.86378900	0.50489700
O	4.02105700	0.83388900	1.95286600
C	3.35411800	0.05845100	2.96257300
C	5.96924500	-0.89737900	-1.74385600
H	4.09681200	3.31628700	0.31399600
H	1.61605500	3.11684400	-2.75327800
H	0.66737800	2.40987300	-1.28522800
C	6.11144600	1.67432900	0.22315900
H	5.60663200	-1.55705800	-0.95181900
H	5.98712200	-1.43780400	-2.69409300
H	6.97516100	-0.52923400	-1.52242300
H	3.84160900	-0.91546700	3.07846900
H	3.43765300	0.64103700	3.88225900
H	2.30027800	-0.08619600	2.69014200
H	6.56652700	2.34709600	-0.51297100
H	6.04061800	2.19819200	1.18428100
H	6.76871100	0.80778800	0.36401300
Cl	0.31845800	-2.04064800	2.44177700
Cl	0.35264800	1.03305100	1.09256800
C	0.13988400	-0.73907100	-1.92732100
C	1.37195800	-1.18978600	-1.35985400
C	1.39666500	-2.39050000	-0.64389800
C	0.20520000	-3.18391000	-0.51640200
C	-0.97607300	-2.81861000	-1.19623000
C	-1.00732000	-1.57747500	-1.89183000
H	0.09078900	0.23830900	-2.40360900
H	2.26265600	-0.55874500	-1.38445900
H	2.28643000	-2.65241700	-0.07868400
H	0.21144600	-4.05792800	0.12881500
H	-1.87660100	-3.42001500	-1.10269900
H	-1.94307700	-1.22597800	-2.32068200
Ru	-0.35768300	-1.15711100	0.20722900
C	-4.10197000	1.46424300	-0.33343000
C	-2.72440300	0.84665300	-0.51978800
C	-2.24436500	-0.13651300	0.22370500
C	-5.05626800	0.60436800	-1.16292800
S	-4.69370500	1.42243700	1.46918500

C	-2.27040000	-1.00053600	1.29386600
O	-5.37712000	0.86593200	-2.30278700
O	-5.43266400	-0.50437700	-0.52155800
C	-6.26878300	-1.38772900	-1.26983900
C	-3.39016600	2.50602000	2.23716200
H	-2.13019100	1.27878900	-1.33143100
H	-2.03553600	-0.62173200	2.28997700
H	-2.79908000	-1.95356400	1.24474100
C	-4.09325800	2.88812900	-0.87172500
H	-2.39409600	2.18438900	1.90892900
H	-3.55697800	3.55974300	1.99808100
H	-3.47783000	2.35814000	3.31681800
H	-5.75027100	-1.74082200	-2.16864000
H	-6.49311900	-2.22428500	-0.60547200
H	-7.19181900	-0.88059000	-1.56874900
H	-3.34119700	3.48878000	-0.34697500
H	-3.84101100	2.88434000	-1.93941800
H	-5.07511700	3.35886500	-0.75063800

3.2 RU-CATALYST TS1

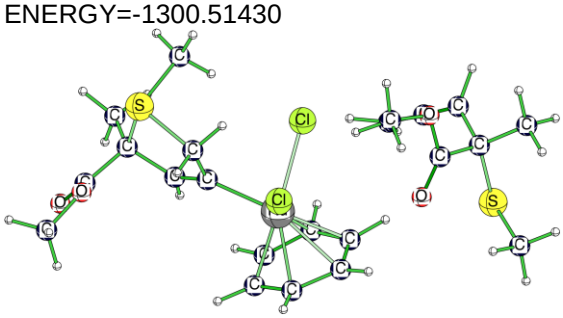
ENERGY=-1300.50134 LOWEST
FREQUENCY=-223.89



C	4.98630800	0.86183900	-0.41016800
C	4.38208200	1.92534700	-1.30651200
C	3.37846500	1.73421200	-2.13496800
C	4.06694900	0.62866400	0.79929700
S	5.14158700	-0.70100400	-1.46256100
C	2.36485300	1.57487500	-2.95321400
O	3.65252200	-0.44470500	1.18283300
O	3.82497200	1.78301100	1.41260500
C	2.95974800	1.70847000	2.55672000
C	5.96117000	-1.89106800	-0.28931500
H	4.79423000	2.93195700	-1.19880000
H	2.51130400	1.31613200	-4.00165200
H	1.35064000	1.70876600	-2.56983100
C	6.35326800	1.32012100	0.09559600
H	5.35773100	-1.98738500	0.61635800
H	5.99933800	-2.84794300	-0.81715200
H	6.98058900	-1.57141400	-0.05387500
H	3.35669800	0.99623900	3.28823100
H	2.93742100	2.71783700	2.97311700
H	1.95616800	1.39424200	2.24521200
H	7.03620100	1.45390300	-0.75150300
H	6.25246000	2.27610100	0.62499600
H	6.79360000	0.59540400	0.79133000
Cl	-0.05884300	-0.60952500	2.81337300
Cl	0.35933600	1.50339200	0.04359600
C	0.24449800	-1.44177900	-1.74375400
C	1.42377500	-1.51790300	-0.93162200
C	1.43629100	-2.30169800	0.23451200
C	0.24092900	-2.97852200	0.63741000
C	-0.91532600	-2.96893700	-0.18228500
C	-0.90680400	-2.18523800	-1.37711300
H	0.21932400	-0.77406500	-2.60228300
H	2.28328500	-0.88737100	-1.16004800
H	2.28939600	-2.23361600	0.90395800
H	0.19980100	-3.45299300	1.61440700
H	-1.82674000	-3.46101000	0.14588200
H	-1.82223300	-2.08391500	-1.95583200
Ru	-0.33682500	-0.88222200	0.29211400
C	-4.33386000	1.02569200	-0.82201300
C	-2.98559900	0.33128800	-0.98752000
C	-2.25925000	-0.00129400	0.07677700
C	-5.38808400	-0.07453800	-0.94215400
S	-4.46153500	1.75972400	0.92389400
C	-2.50387300	0.26324500	1.42542900
O	-5.93039300	-0.36663900	-1.98507100
O	-5.57078700	-0.72801800	0.20816500
C	-6.46835300	-1.83971300	0.14841100
C	-3.31580000	3.21549400	0.74757500
H	-2.68489900	0.13472200	-2.01984800
H	-1.95900700	1.06318200	1.92669700
H	-2.96650400	-0.48199900	2.07303100
C	-4.54090000	2.08050400	-1.89669500
H	-2.38948700	2.89822700	0.25306000
H	-3.80836700	4.01789500	0.19419100
H	-3.09543300	3.54678100	1.76563800
H	-6.09885900	-2.58794700	-0.56102900
H	-6.50219600	-2.25297500	1.15799900
H	-7.46512600	-1.51166300	-0.16357700
H	-3.72510200	2.81140100	-1.88014800
H	-4.53693500	1.59209100	-2.87798900
H	-5.49966000	2.59839600	-1.77798400

3.3 RU-CATALYST S-Cycle

ENERGY=-1300.51430

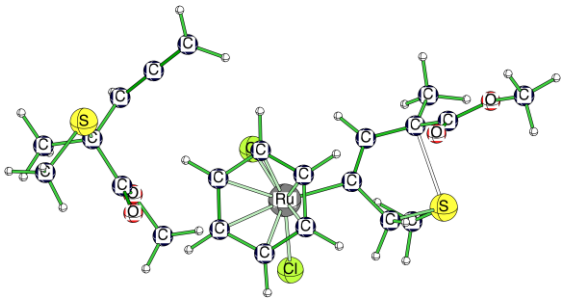


C	5.04423700	0.87872000	-0.12493700
C	4.47906100	1.92006300	-1.07277400
C	3.55345000	1.69316300	-1.97980900
C	3.99165700	0.57204900	0.95218700
S	5.41377900	-0.65162600	-1.16817600
C	2.61101900	1.50177300	-2.87259400
O	3.49732900	-0.51074200	1.18109100
O	3.70631200	1.68063400	1.63243700
C	2.66480500	1.54528600	2.61238800
C	6.12765500	-1.81554200	0.09695000
H	4.84683100	2.94028100	-0.93575400
H	2.84440300	1.24539400	-3.90583500

H	1.56723500	1.59810000	-2.55838300
C	6.31426500	1.41016900	0.53565400
H	5.40949900	-1.96496200	0.90729300
H	6.29596000	-2.76005000	-0.42763700
H	7.08336500	-1.44376500	0.47858300
H	2.94969500	0.80816100	3.37100700
H	2.55255700	2.53515300	3.06044300
H	1.73380500	1.22703700	2.12818600
H	7.07607900	1.60219800	-0.22924900
H	6.09913300	2.34686700	1.06490400
H	6.72112200	0.69925200	1.26521800
Cl	-0.32936600	-0.62371000	2.57644500
Cl	0.30349100	1.53612300	-0.20115100
C	0.52823600	-1.41543400	-1.87763700
C	1.57619700	-1.65316200	-0.92403400
C	1.32640000	-2.45082800	0.19494800
C	0.01872400	-3.01672900	0.38454100
C	-0.98663900	-2.88212500	-0.60770900
C	-0.72420300	-2.06860800	-1.75499900
H	0.69224700	-0.70868300	-2.68844200
H	2.52133300	-1.11571900	-1.00249900
H	2.06736700	-2.50787900	0.98714100
H	-0.21426400	-3.52233400	1.31836100
H	-1.97609100	-3.30356200	-0.44670700
H	-1.50546900	-1.88716700	-2.48907300
Ru	-0.35889300	-0.89763700	0.05393900
C	-4.39770600	0.83120200	-0.85766800
C	-3.12073500	0.02699900	-0.98454500
C	-2.25125800	-0.04209100	0.04169100
C	-5.52709000	-0.14081700	-0.52158600
S	-4.06588600	1.91724800	0.68610300
C	-2.63983600	0.73854600	1.25195000
O	-6.19036900	-0.68501700	-1.37473900
O	-5.62011100	-0.38174600	0.78672500
C	-6.55679500	-1.39814500	1.16558400
C	-2.99370800	3.25949500	-0.02407400
H	-2.98750900	-0.45689100	-1.95304900
H	-1.85317900	1.40096400	1.62533400
H	-3.05855800	0.14156600	2.06649600
C	-4.73039400	1.66021300	-2.08188400
H	-2.14855500	2.79421300	-0.54635700
H	-3.60921900	3.88348500	-0.67438200
H	-2.64046700	3.83574500	0.83417100
H	-6.27886300	-2.35314400	0.70857600
H	-6.50294700	-1.46430400	2.25312200
H	-7.56645400	-1.12215900	0.84566800
H	-3.86144400	2.24312600	-2.40528300
H	-4.99537600	0.96842700	-2.88923700
H	-5.58667300	2.32549700	-1.91671900

