MATERIAL SUPLEMENTARIO

"Reacciones de isomerización de alcoholes alílicos y formación de enlaces carbono-carbono en agua promovidas por catalizadores bifuncionales de rutenio(IV)"

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MATERIAL SUPLEMENTARIO

CAPÍTULO 1

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	1.2a	**1.2b**	**1.2c**	**1.2e**	**1.2f**	**1.2g**	**1.2i**	**1.2j**	**1.2k**	**1.2l**
Chem formula	$C_{13}H_{20}Cl_2N_2Ru$	$C_{14}H_{22}Cl_2N_2Ru$	$C_{15}H_{24}Cl_2N_2Ru$	$C_{19}H_{24}Cl_2N_2ORu$	$C_{17}H_{22}Cl_2N_2Ru$	$C_{13}H_{19}Cl_2N_3O_2Ru$	$C_{19}H_{23}ClN_2ORu$	$C_{13}H_{20}Cl_2N_2Ru$	$C_{17}H_{22}Cl_2N_2Ru$	$C_{14}H_{22}Cl_2N_2Ru$
fw	376.28	390.31	404.33	486.37	426.34	421.28	431.91	376.28	426.34	390.31
T (K)	293(2)	293(2)	293(2)	293(2)	200(2)	293(2)	293(2)	293(2)	293(2)	293(2)
wavelength (Å)	1.5418	1.5418	1.5418	0.7107	1.5418	1.5418	1.5418	0.71073	1.54184	0.71073
space group	Fdd2	$Pna2_1$	$P2_1/c$	$P2_1/c$	Cc	$P2_1/c$	Pbca	Cc	Pbca	$P2_1/c$
a, Å	33.2559(8)	7.6952(1)	9.1513(1)	16.2255(8)	13.4322(4)	12.3933(7)	8.8541(1)	12.1026(5)	14.9645(1)	16.9808(3)
b, Å	24.4116(6)	22.8324(3)	22.9768(2)	8.3163(4)	11.8175(3)	8.5805(4)	13.8896(1)	11.1887(5)	14.1657(1)	8.2512(1)
c, Å	11.1014(2)	9.0117(1)	7.8822(1)	14.5735(4)	12.9173(4)	15.8735(10)	29.3729(2)	11.2215(3)	15.9196(1)	27.3173(5)
α, deg	90	90	90	90	90	90	90	90	90	90
β, deg	90	90	93.313(1)	91.335(3)	120.241(2)	95.632(3)	90	93.417(2)	90	122.317(1)
γ, deg	90	90	90	90	90	90	90	90	90	90
Z	24	4	4	4	4	4	8	4	8	8
V, Å^3	9012.4(3)	1583.35(3)	1654.60(3)	1965.96(15)	1771.39(9)	1679.85(16)	3612.28(5)	1516.83(10)	3374.68	3234.61(9)
ρ_{calcd}, gcm^{-3}	1.664	1.637	1.623	1.582	1.599	1.666	1.588	1.648	1.678	1.603
μ, mm^{-1}	11.586	11.014	10.562	1.079	9.906	1.258	8.441	1.371	10.399	1.289
goodness of fit on F^2	1.019	1.083	1.067	0.866	1.094	0.956	1.035	1.245	1.035	0.971
weight function (a,b)	0.0195,8.5210	0.0689,0.0	0.0691,0.0677	0.0474,0.0	0.0809,5.4383	0.0541,0.0	0.0355,1.3321	0.0616,0.0	0.0337,1.7322	0.0619,0.0
R1[a] ($I > 2\sigma(I)$)	0.0426	0.0329	0.0347	0.0375	0.0414	0.0336	0.0235	0.0319	0.0208	0.0333
wR2[a] ($I > 2\sigma(I)$)	0.1151	0.0904	0.0920	0.1009	0.1132	0.0922	0.0613	0.0971	0.0550	0.0900
R1[a] (all data)	0.0443	0.0343	0.0386	0.0645	0.0415	0.0494	0.0255	0.0356	0.0218	0.0552
wR2[a] (all data)	0.1169	0.0915	0.0949	0.1068	0.1134	0.1119	0.0629	0.1101	0.0556	0.1280
F(0)	4560	792	824	952	864	848	1760	760	1728	1584

[a] $R1 = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|$; $wR2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/ \Sigma[w(F_o^2)^2]\}^{1/2}$.