3.4 RU-CATALYST TS2

ENERGY=-1300.49902 LOWEST
FREQUENCY=-278.43

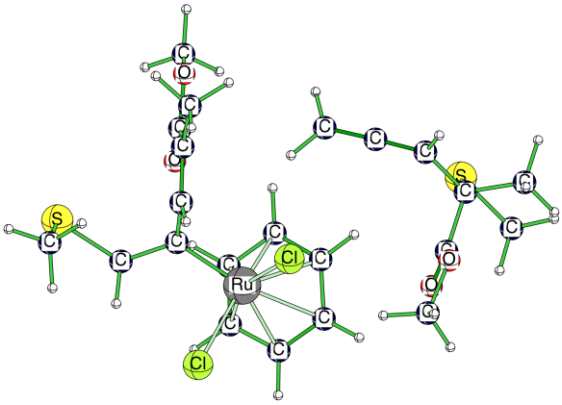


C	-4.95166100	0.91157300	-0.68461800
C	-4.18845500	2.04390000	-1.34315600
C	-3.26509600	2.77636500	-0.76063400
C	-4.13417500	-0.38361700	-0.81535300
S	-5.18306100	1.37844000	1.13097900
C	-2.32660000	3.50290200	-0.20056000
O	-3.82912200	-1.12632500	0.09462200
O	-3.83663700	-0.60902900	-2.09116900
C	-3.00975400	-1.75571000	-2.34339900
C	-6.24653700	-0.01743100	1.75109100
H	-4.39413700	2.19473400	-2.40606500
H	-2.55027100	4.44778000	0.29375900
H	-1.29597300	3.14182600	-0.22849000
C	-6.29756500	0.72069500	-1.38315800
H	-5.76112800	-0.97459200	1.54532900
H	-6.32802500	0.12967000	2.83154400
H	-7.24609500	0.02319900	1.30866400
H	-3.47833900	-2.65894700	-1.93746300
H	-2.92400200	-1.82346100	-3.42977400
H	-2.01866600	-1.61273300	-1.89366200
H	-6.90817700	1.62347700	-1.26387700
H	-6.13728200	0.54097400	-2.45384800
H	-6.85065600	-0.13589800	-0.97883200
Cl	0.49730300	-2.69265500	-1.03756100
Cl	-0.54900700	0.62861800	-1.26192100
C	-1.48940500	-0.18104900	1.85722500
C	-1.45294500	-1.58115100	1.85787500
C	-0.21810500	-2.23904200	2.15445800
C	0.91509400	-1.51161300	2.60759100
C	0.85997100	-0.08201300	2.61382200
C	-0.32380700	0.58426700	2.20338800
H	-2.38585800	0.32486900	1.49443000
H	-2.30348100	-2.13399500	1.47073200
H	-0.13736300	-3.31497600	2.01890500
H	1.83700300	-2.03301600	2.85332800
H	1.75735800	0.49447400	2.83370100
H	-0.34442400	1.66836500	2.12761200
Ru	0.34096400	-0.77781300	0.59934000
C	3.93436400	1.27334000	-0.77951000
C	2.56970600	0.92359500	-0.56461300
C	2.18310600	-0.26622800	-0.00071900
C	4.82865100	1.40173100	0.44047200
S	4.71435700	-0.97202700	-1.01463500
C	3.24360900	-1.33121800	0.13279200
O	4.51544400	1.05522000	1.56001600
O	6.00271200	1.95193200	0.12723000
C	6.92183900	2.09240700	1.21448800
C	3.84400300	-1.35900000	-2.60652800
H	1.80661900	1.53771800	-1.05421800
H	2.84670600	-2.30761000	-0.16962500
H	3.66056800	-1.38323100	1.14629300

C	4.28638100	2.10681100	-1.97171000
H	3.67427300	-2.43749800	-2.64887700
H	2.87749800	-0.83661200	-2.60418400
H	4.48433400	-1.02895000	-3.42683500
H	7.18720100	1.10851800	1.61599200
H	7.80334800	2.58503600	0.80059500
H	6.48074800	2.69841700	2.01229200
H	3.63917300	1.85921900	-2.81974800
H	4.13303000	3.16710300	-1.72436200
H	5.33695000	1.99447200	-2.25564900

3.5 RU-CATALYST Carbenoid

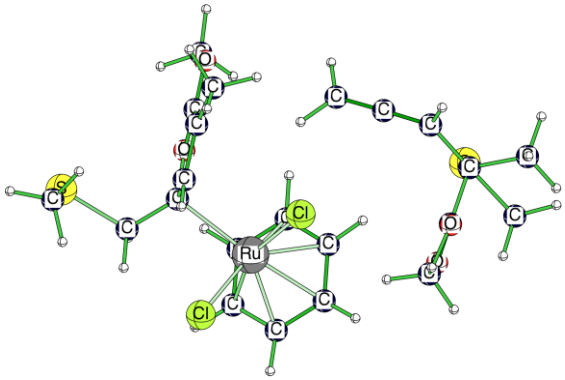
This structure was obtained as a shoulder
ENERGY=-1300.52238



C	4.50439100	0.95934900	0.48619300
C	3.54086200	1.91615600	1.16553100
C	2.34189600	2.22499300	0.72076800
C	4.04970200	-0.47304800	0.80672900
S	4.39436100	1.30665800	-1.36631700
C	1.12296100	2.50363700	0.32316100
O	3.68881700	-1.30639100	0.00226100
O	4.11502700	-0.68849100	2.11907200
C	3.59968500	-1.95291100	2.56025100
C	5.61272800	0.08269000	-2.05838000
H	3.87098200	2.32111100	2.12562000
H	0.90217100	3.36551400	-0.30806300
H	0.31095100	1.84248200	0.64747100
C	5.92149500	1.18920000	1.00527000
H	5.32338000	-0.93158600	-1.77328700
H	5.55720400	0.19048000	-3.14488900
H	6.63030300	0.31179600	-1.72869400
H	4.13977300	-2.77395000	2.07671800
H	3.75495500	-1.97605500	3.64054700
H	2.52918500	-2.01564600	2.32418700
H	6.24595000	2.20417600	0.74780000
H	5.94757600	1.07585500	2.09590800
H	6.63412100	0.47380700	0.57735000
Cl	-1.92271900	-3.20044800	0.83027600
Cl	0.27407500	-0.65366000	1.76036900
C	-0.07886500	-0.03379200	-2.08013200
C	1.02469400	-0.66821100	-1.46989600
C	1.10420500	-2.09398100	-1.39708000
C	0.01827000	-2.85986200	-1.83652500
C	-1.15261600	-2.23375200	-2.38319300
C	-1.18368800	-0.82551000	-2.52355600
H	-0.13330700	1.05076400	-2.12279700
H	1.82610600	-0.07050500	-1.03787100
H	1.95076700	-2.54452000	-0.88712300
H	0.00210700	-3.93110000	-1.65198900
H	-2.01499700	-2.83576000	-2.65889200
H	-2.07338900	-0.33235700	-2.90840800
Ru	-0.86411000	-1.29570800	-0.39048800
C	-2.29075900	2.04335600	1.09536100
C	-2.32982100	0.70361400	1.24050900
C	-2.43530300	-0.25298200	0.15520100
C	-2.35873500	2.48339300	-0.30602800
S	-5.30254900	0.27526400	0.12597100
C	-3.77596000	-0.71217400	-0.31153000
O	-2.47845800	1.69898600	-1.24311900
O	-2.25388400	3.80185200	-0.46201100
C	-2.27138700	4.26389100	-1.81404500
C	-5.48724500	-0.26233000	1.89873200
H	-2.21826300	0.24264400	2.22672800
H	-3.89041900	-1.73017900	0.10177600
H	-3.78258700	-0.82397300	-1.40144100
C	-2.11972800	3.02126200	2.21176700
H	-4.71860800	0.20139500	2.52527300
H	-6.47478200	0.06788200	2.23013000
H	-5.42365000	-1.35293900	1.96653300
H	-3.19646000	3.95731000	-2.31283700
H	-2.20566000	5.35194700	-1.76301200
H	-1.41495300	3.85725300	-2.36573900
H	-2.08680800	2.50163600	3.17486900
H	-1.18571700	3.58777900	2.09684700
H	-2.93984400	3.74941100	2.22907100

3.6 RU-CATALYST Cycle-O MLn-F

ENERGY=-1300.54681

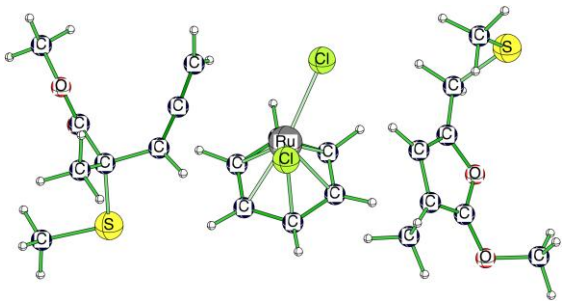


C	4.50854200	0.91079300	0.32667100
C	3.55829300	1.95250700	0.88788300
C	2.41222100	2.30198300	0.34720500
C	4.04296200	-0.46652300	0.82612500
S	4.39914100	1.02372100	-1.55395800
C	1.24612100	2.63103600	-0.15702500
O	3.71948400	-1.41001300	0.13514600
O	4.05278300	-0.49135100	2.15754100
C	3.52820900	-1.68519800	2.75314600
C	5.62082900	-0.27290100	-2.08874500
H	3.84139100	2.37757100	1.85419600
H	1.12588900	3.47379600	-0.83784600
H	0.37770100	2.02636100	0.12920700
C	5.92986900	1.18121500	0.81563500

H	5.33205700	-1.24486600	-1.68266300
H	5.56509600	-0.29799500	-3.18029000
H	6.63803200	-0.00357800	-1.78969400
H	4.12861900	-2.55380800	2.46133400
H	3.58350200	-1.52789700	3.83199700
H	2.48555200	-1.82230800	2.44095200
H	6.26930100	2.15601200	0.44649500
H	5.95391900	1.18970400	1.91240900
H	6.63077900	0.41121100	0.47088500
Cl	-2.06349500	-2.68716500	1.32420900
Cl	0.37630200	-0.23358000	1.67331200
C	0.02583500	-0.34125900	-2.14459100
C	1.05183400	-0.96779900	-1.39776700
C	0.95548400	-2.34184500	-1.02227500
C	-0.21880100	-3.05959300	-1.34136700
C	-1.27934200	-2.44231900	-2.07920000
C	-1.15126300	-1.08233900	-2.46766400
H	0.09482700	0.71960300	-2.37507200
H	1.89901500	-0.37992800	-1.04763400
H	1.72013800	-2.76734100	-0.37780000
H	-0.36877000	-4.05530600	-0.93121600
H	-2.20705100	-2.98124200	-2.25813200
H	-1.98146800	-0.58080300	-2.96207800
Ru	-0.84959900	-1.22224300	-0.30664800
C	-2.16623800	1.96618400	1.26558400
C	-2.46973900	0.61666700	1.25657300
C	-2.63585100	0.14746700	-0.08607200
C	-2.20563100	2.32644400	-0.08947400
S	-5.47381700	0.37480200	-0.29303200
C	-3.86955500	-0.58633500	-0.53244100
O	-2.46668300	1.33208000	-0.90440600
O	-1.95888500	3.51944500	-0.56521300
C	-2.06610200	3.70493200	-1.98236800
C	-5.68750600	0.13163500	1.53982000
H	-2.54207900	-0.04025100	2.11849600
H	-3.95171300	-1.53330500	0.01175100
H	-3.83951700	-0.79523300	-1.60751100
C	-1.76595600	2.85617600	2.39161600
H	-5.04544300	0.81753100	2.10121100
H	-6.73527600	0.33743900	1.77229100
H	-5.45152000	-0.90595900	1.79966000
H	-3.04924200	3.37961300	-2.33747500
H	-1.93341900	4.77392300	-2.15254700
H	-1.27870400	3.14217600	-2.49812700
H	-1.91391500	2.34630700	3.34849800
H	-0.70198100	3.11946300	2.31778200
H	-2.34512400	3.78721400	2.39523400

3.7 RU-REGENERATION TSx

ENERGY=-1300.52526 LOWEST
FREQUENCY=-60.75

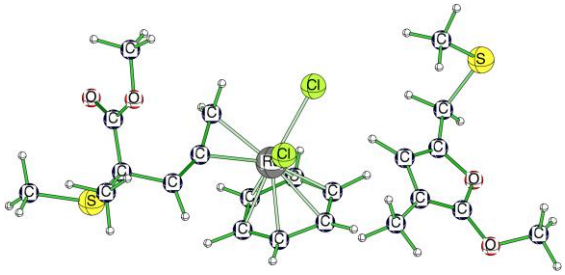


C	3.82689100	-1.46323200	1.12694600
C	3.52423600	-0.07522800	0.90089100
C	4.26861300	0.33378700	-0.16974600
C	4.73537200	-1.78129400	0.15618600
S	5.87423800	2.65695200	-0.14118100
C	4.43886100	1.63636600	-0.83407400
O	5.01838900	-0.71630700	-0.64121600
O	5.30160600	-2.95248800	-0.15713400
C	6.72330300	-2.90997700	-0.28047800
C	5.13261200	2.98120300	1.53344000
H	2.81826400	0.53697400	1.45553000
H	4.67118000	1.51960200	-1.89866900
H	3.52514200	2.23503100	-0.71852300
C	3.25893700	-2.37232800	2.16417600
H	5.03034700	2.04232400	2.08719300
H	5.81175300	3.65340500	2.06387200
H	4.15219400	3.45648800	1.41834400
H	7.17821100	-2.51951700	0.63999200
H	7.05334900	-3.93821000	-0.44813800
H	7.02488100	-2.28414300	-1.12919700
H	2.16418600	-2.42793900	2.08127500
H	3.67167100	-3.38262600	2.06361500
H	3.47847400	-2.00977000	3.17601200
Cl	0.93639200	2.33283300	0.03711200
Cl	-0.02213100	-0.32730300	2.01732200
C	0.15737100	-2.00110300	-0.85549200
C	1.28052000	-1.24798700	-1.31853800
C	1.09024900	-0.13557900	-2.19812600
C	-0.21837500	0.25712300	-2.57188900
C	-1.33155000	-0.44742000	-2.03091100
C	-1.14858100	-1.60184300	-1.21008900
H	0.30594300	-2.77809000	-0.10928400
H	2.27336600	-1.46537700	-0.92692100
H	1.94438500	0.48606100	-2.45874600
H	-0.37289700	1.17588500	-3.13148200
H	-2.34186500	-0.06883600	-2.18684700
H	-2.01677400	-2.07807600	-0.75581900
Ru	-0.04142400	0.13079500	-0.36683600
C	-4.85900000	-0.42248600	0.78953700
C	-3.41546700	-0.01064000	0.96659900
C	-2.90441400	1.08839600	0.45525400
C	-5.54345800	0.62611700	-0.09215800
S	-4.74757600	-2.07992900	-0.12370900
C	-2.47792300	2.23565800	-0.02633200
O	-5.59872800	0.60912300	-1.30141900
O	-6.02843800	1.62050400	0.65871100
C	-6.55537600	2.72992800	-0.07191500
C	-6.54847900	-2.46845000	-0.37784500
H	-2.77564500	-0.68649800	1.54562000
H	-2.48113600	3.13168300	0.59412100
H	-2.07427200	2.33370500	-1.03441800

C	-5.52592100	-0.60237100	2.14990500
H	-7.05007000	-2.63338200	0.57982100
H	-7.02721900	-1.66167700	-0.94028300
H	-6.58066700	-3.38884900	-0.96613100
H	-7.40777100	2.41788800	-0.68471400
H	-6.87005300	3.46107700	0.67503500
H	-5.78292200	3.15378400	-0.72361300
H	-5.48650100	0.33455800	2.71650900
H	-6.57801200	-0.89691200	2.05083800
H	-4.99707800	-1.37844700	2.71508600

3.8 RU-REGENERATION Furane

ENERGY=-1300.54093

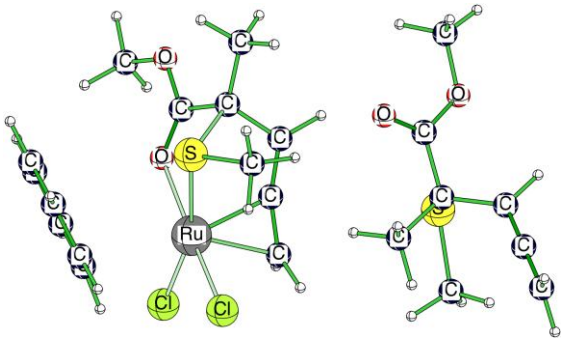


C	3.80613600	-1.18934600	1.44053200
C	3.36358700	-0.02688000	0.71679300
C	4.32184500	0.25947300	-0.21347300
C	5.00735800	-1.51193600	0.87295800
S	5.54656200	2.78116700	-0.56673900
C	4.46620200	1.35554000	-1.18527200
O	5.34313200	-0.65603900	-0.12657600
O	5.82462400	-2.54584300	1.10363800
C	7.20517700	-2.20490400	1.21928200
C	4.41670100	3.34575500	0.79956800
H	2.43724900	0.52336100	0.87203800
H	4.94858900	1.02605000	-2.11253700
H	3.47777700	1.77857700	-1.40963300
C	3.11437300	-1.89842500	2.55691200
H	4.34679200	2.57556300	1.57425700
H	4.84752100	4.25866500	1.21842000
H	3.42110400	3.55448300	0.39231600
H	7.35202200	-1.44096900	1.99490800
H	7.72973300	-3.12157000	1.50026200
H	7.60021900	-1.83307100	0.26614200
H	2.14349900	-2.30593800	2.23874500
H	3.72844700	-2.72581100	2.93024300
H	2.90348400	-1.21674000	3.38982400
Cl	0.74920300	2.02618400	-0.93415900
Cl	-0.10154300	0.05712100	1.68070400
C	-0.23129000	-2.36499700	-0.67279300
C	1.08845700	-1.86372600	-0.92723100
C	1.29933400	-0.99251700	-2.00025600
C	0.20420900	-0.58001000	-2.83251900
C	-1.06892900	-1.16899100	-2.65746100
C	-1.27862600	-2.07975300	-1.58156700
H	-0.42223000	-2.96939200	0.21101600
H	1.90070600	-2.06324900	-0.22988900
H	2.27074400	-0.51403100	-2.10950800
H	0.35600300	0.18556800	-3.58812300
H	-1.90888000	-0.86250300	-3.27681100
H	-2.27978200	-2.46092900	-1.39324800
Ru	-0.45332100	-0.15215900	-0.75380300
C	-4.74206600	-0.43068900	0.80798600
C	-3.28561600	-0.73946500	0.56443100
C	-2.49699300	0.06969800	-0.12095200
C	-4.98451400	1.08259700	0.77702100
S	-5.60476800	-1.28157000	-0.64730700
C	-2.16781300	1.24126900	-0.76285100
O	-5.61522000	1.69521200	-0.05472700
O	-4.38960500	1.65319400	1.82935900
C	-4.49946500	3.07585000	1.90183500
C	-7.39934700	-1.02354500	-0.22593800
H	-2.92459000	-1.69792800	0.94647100
H	-1.87435200	2.10793100	-0.16789600
H	-2.45673900	1.42988900	-1.79765300
C	-5.19401400	-1.01667900	2.14401400
H	-7.67743700	-1.58725100	0.66916000
H	-7.59106200	0.04531900	-0.09824600
H	-7.96850900	-1.39680400	-1.08128900
H	-5.54544500	3.37422800	2.03179600
H	-3.90435900	3.37888900	2.76497000
H	-4.10913300	3.53664600	0.98756300
H	-4.58099300	-0.60987400	2.95625300
H	-6.24372200	-0.77851000	2.35537700
H	-5.08114500	-2.10745100	2.12622700