Figura S1.1. Espectros del complejo **1.2a**.

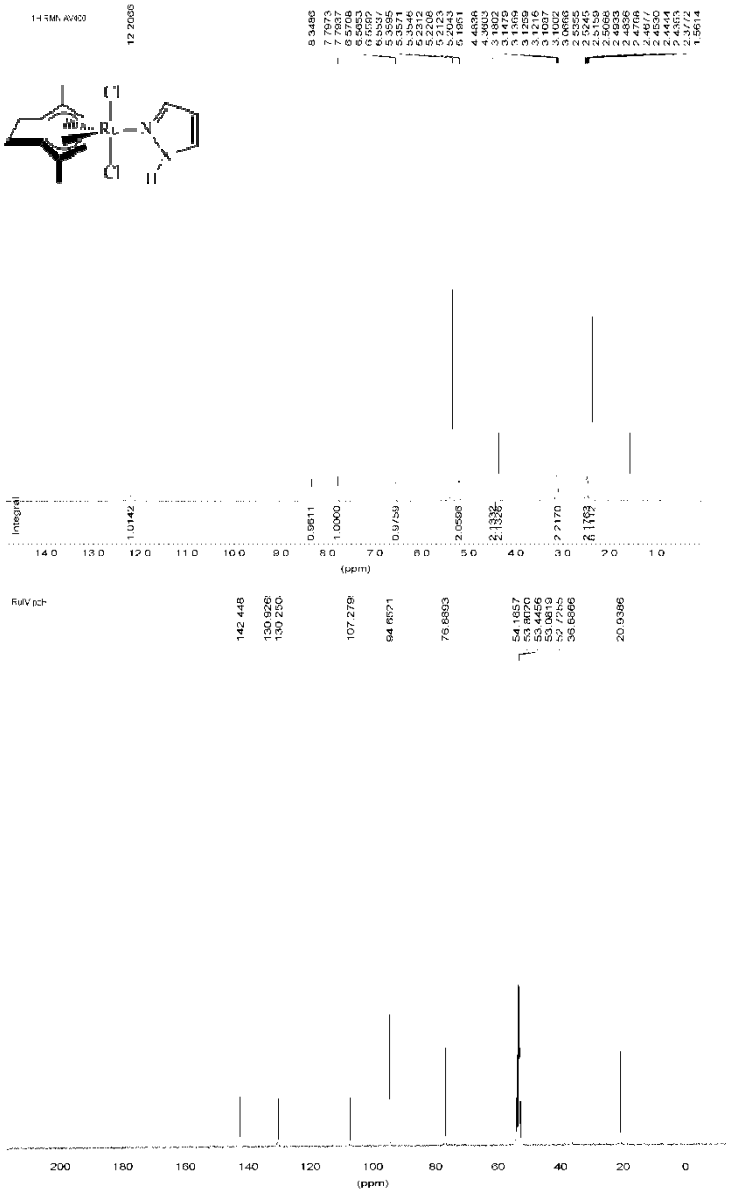


Figura S1.2. Espectros del complejo **1.2b**.