4 Coordination of the Sulfur on the Ru CATALYST

4.1 SO-complexe bimolecular

ENERGY=-1300.52943

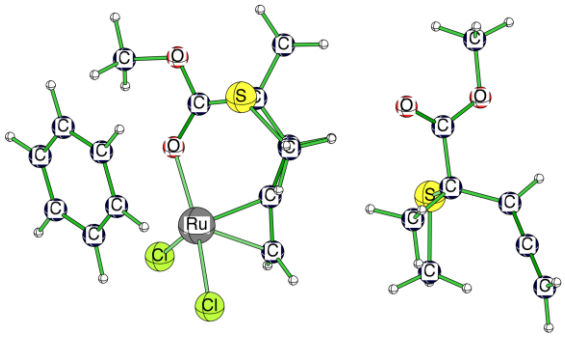


C	-0.70027900	2.03379900	0.17952300
C	0.40150400	1.36896500	-0.59438500
C	0.16122600	0.10679100	-0.94821300
C	-1.86653000	2.08766700	-0.79429800
S	-1.36540700	0.69223300	1.44180300
C	0.27821400	-1.11123900	-1.58712800
O	-2.35644000	1.07172700	-1.29912000
O	-2.27435200	3.29818000	-1.10084300
C	-3.29910400	3.38426900	-2.10732900
C	0.14514300	0.31321300	2.44786800
H	1.29333100	1.93246300	-0.87678800
H	0.83225100	-1.93494800	-1.13288000
H	0.08880600	-1.18634800	-2.65861800
C	-0.33069600	3.33227000	0.85240600
H	0.09003000	-0.75976000	2.65850600

H	1.03945700	0.53753900	1.85666200
H	0.11376000	0.90990900	3.36163700
H	-3.52528300	4.44633300	-2.20767400
H	-2.92891500	2.97372100	-3.05154000
H	-4.18551400	2.82558100	-1.79213000
H	0.51072000	3.16474500	1.53688300
H	-0.01532500	4.06480300	0.09825900
H	-1.17084800	3.75540200	1.41342500
Cl	-2.42842100	-2.07657500	-2.42131100
Cl	-0.70151400	-2.74828700	0.77513500
C	-3.78934800	-1.68549200	2.06732200
C	-4.31287700	-0.62016200	2.79012800
C	-4.91479700	0.45686000	2.11702500
C	-4.99090100	0.46130800	0.72697800
C	-4.47843900	-0.62138100	-0.00688300
C	-3.87449700	-1.69509300	0.66081700
H	-3.31869400	-2.52323600	2.57838800
H	-4.25603000	-0.61713900	3.87759400
H	-5.32406700	1.29042300	2.68668800
H	-5.46830200	1.29161400	0.20741700
H	-4.56668200	-0.65080900	-1.09201500
H	-3.55483300	-2.57343300	0.09996500
Ru	-1.56862700	-0.83230000	-0.48234500
C	4.17792500	-0.12728600	0.15770500
C	5.65265800	-0.35212900	0.38093200
C	6.14682500	-1.40017200	1.00744800
C	3.81751100	1.28024800	0.62748800
S	3.86502200	-0.09408800	-1.74046700
C	6.63808000	-2.44112400	1.63771900
O	3.01307900	1.52993700	1.50116300
O	4.51045200	2.21756200	-0.02301600
C	4.24227500	3.56464900	0.37136200
C	4.12711400	-1.89342800	-2.12150800
H	6.32798700	0.39645300	-0.03862000
H	6.81771200	-2.41497700	2.71246400
H	6.88369800	-3.36059700	1.10624700
C	3.28770300	-1.14770000	0.83952900
H	5.05269300	-2.23804700	-1.64669300
H	3.27735000	-2.50098900	-1.79887700
H	4.23334800	-1.95786700	-3.20733600
H	4.88580100	4.19285600	-0.24695600
H	3.18827600	3.81215800	0.19767200
H	4.47101100	3.70595800	1.43279300
H	3.55870100	-2.16792500	0.54723900
H	3.39519200	-1.07109400	1.92891800
H	2.23483900	-0.97753600	0.58364500

4.2 TSso1 bimolecular

ENERGY=-1300.50397 LOWEST
FREQUENCY=-24.86

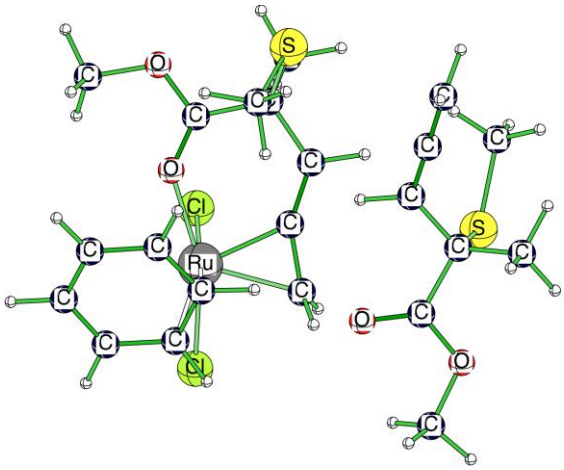


C	-0.35399000	2.00063500	-0.14626100
C	0.46827600	0.83184000	-0.58173100
C	0.00281200	-0.41045700	-0.65777900
C	-1.74570000	1.86336800	-0.73052800
S	-0.70798600	2.02974600	1.76736200
C	0.06645800	-1.76361000	-0.95924900
O	-2.36433800	0.80508100	-0.87379500
O	-2.27156800	3.00801300	-1.10698200
C	-3.57334600	2.95716500	-1.71317500
C	0.48078900	0.76344100	2.43523000
H	1.50679700	1.02995700	-0.86726400
H	0.56674200	-2.46236700	-0.28548500
H	-0.06485900	-2.09640600	-1.99087200
C	0.33204800	3.31031200	-0.50169500
H	0.20907900	-0.25058200	2.11966700
H	1.50198600	1.00879200	2.12844100
H	0.38386900	0.84245300	3.52221800
H	-3.80427200	3.98443600	-1.99822600
H	-3.55412600	2.30229100	-2.58960000
H	-4.30508700	2.57561800	-0.99332200
H	1.31258600	3.32818200	-0.01071500
H	0.47643300	3.38481400	-1.58837900
H	-0.24378000	4.17594200	-0.16196300
Cl	-2.70679100	-1.88186800	-2.20012600
Cl	-1.48031300	-3.10734000	1.21161200
C	-3.76559500	-0.64925400	1.80138800
C	-4.13586100	0.68764300	2.02634900
C	-5.07440500	1.29254900	1.19678900
C	-5.63952000	0.57998600	0.12468700
C	-5.25839500	-0.73373900	-0.11788500
C	-4.32223600	-1.35872200	0.72596400
H	-3.09293500	-1.15706900	2.49293600
H	-3.69605800	1.23916300	2.85491700
H	-5.37837400	2.32246000	1.38452800
H	-6.37850800	1.05924300	-0.51688400
H	-5.68185700	-1.28869900	-0.95208500
H	-4.09518200	-2.41693500	0.59509000
Ru	-1.79957300	-1.11810900	-0.11856000
C	4.43461000	-0.19168200	0.08353300
C	5.88381100	-0.57302800	0.21401300
C	6.31057000	-1.60641000	0.91032700
C	4.24159800	1.30800200	0.29388900
S	3.92612000	-0.40209200	-1.76669600
C	6.74216100	-2.62830000	1.61159200
O	3.34901300	1.79987300	0.95337700
O	5.16060600	2.02237700	-0.35648300
C	5.02144700	3.44184500	-0.25789000
C	3.91254700	-2.25655400	-1.87348000
H	6.59900100	0.03752000	-0.33954600
H	7.02501000	-2.51326500	2.65796100

H	6.83540500	-3.62048700	1.16968000
C	3.50493400	-0.97314700	0.99062300
H	4.82640200	-2.65548500	-1.41917000
H	3.02368200	-2.67763600	-1.39570600
H	3.90532200	-2.49647700	-2.93957000
H	5.85721800	3.86550700	-0.81727400
H	4.06961500	3.76257800	-0.69604400
H	5.05895300	3.75933400	0.78911800
H	3.63944500	-2.05149300	0.85253700
H	3.72265500	-0.73938200	2.04096400
H	2.45887600	-0.71520500	0.78756600

4.3 O-Complexe bimolecular

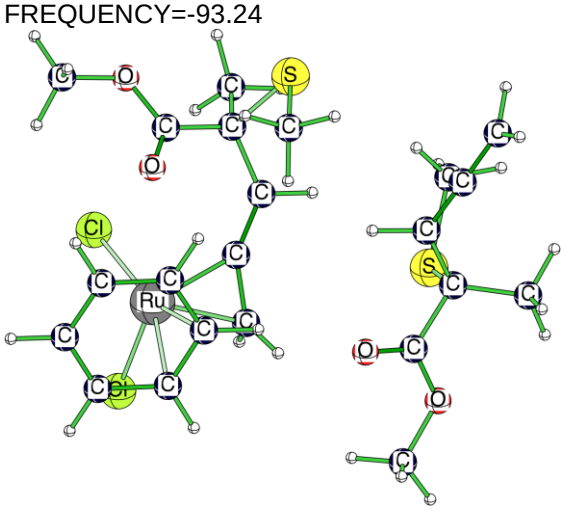
ENERGY=-1300.51643



C	-0.51215500	2.41334800	-0.81814400
C	0.26637900	1.16552100	-1.07007600
C	-0.18038000	-0.07904200	-0.96855900
C	-1.84440300	2.14532100	-0.14931500
S	0.47542400	3.56008200	0.36347800
C	-0.05405000	-1.45412100	-1.18727200
O	-2.17305700	1.08231000	0.39413900
O	-2.63577700	3.18944600	-0.10778700
C	-3.93666800	2.97989900	0.46461900
C	0.44338800	2.52444600	1.90515500
H	1.27934900	1.30675600	-1.45944600
H	0.50296000	-2.08530200	-0.48848500
H	-0.16002400	-1.84264200	-2.20167000
C	-0.66302200	3.22657500	-2.10224600
H	-0.45602600	2.73797700	2.49193400
H	0.45921200	1.46663100	1.61545000
H	1.34069400	2.76344200	2.48247600
H	-4.46653800	3.92482300	0.33973100
H	-4.44731400	2.17100400	-0.06865900
H	-3.84571800	2.72472200	1.52587400
H	0.33180900	3.40356200	-2.53049000
H	-1.25714200	2.65178100	-2.82232400
H	-1.14684200	4.19139600	-1.91529600
Cl	-2.88402400	0.18245800	-2.39045900
Cl	-2.54648900	-3.00820400	-1.40332700
C	-1.68693400	-2.31152600	1.45632600
C	-0.87056500	-1.27195000	1.94478300
C	-1.39491600	-0.35242300	2.88286900
C	-2.72580600	-0.41510700	3.25247500
C	-3.57117600	-1.40680400	2.70379100
C	-3.05481900	-2.36138800	1.84414200
H	-1.24854600	-3.15789400	0.93168300
H	0.19523900	-1.27056600	1.71179600
H	-0.73830500	0.39580100	3.32372500
H	-3.12552700	0.29671600	3.97330300
H	-4.62130300	-1.44277000	2.98804800
H	-3.68303500	-3.15996000	1.45554300
Ru	-1.93167900	-0.86982000	-0.40791500
C	4.02848300	-0.50794100	0.16185300
C	3.37311900	0.57590100	0.95787700
C	4.00259200	1.59729700	1.49649900
C	3.30270700	-1.82328900	0.43266800
S	3.64856200	-0.23132500	-1.71530200
C	4.61149300	2.63363500	2.02443700
O	2.29883300	-1.93632400	1.10753900
O	3.89670600	-2.84203200	-0.18402300
C	3.25006000	-4.11144700	-0.04678600
C	4.02268600	1.58305500	-1.88113600
H	2.28488300	0.50906700	1.04449300
H	4.98753900	2.61131700	3.04716500
H	4.75621800	3.54981100	1.45043100
C	5.52977200	-0.62006100	0.37536000
H	3.37288200	2.18109700	-1.23213800
H	5.07415600	1.78805900	-1.65746700
H	3.82067700	1.82279900	-2.92907800
H	3.84851500	-4.81588000	-0.62655300
H	3.21493900	-4.41080400	1.00575500
H	2.22957400	-4.06421800	-0.44270500
H	5.95421200	-1.39591400	-0.26757300
H	6.01762200	0.33476400	0.14662200
H	5.74631500	-0.86255100	1.42479500

4.4 TSso2 bimolecular

ENERGY=-1300.50147 LOWEST
FREQUENCY=-93.24

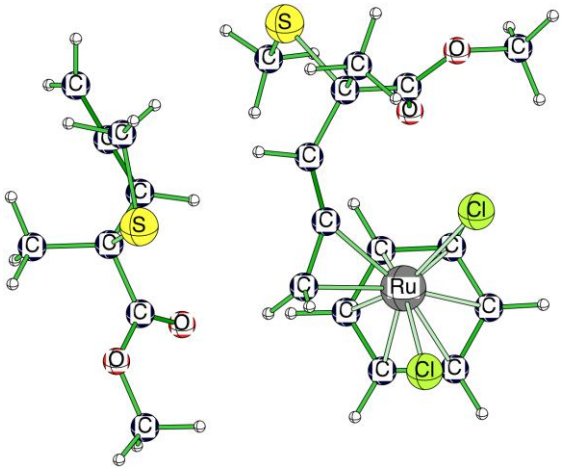


C	-0.38421600	2.54137100	-0.71984400
C	0.20567900	1.19151800	-0.95965000
C	-0.30442900	-0.03004800	-0.85056000
C	-1.71141700	2.51845900	0.01287800
S	0.79034300	3.54206200	0.42943800
C	-0.10256200	-1.39280800	-1.10379500
O	-1.98235800	1.72006000	0.89424600

O	-2.51268500	3.51402200	-0.34671800
C	-3.79221500	3.52738400	0.28968700
C	0.75416300	2.51493500	1.97796400
H	1.21989500	1.21780300	-1.37645400
H	0.53918800	-1.99978200	-0.45876500
H	-0.24104800	-1.76889100	-2.11818500
C	-0.40394300	3.33158600	-2.02375400
H	-0.12492200	2.75701300	2.58074500
H	0.73773800	1.45295400	1.70580400
H	1.67132800	2.74361000	2.52840000
H	-4.34439800	4.34988500	-0.16871600
H	-4.30334100	2.57400100	0.11240400
H	-3.68336600	3.69356500	1.36719300
H	0.59254100	3.30406800	-2.48371500
H	-1.12211100	2.87202700	-2.71343900
H	-0.68832900	4.37626300	-1.85825000
Cl	-3.15408100	0.47196800	-1.78183100
Cl	-2.66975800	-2.76192600	-1.68981300
C	-1.67153300	-2.65551000	1.27550000
C	-0.94822300	-1.54401900	1.78060200
C	-1.62789400	-0.54166100	2.52197600
C	-3.00478200	-0.59628600	2.68218800
C	-3.73759200	-1.67894800	2.13946400
C	-3.07875600	-2.71410700	1.48551100
H	-1.15150700	-3.49569300	0.81897100
H	0.13940500	-1.52353300	1.70576600
H	-1.06466500	0.29457700	2.92859600
H	-3.52197900	0.20294900	3.20807200
H	-4.81927400	-1.71243500	2.24804700
H	-3.63941700	-3.55560400	1.08693500
Ru	-1.97739700	-0.97940200	-0.20465600
C	4.04645500	-0.63943900	0.08242500
C	3.51318900	0.45965800	0.94439200
C	4.23833700	1.42431100	1.46675000
C	3.25721400	-1.91269400	0.37533500
S	3.56624500	-0.29069300	-1.75982700
C	4.94084100	2.40745100	1.97953900
O	2.29222000	-1.97841300	1.11134000
O	3.74496400	-2.95388700	-0.29548000
C	3.04008700	-4.18745800	-0.12665600
C	3.95374800	1.52503100	-1.88437600
H	2.43055500	0.45557800	1.10055000
H	5.37810500	2.33395100	2.97516300
H	5.10367100	3.32947900	1.41986900
C	5.54935800	-0.84433400	0.19039100
H	3.31104600	2.11585700	-1.22120900
H	5.00790000	1.71505100	-1.65957000
H	3.75126700	1.78750500	-2.92700300
H	3.58940600	-4.92867400	-0.70922700
H	3.01327400	-4.47140400	0.93035200
H	2.01451600	-4.09749200	-0.50309900
H	5.88599600	-1.62825300	-0.49331400
H	6.07511400	0.08537000	-0.05813700
H	5.82255000	-1.11929700	1.21834400

4.5 cis-Allene bimolecular

ENERGY=-1300.51980

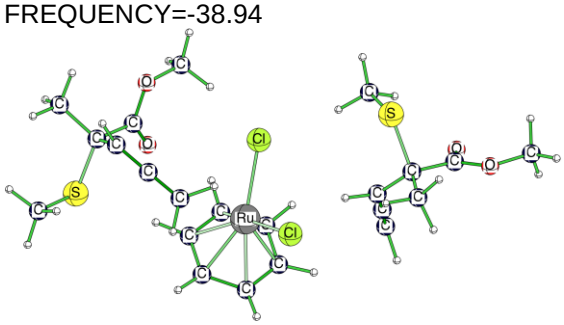


C	0.68013600	2.58413900	0.76060900
C	-0.03035600	1.26586100	0.83305400
C	0.30336500	-0.00947600	0.66701600
C	1.90760500	2.64321000	-0.12806800
S	-0.51178100	3.89337000	0.01793000
C	-0.13326400	-1.29806900	0.94254800
O	1.95974300	2.17007000	-1.24882400
O	2.88838600	3.36441500	0.41107100
C	4.09560800	3.41078200	-0.34422600
C	-0.82887200	3.19794400	-1.67558500
H	-1.02567600	1.36627100	1.28856200
H	-0.83452900	-1.82556100	0.29451200
H	-0.02535400	-1.68760700	1.95470400
C	0.92791400	3.06463200	2.18890500
H	0.05643600	3.30394300	-2.30620500
H	-1.10503700	2.14153000	-1.58550100
H	-1.67020400	3.76045900	-2.08908900
H	4.77832600	4.05025600	0.21884500
H	4.51263300	2.39887000	-0.43004800
H	3.91757700	3.82512700	-1.34272100
H	-0.00387700	2.99954200	2.76489300
H	1.68079800	2.41668900	2.65331900
H	1.28514700	4.10024500	2.20891000
Cl	3.26873100	0.19044800	1.29558500
Cl	2.25201200	-2.96838200	1.78377000
C	1.41395900	-2.95353800	-1.48032700
C	0.70121700	-1.79405800	-1.89133100
C	1.39522100	-0.57681800	-2.12815100
C	2.78402100	-0.51487400	-1.88927400
C	3.52006900	-1.70629700	-1.57091600
C	2.84158200	-2.91829000	-1.40534100
H	0.87539900	-3.86510800	-1.23266800
H	-0.38692300	-1.82000800	-1.94528600
H	0.85233700	0.33877600	-2.34661400
H	3.28222100	0.44984600	-1.93258000
H	4.58895300	-1.64772200	-1.38545500
H	3.38168700	-3.79988500	-1.06996600
Ru	1.82753000	-1.32531100	-0.02154100
C	-3.97320700	-0.46152400	-0.08984100
C	-3.36666400	0.55537400	-1.00570300
C	-4.00376200	1.61008800	-1.46578500
C	-3.36120500	-1.82571200	-0.39121500
S	-3.38433400	-0.11104900	1.71801100
C	-4.63216200	2.67925000	-1.89526700
O	-2.53805500	-2.04009200	-1.26068900

O	-3.83008200	-2.76469700	0.42497900
C	-3.26707400	-4.07035400	0.26174400
C	-3.72223400	1.71405600	1.83906100
H	-2.30825200	0.41213300	-1.24754900
H	-5.16370700	2.68671600	-2.84653700
H	-4.63095200	3.59775000	-1.30560200
C	-5.49393600	-0.50938300	-0.13543300
H	-3.07424100	2.28830300	1.16621700
H	-4.77557800	1.92829400	1.63239600
H	-3.49713300	1.97619700	2.87711000
H	-3.78064800	-4.70907200	0.98173900
H	-3.42747700	-4.43249900	-0.75875800
H	-2.19171800	-4.05099600	0.47545700
H	-5.88008400	-1.24309800	0.57773300
H	-5.91043100	0.47510400	0.10932000
H	-5.83346800	-0.77232700	-1.14659600