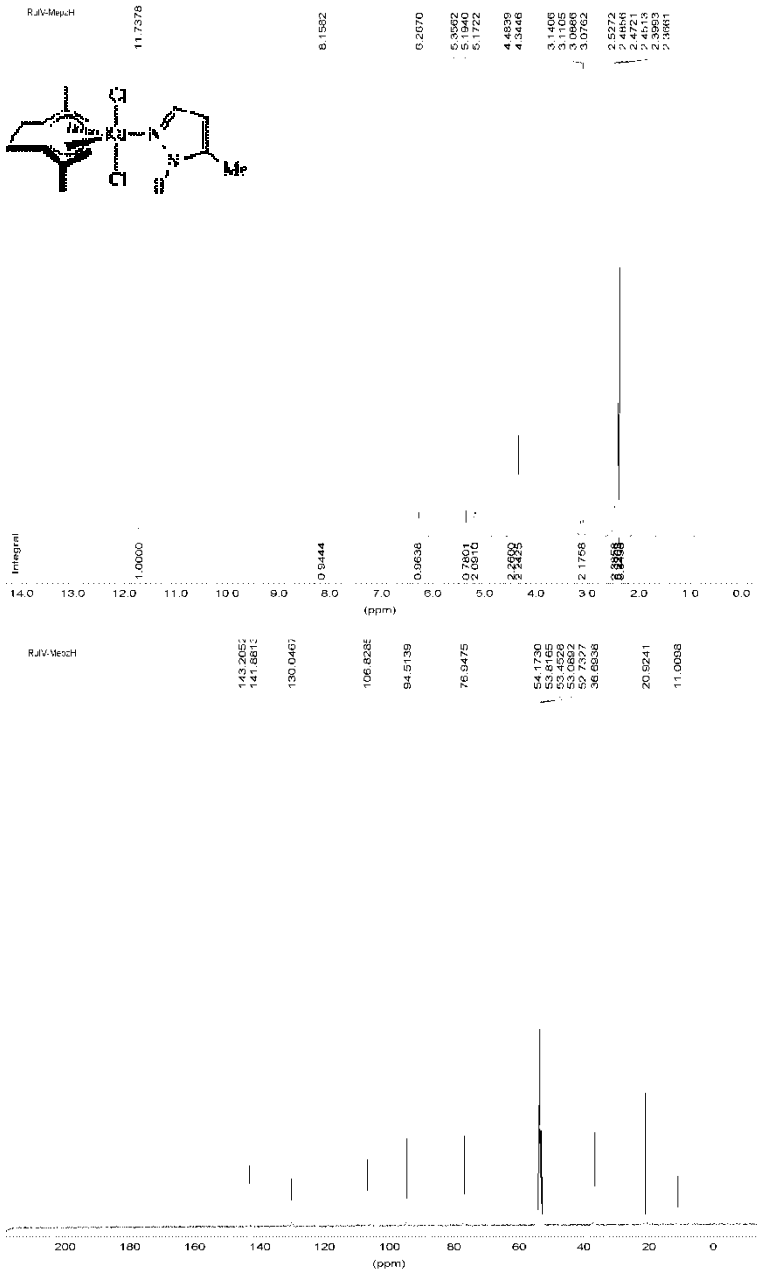


Figura S1.3. Espectros del complejo **1.2c**.