4.6 TSso3 bimolecular

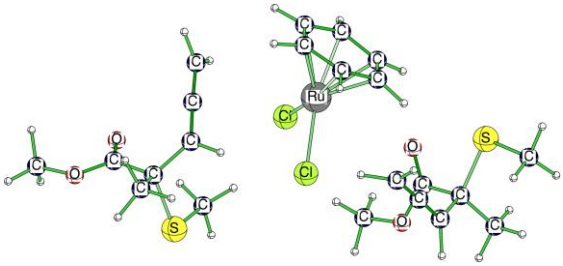
ENERGY=-1300.49936 LOWEST
FREQUENCY=-38.94



C	-4.96220500	1.24558900	0.18101900
C	-4.37537000	1.06880900	1.56716100
C	-3.40989900	0.24385900	1.91096500
C	-3.86755100	1.71173800	-0.78259300
S	-5.59880400	-0.39949100	-0.53865100
C	-2.45656700	-0.54874400	2.35027100
O	-3.43396600	1.06968000	-1.71758900
O	-3.46090100	2.93544300	-0.46522300
C	-2.42551000	3.47705400	-1.29511800
C	-6.72834500	-0.92085100	0.84066900
H	-4.79562400	1.70688800	2.35030500
H	-2.67039100	-1.54784800	2.73230200
H	-1.42678400	-0.18842800	2.41872900
C	-6.09036600	2.27291700	0.22101200
H	-6.18417500	-0.93028300	1.79038200
H	-7.60666200	-0.27255500	0.90420400
H	-7.04927400	-1.93666600	0.59582900
H	-2.79015500	3.59419300	-2.32154400
H	-2.17794400	4.44841500	-0.86362400
H	-1.55046200	2.81744600	-1.27922700
H	-6.88998300	1.93487700	0.89173300
H	-5.71318100	3.23092400	0.59923000
H	-6.51630300	2.42832900	-0.77629400
Cl	-0.07421200	1.21358800	0.34926300
Cl	0.87624800	-1.61886400	2.08169900
C	-0.45608800	-3.29446900	-0.49501600
C	-1.79375000	-2.83546500	-0.47217500
C	-2.17816200	-1.67454200	-1.21804400
C	-1.22325300	-0.96015800	-1.97613400
C	0.14082600	-1.36753600	-1.93449600
C	0.52353400	-2.53519500	-1.19890400
H	-0.14336500	-4.10285600	0.16001400
H	-2.51651400	-3.30253700	0.19337900
H	-3.18458800	-1.26611200	-1.10973900
H	-1.51115300	-0.00999100	-2.41928000
H	0.91918600	-0.74144000	-2.36875300
H	1.58127000	-2.77319700	-1.09330600
Ru	-0.48342300	-1.16965200	0.10077900
C	4.53916400	0.26083800	0.57233900
C	3.49761600	-0.40820400	-0.27534600
C	3.64895300	-0.88260700	-1.49285300
C	5.82644900	0.56236600	-0.17562000
S	3.91301300	1.98507500	1.11875800
C	3.74845100	-1.38526300	-2.70349200
O	5.88857200	0.92773100	-1.33199500
O	6.90094200	0.43004900	0.61335000
C	8.14103700	0.80756100	0.01896600
C	3.25561000	2.64822800	-0.49071800
H	2.52858300	-0.53041500	0.22763500
H	3.53761700	-0.77854700	-3.58472200
H	4.08609400	-2.40925100	-2.86589600
C	4.72386300	-0.51992600	1.86864600
H	4.01354100	2.53450900	-1.27208800
H	2.32650000	2.12931200	-0.75163500
H	3.05065200	3.70796900	-0.31539200
H	8.11505600	1.85761600	-0.29210200
H	8.90173400	0.65926900	0.78842900
H	8.35772200	0.18402100	-0.85520500
H	3.74168400	-0.69173900	2.32562000
H	5.19069800	-1.49043000	1.65891500
H	5.35707900	0.02433900	2.57815200

4.7 cis-Allene-MLn-A-intermediary bimolecular

ENERGY=-1300.50213

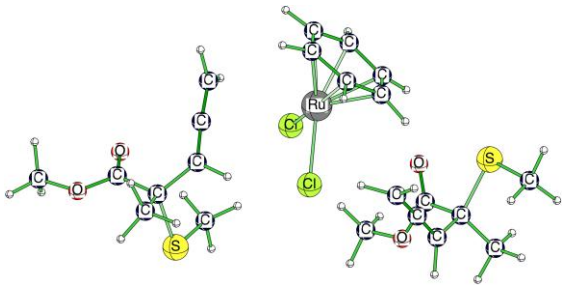


C	4.65423000	-1.52774900	-0.17103100
C	4.05219300	-2.22002700	1.03707900
C	3.41503000	-1.62825300	2.02380100
C	3.52291800	-1.21358400	-1.15612900
S	5.41468600	0.15798600	0.25112400
C	2.76210000	-1.07137900	3.01663900
O	3.23223000	-0.10312600	-1.55019200
O	2.90987100	-2.33213100	-1.52727700
C	1.77101400	-2.17894400	-2.38994800
C	6.69794500	-0.38629300	1.48040900
H	4.09901800	-3.31281700	1.02697600
H	3.26119300	-0.78144900	3.94129300
H	1.68562200	-0.90860000	2.91777200
C	5.68245400	-2.43551900	-0.84227400

H	6.23927500	-1.00435400	2.25856900
H	7.51175400	-0.92581700	0.98809200
H	7.09301000	0.52901800	1.92877800
H	2.02706300	-1.56263200	-3.25781500
H	1.50048100	-3.19014500	-2.70000900
H	0.94410100	-1.71242300	-1.83928600
H	6.49545400	-2.67746100	-0.14692600
H	5.20846000	-3.37780500	-1.14432000
H	6.11082400	-1.95558300	-1.72948800
Cl	-0.57008100	0.81343100	-2.32312900
Cl	0.04812700	-0.86972700	0.63510900
C	1.10880000	2.18432300	1.75504600
C	2.18531000	1.93673500	0.86981900
C	2.17262200	2.49697500	-0.44804500
C	1.10839600	3.34836300	-0.86105600
C	0.00578200	3.54656300	0.00237900
C	-0.00777800	2.93675400	1.29921700
H	1.05247700	1.65316900	2.70171700
H	2.96565900	1.21859100	1.12906400
H	2.93013600	2.16982200	-1.15644800
H	1.05483800	3.68516700	-1.89246800
H	-0.88795500	4.04701900	-0.36215600
H	-0.91077000	2.98812700	1.90351300
Ru	0.35201000	1.39487800	-0.17127400
C	-4.50836500	-0.91391000	0.94114500
C	-3.38946200	0.08374000	0.96653900
C	-3.33785900	1.25561900	0.37242800
C	-5.68822200	-0.48938700	0.08410800
S	-3.88499300	-2.52406700	0.10730100
C	-3.23642500	2.42465400	-0.21934800
O	-5.60365500	0.11990800	-0.96136300
O	-6.85279900	-0.91589800	0.59454900
C	-7.99717300	-0.65576000	-0.21656400
C	-3.03215500	-1.82980700	-1.39591700
H	-2.50979600	-0.24595600	1.53180400
H	-2.83808700	2.48514100	-1.23397400
H	-3.58927900	3.34008900	0.25764800
C	-4.88011900	-1.32367100	2.36123600
H	-3.71381500	-1.16087300	-1.93107200
H	-2.12226400	-1.29925700	-1.09701600
H	-2.77994200	-2.69176100	-2.02010000
H	-7.87888000	-1.11108000	-1.20587900
H	-8.84586000	-1.10050800	0.30748000
H	-8.14709000	0.42256900	-0.33877100
H	-3.97159300	-1.60901200	2.90493600
H	-5.35539400	-0.48487400	2.88485800
H	-5.57156300	-2.17327000	2.36786200

4.8 TSso4 bimolecular

ENERGY=-1300.50156 LOWEST
FREQUENCY=-26.46

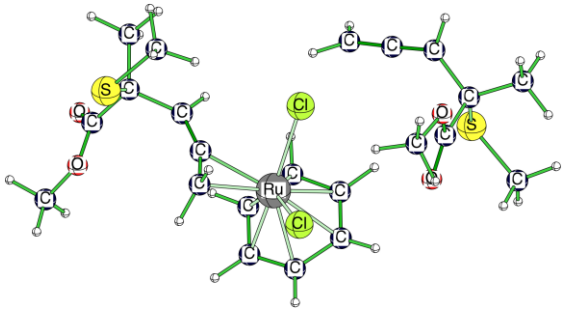


C	4.51253700	-1.65643900	-0.14946000
C	3.80674200	-2.30798000	1.02407200
C	3.22146300	-1.67740600	2.01823900
C	3.45950200	-1.27412000	-1.19536900
S	5.35457700	-0.02035500	0.31154300
C	2.61973600	-1.07441800	3.01638600
O	3.27578000	-0.15223200	-1.61934400
O	2.78074400	-2.34641500	-1.58701100
C	1.71362900	-2.10171700	-2.51785700
C	6.52432800	-0.63867900	1.61724900
H	3.72832300	-3.39814100	0.97910300
H	3.12935600	-0.87068800	3.95818000
H	1.57217300	-0.78430600	2.90108400
C	5.51587600	-2.62751500	-0.76826800
H	5.98169100	-1.22898900	2.36259100
H	7.33340600	-1.22646700	1.17484100
H	6.94415000	0.25151300	2.09278000
H	2.11393400	-1.69059700	-3.45096200
H	1.24932400	-3.07405500	-2.69312200
H	0.98866300	-1.39825800	-2.09059200
H	6.28226700	-2.90672200	-0.03507300
H	5.00405800	-3.54506500	-1.08469200
H	6.00915900	-2.17985700	-1.63859100
Cl	-0.49440500	0.97198300	-2.37548000
Cl	0.05614500	-0.76618000	0.55210300
C	1.14892000	2.27333400	1.76055000
C	2.16852900	1.89095000	0.85074700
C	2.19409600	2.43786700	-0.47104800
C	1.22160500	3.40457600	-0.86767600
C	0.17984800	3.75075800	0.02192900
C	0.12825500	3.15849400	1.32564700
H	1.05627100	1.76706500	2.71807700
H	2.87002700	1.09281900	1.10481500
H	2.89793000	2.02461500	-1.19074400
H	1.18285800	3.73550700	-1.90177700
H	-0.64689300	4.36609800	-0.32415900
H	-0.73977300	3.33023500	1.95763000
Ru	0.27168600	1.55753200	-0.14297600
C	-4.41699300	-1.03706100	0.93103500
C	-3.24746900	-0.10493100	0.98786600
C	-3.12710200	1.09519100	0.46974000
C	-5.59681400	-0.49875000	0.14071300
S	-3.88221200	-2.59995900	-0.04562000
C	-2.91278100	2.28491600	-0.05409500
O	-5.51079700	0.20612400	-0.84299900
O	-6.76293600	-0.94461100	0.62844400
C	-7.91224100	-0.59000100	-0.13904200
C	-3.01142600	-1.82400600	-1.50005000
H	-2.35846600	-0.52551800	1.47440000
H	-2.57081900	2.36898600	-1.08741900
H	-3.14960600	3.19993200	0.49172200

C	-4.76971200	-1.53775900	2.32612500
H	-3.65807800	-1.06657400	-1.95433500
H	-2.06217800	-1.38211400	-1.17866300
H	-2.83337900	-2.63820700	-2.20823100
H	-7.82539600	-0.97990500	-1.15911400
H	-8.76602300	-1.04281500	0.36947200
H	-8.02671900	0.49843000	-0.18386200
H	-3.85992200	-1.89602900	2.82217600
H	-5.19907500	-0.72237200	2.92140200
H	-5.49435900	-2.35829000	2.28932300

4.9 Ru-Ln-A bimolecular

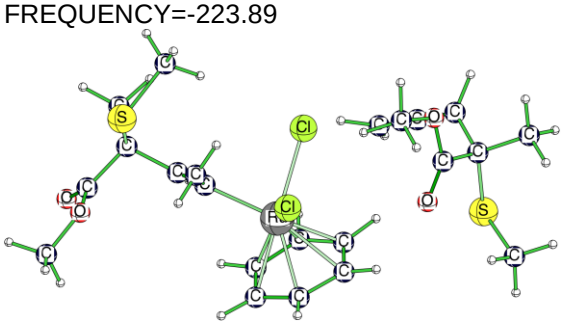
ENERGY=-1300.51524



C	4.71954300	1.26117300	-0.24960800
C	3.81874800	2.47859600	-0.33105100
C	2.72175400	2.57141800	-1.05055700
C	4.10269700	0.27125500	0.75128500
S	4.78270900	0.51538700	-1.98333400
C	1.61484100	2.70636800	-1.74378400
O	3.75080800	-0.86378900	0.50489700
O	4.02105700	0.83388900	1.95286600
C	3.35411800	0.05845100	2.96257300
C	5.96924500	-0.89737900	-1.74385600
H	4.09681200	3.31628700	0.31399600
H	1.61605500	3.11684400	-2.75327800
H	0.66737800	2.40987300	-1.28522800
C	6.11144600	1.67432900	0.22315900
H	5.60663200	-1.55705800	-0.95181900
H	5.98712200	-1.43780400	-2.69409300
H	6.97516100	-0.52923400	-1.52242300
H	3.84160900	-0.91546700	3.07846900
H	3.43765300	0.64103700	3.88225900
H	2.30027800	-0.08619600	2.69014200
H	6.56652700	2.34709600	-0.51297100
H	6.04061800	2.19819200	1.18428100
H	6.76871100	0.80778800	0.36401300
Cl	0.31845800	-2.04064800	2.44177700
Cl	0.35264800	1.03305100	1.09256800
C	0.13988400	-0.73907100	-1.92732100
C	1.37195800	-1.18978600	-1.35985400
C	1.39666500	-2.39050000	-0.64389800
C	0.20520000	-3.18391000	-0.51640200
C	-0.97607300	-2.81861000	-1.19623000
C	-1.00732000	-1.57747500	-1.89183000
H	0.09078900	0.23830900	-2.40360900
H	2.26265600	-0.55874500	-1.38445900
H	2.28643000	-2.65241700	-0.07868400
H	0.21144600	-4.05792800	0.12881500
H	-1.87660100	-3.42001500	-1.10269900
H	-1.94307700	-1.22597800	-2.32068200
Ru	-0.35768300	-1.15711100	0.20722900
C	-4.10197000	1.46424300	-0.33343000
C	-2.72440300	0.84665300	-0.51978800
C	-2.24436500	-0.13651300	0.22370500
C	-5.05626800	0.60436800	-1.16292800
S	-4.69370500	1.42243700	1.46918500
C	-2.27040000	-1.00053600	1.29386600
O	-5.37712000	0.86593200	-2.30278700
O	-5.43266400	-0.50437700	-0.52155800
C	-6.26878300	-1.38772900	-1.26983900
C	-3.39016600	2.50602000	2.23716200
H	-2.13019100	1.27878900	-1.33143100
H	-2.03553600	-0.62173200	2.28997700
H	-2.79908000	-1.95356400	1.24474100
C	-4.09325800	2.88812900	-0.87172500
H	-2.39409600	2.18438900	1.90892900
H	-3.55697800	3.55974300	1.99808100
H	-3.47783000	2.35814000	3.31681800
H	-5.75027100	-1.74082200	-2.16864000
H	-6.49311900	-2.22428500	-0.60547200
H	-7.19181900	-0.88059000	-1.56874900
H	-3.34119700	3.48878000	-0.34697500
H	-3.84101100	2.88434000	-1.93941800
H	-5.07511700	3.35886500	-0.75063800

4.10 TSso5 bimolecular

ENERGY=-1300.50134 LOWEST
FREQUENCY=-223.89

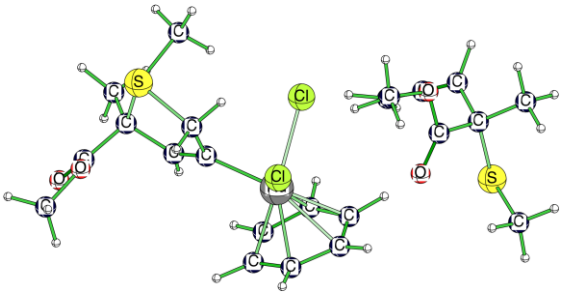


C	4.98630800	0.86183900	-0.41016800
C	4.38208200	1.92534700	-1.30651200
C	3.37846500	1.73421200	-2.13496800
C	4.06694900	0.62866400	0.79929700
S	5.14158700	-0.70100400	-1.46256100
C	2.36485300	1.57487500	-2.95321400
O	3.65252200	-0.44470500	1.18283300
O	3.82497200	1.78301100	1.41260500
C	2.95974800	1.70847000	2.55672000
C	5.96117000	-1.89106800	-0.28931500
H	4.79423000	2.93195700	-1.19880000
H	2.51130400	1.31613200	-4.00165200
H	1.35064000	1.70876600	-2.56983100
C	6.35326800	1.32012100	0.09559600
H	5.35773100	-1.98738500	0.61635800
H	5.99933800	-2.84794300	-0.81715200
H	6.98058900	-1.57141400	-0.05387500
H	3.35669800	0.99623900	3.28823100
H	2.93742100	2.71783700	2.97311700
H	1.95616800	1.39424200	2.24521200

H	7.03620100	1.45390300	-0.75150300
H	6.25246000	2.27610100	0.62499600
H	6.79360000	0.59540400	0.79133000
Cl	-0.05884300	-0.60952500	2.81337300
Cl	0.35933600	1.50339200	0.04359600
C	0.24449800	-1.44177900	-1.74375400
C	1.42377500	-1.51790300	-0.93162200
C	1.43629100	-2.30169800	0.23451200
C	0.24092900	-2.97852200	0.63741000
C	-0.91532600	-2.96893700	-0.18228500
C	-0.90680400	-2.18523800	-1.37711300
H	0.21932400	-0.77406500	-2.60228300
H	2.28328500	-0.88737100	-1.16004800
H	2.28939600	-2.23361600	0.90395800
H	0.19980100	-3.45299300	1.61440700
H	-1.82674000	-3.46101000	0.14588200
H	-1.82223300	-2.08391500	-1.95583200
Ru	-0.33682500	-0.88222200	0.29211400
C	-4.33386000	1.02569200	-0.82201300
C	-2.98559900	0.33128800	-0.98752000
C	-2.25925000	-0.00129400	0.07677700
C	-5.38808400	-0.07453800	-0.94215400
S	-4.46153500	1.75972400	0.92389400
C	-2.50387300	0.26324500	1.42542900
O	-5.93039300	-0.36663900	-1.98507100
O	-5.57078700	-0.72801800	0.20816500
C	-6.46835300	-1.83971300	0.14841100
C	-3.31580000	3.21549400	0.74757500
H	-2.68489900	0.13472200	-2.01984800
H	-1.95900700	1.06318200	1.92669700
H	-2.96650400	-0.48199900	2.07303100
C	-4.54090000	2.08050400	-1.89669500
H	-2.38948700	2.89822700	0.25306000
H	-3.80836700	4.01789500	0.19419100
H	-3.09543300	3.54678100	1.76563800
H	-6.09885900	-2.58794700	-0.56102900
H	-6.50219600	-2.25297500	1.15799900
H	-7.46512600	-1.51166300	-0.16357700
H	-3.72510200	2.81140100	-1.88014800
H	-4.53693500	1.59209100	-2.87798900
H	-5.49966000	2.59839600	-1.77798400

4.11 S-Cycle bimolecular

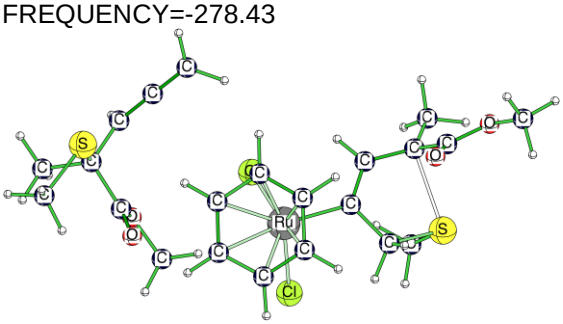
ENERGY=-1300.51430



C	5.04423700	0.87872000	-0.12493700
C	4.47906100	1.92006300	-1.07277400
C	3.55345000	1.69316300	-1.97980900
C	3.99165700	0.57204900	0.95218700
S	5.41377900	-0.65162600	-1.16817600
C	2.61101900	1.50177300	-2.87259400
O	3.49732900	-0.51074200	1.18109100
O	3.70631200	1.68063400	1.63243700
C	2.66480500	1.54528600	2.61238800
C	6.12765500	-1.81554200	0.09695000
H	4.84683100	2.94028100	-0.93575400
H	2.84440300	1.24539400	-3.90583500
H	1.56723500	1.59810000	-2.55838300
C	6.31426500	1.41016900	0.53565400
H	5.40949900	-1.96496200	0.90729300
H	6.29596000	-2.76005000	-0.42763700
H	7.08336500	-1.44376500	0.47858300
H	2.94969500	0.80816100	3.37100700
H	2.55255700	2.53515300	3.06044300
H	1.73380500	1.22703700	2.12818600
H	7.07607900	1.60219800	-0.22924900
H	6.09913300	2.34686700	1.06490400
H	6.72112200	0.69925200	1.26521800
Cl	-0.32936600	-0.62371000	2.57644500
Cl	0.30349100	1.53612300	-0.20115100
C	0.52823600	-1.41543400	-1.87763700
C	1.57619700	-1.65316200	-0.92403400
C	1.32640000	-2.45082800	0.19494800
C	0.01872400	-3.01672900	0.38454100
C	-0.98663900	-2.88212500	-0.60770900
C	-0.72420300	-2.06860800	-1.75499900
H	0.69224700	-0.70868300	-2.68844200
H	2.52133300	-1.11571900	-1.00249900
H	2.06736700	-2.50787900	0.98714100
H	-0.21426400	-3.52233400	1.31836100
H	-1.97609100	-3.30356200	-0.44670700
H	-1.50546900	-1.88716700	-2.48907300
Ru	-0.35889300	-0.89763700	0.05393900
C	-4.39770600	0.83120200	-0.85766800
C	-3.12073500	0.02699900	-0.98454500
C	-2.25125800	-0.04209100	0.04169100
C	-5.52709000	-0.14081700	-0.52158600
S	-4.06588600	1.91724800	0.68610300
C	-2.63983600	0.73854600	1.25195000
O	-6.19036900	-0.68501700	-1.37473900
O	-5.62011100	-0.38174600	0.78672500
C	-6.55679500	-1.39814500	1.16558400
C	-2.99370800	3.25949500	-0.02407400
H	-2.98750900	-0.45689100	-1.95304900
H	-1.85317900	1.40096400	1.62533400
H	-3.05855800	0.14156600	2.06649600
C	-4.73039400	1.66021300	-2.08188400
H	-2.14855500	2.79421300	-0.54635700
H	-3.60921900	3.88348500	-0.67438200
H	-2.64046700	3.83574500	0.83417100
H	-6.27886300	-2.35314400	0.70857600
H	-6.50294700	-1.46430400	2.25312200
H	-7.56645400	-1.12215900	0.84566800
H	-3.86144400	2.24312600	-2.40528300
H	-4.99537600	0.96842700	-2.88923700
H	-5.58667300	2.32549700	-1.91671900

4.12 TSso6 bimolecular

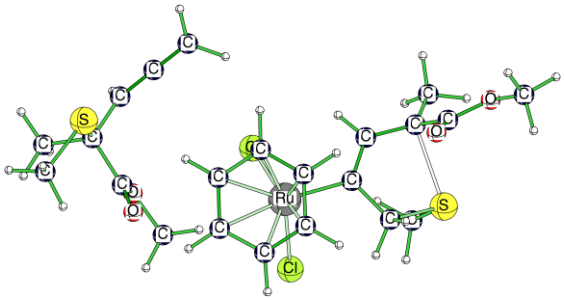
ENERGY=-1300.49902 LOWEST
FREQUENCY=-278.43



C	-4.95166100	0.91157300	-0.68461800
C	-4.18845500	2.04390000	-1.34315600
C	-3.26509600	2.77636500	-0.76063400
C	-4.13417500	-0.38361700	-0.81535300
S	-5.18306100	1.37844000	1.13097900
C	-2.32660000	3.50290200	-0.20056000
O	-3.82912200	-1.12632500	0.09462200
O	-3.83663700	-0.60902900	-2.09116900
C	-3.00975400	-1.75571000	-2.34339900
C	-6.24653700	-0.01743100	1.75109100
H	-4.39413700	2.19473400	-2.40606500
H	-2.55027100	4.44778000	0.29375900
H	-1.29597300	3.14182600	-0.22849000
C	-6.29756500	0.72069500	-1.38315800
H	-5.76112800	-0.97459200	1.54532900
H	-6.32802500	0.12967000	2.83154400
H	-7.24609500	0.02319900	1.30866400
H	-3.47833900	-2.65894700	-1.93746300
H	-2.92400200	-1.82346100	-3.42977400
H	-2.01866600	-1.61273300	-1.89366200
H	-6.90817700	1.62347700	-1.26387700
H	-6.13728200	0.54097400	-2.45384800
H	-6.85065600	-0.13589800	-0.97883200
Cl	0.49730300	-2.69265500	-1.03756100
Cl	-0.54900700	0.62861800	-1.26192100
C	-1.48940500	-0.18104900	1.85722500
C	-1.45294500	-1.58115100	1.85787500
C	-0.21810500	-2.23904200	2.15445800
C	0.91509400	-1.51161300	2.60759100
C	0.85997100	-0.08201300	2.61382200
C	-0.32380700	0.58426700	2.20338800
H	-2.38585800	0.32486900	1.49443000
H	-2.30348100	-2.13399500	1.47073200
H	-0.13736300	-3.31497600	2.01890500
H	1.83700300	-2.03301600	2.85332800
H	1.75735800	0.49447400	2.83370100
H	-0.34442400	1.66836500	2.12761200
Ru	0.34096400	-0.77781300	0.59934000
C	3.93436400	1.27334000	-0.77951000
C	2.56970600	0.92359500	-0.56461300
C	2.18310600	-0.26622800	-0.00071900
C	4.82865100	1.40173100	0.44047200
S	4.71435700	-0.97202700	-1.01463500
C	3.24360900	-1.33121800	0.13279200
O	4.51544400	1.05522000	1.56001600
O	6.00271200	1.95193200	0.12723000
C	6.92183900	2.09240700	1.21448800
C	3.84400300	-1.35900000	-2.60652800
H	1.80661900	1.53771800	-1.05421800
H	2.84670600	-2.30761000	-0.16962500
H	3.66056800	-1.38323100	1.14629300
C	4.28638100	2.10681100	-1.97171000
H	3.67427300	-2.43749800	-2.64887700
H	2.87749800	-0.83661200	-2.60418400
H	4.48433400	-1.02895000	-3.42683500
H	7.18720100	1.10851800	1.61599200
H	7.80334800	2.58503600	0.80059500
H	6.48074800	2.69841700	2.01229200
H	3.63917300	1.85921900	-2.81974800
H	4.13303000	3.16710300	-1.72436200
H	5.33695000	1.99447200	-2.25564900

4.13 TSso6 bimolecular

ENERGY=-1300.49902 LOWEST
FREQUENCY=-278.43



C	-4.95166100	0.91157300	-0.68461800
C	-4.18845500	2.04390000	-1.34315600
C	-3.26509600	2.77636500	-0.76063400
C	-4.13417500	-0.38361700	-0.81535300
S	-5.18306100	1.37844000	1.13097900
C	-2.32660000	3.50290200	-0.20056000
O	-3.82912200	-1.12632500	0.09462200
O	-3.83663700	-0.60902900	-2.09116900
C	-3.00975400	-1.75571000	-2.34339900
C	-6.24653700	-0.01743100	1.75109100
H	-4.39413700	2.19473400	-2.40606500
H	-2.55027100	4.44778000	0.29375900
H	-1.29597300	3.14182600	-0.22849000
C	-6.29756500	0.72069500	-1.38315800
H	-5.76112800	-0.97459200	1.54532900
H	-6.32802500	0.12967000	2.83154400
H	-7.24609500	0.02319900	1.30866400
H	-3.47833900	-2.65894700	-1.93746300
H	-2.92400200	-1.82346100	-3.42977400
H	-2.01866600	-1.61273300	-1.89366200
H	-6.90817700	1.62347700	-1.26387700
H	-6.13728200	0.54097400	-2.45384800
H	-6.85065600	-0.13589800	-0.97883200
Cl	0.49730300	-2.69265500	-1.03756100
Cl	-0.54900700	0.62861800	-1.26192100
C	-1.48940500	-0.18104900	1.85722500
C	-1.45294500	-1.58115100	1.85787500
C	-0.21810500	-2.23904200	2.15445800
C	0.91509400	-1.51161300	2.60759100
C	0.85997100	-0.08201300	2.61382200
C	-0.32380700	0.58426700	2.20338800
H	-2.38585800	0.32486900	1.49443000

H	-2.30348100	-2.13399500	1.47073200
H	-0.13736300	-3.31497600	2.01890500
H	1.83700300	-2.03301600	2.85332800
H	1.75735800	0.49447400	2.83370100
H	-0.34442400	1.66836500	2.12761200
Ru	0.34096400	-0.77781300	0.59934000
C	3.93436400	1.27334000	-0.77951000
C	2.56970600	0.92359500	-0.56461300
C	2.18310600	-0.26622800	-0.00071900
C	4.82865100	1.40173100	0.44047200
S	4.71435700	-0.97202700	-1.01463500
C	3.24360900	-1.33121800	0.13279200
O	4.51544400	1.05522000	1.56001600
O	6.00271200	1.95193200	0.12723000
C	6.92183900	2.09240700	1.21448800
C	3.84400300	-1.35900000	-2.60652800
H	1.80661900	1.53771800	-1.05421800
H	2.84670600	-2.30761000	-0.16962500
H	3.66056800	-1.38323100	1.14629300
C	4.28638100	2.10681100	-1.97171000
H	3.67427300	-2.43749800	-2.64887700
H	2.87749800	-0.83661200	-2.60418400
H	4.48433400	-1.02895000	-3.42683500
H	7.18720100	1.10851800	1.61599200
H	7.80334800	2.58503600	0.80059500
H	6.48074800	2.69841700	2.01229200
H	3.63917300	1.85921900	-2.81974800
H	4.13303000	3.16710300	-1.72436200
H	5.33695000	1.99447200	-2.25564900