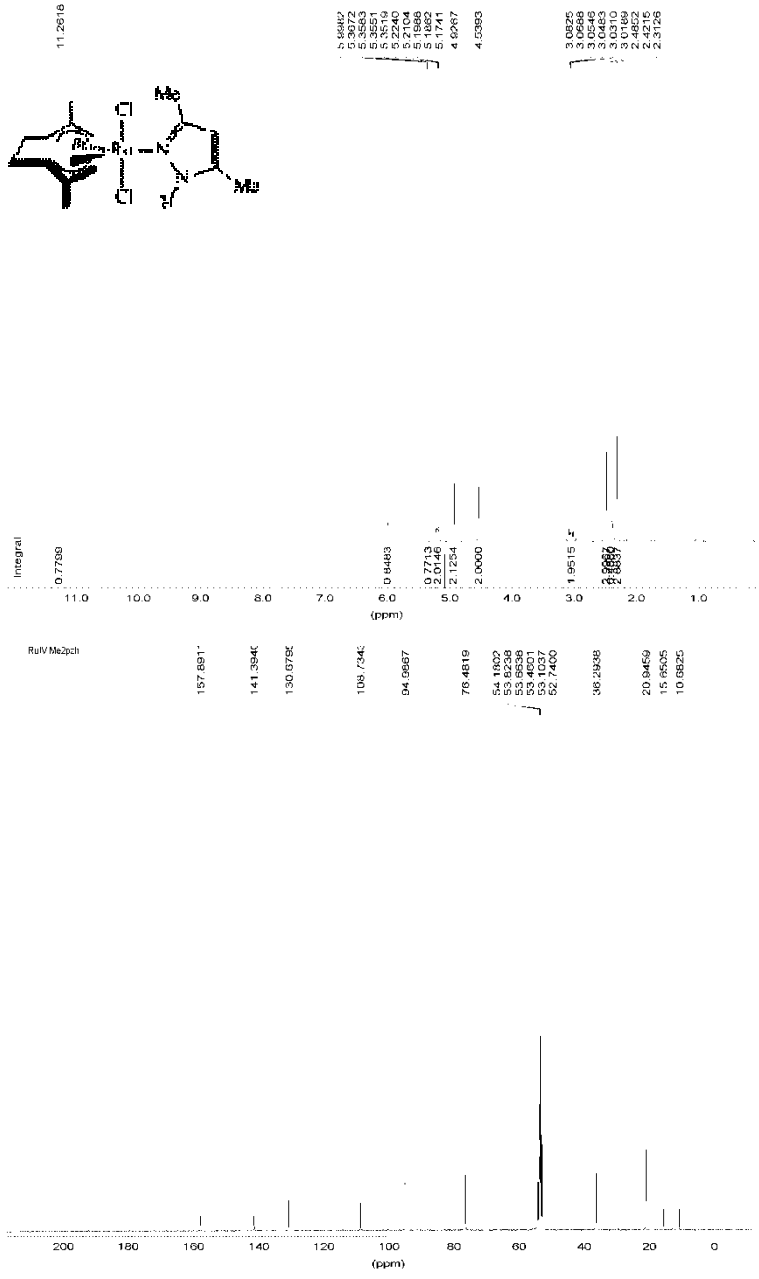


Figura S1.4. Espectros del complejo **1.2d**.

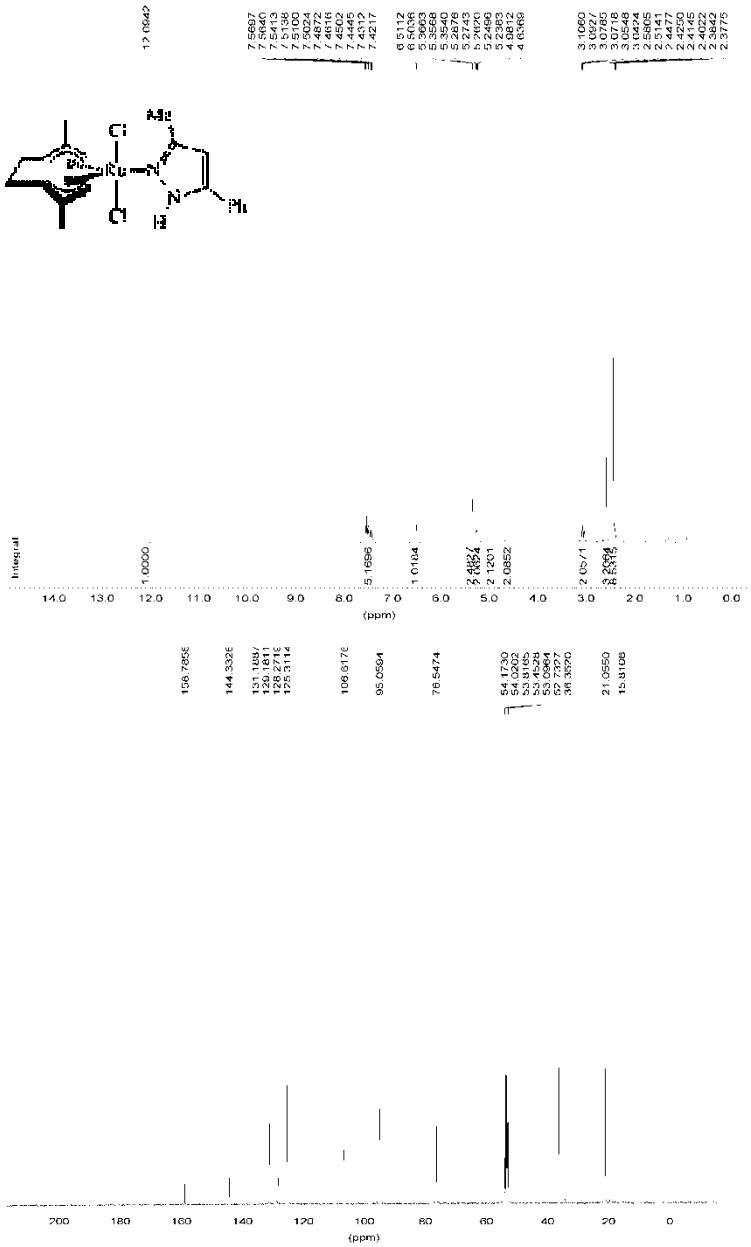


Figura S1.5. Espectros del complejo **1.2e**.

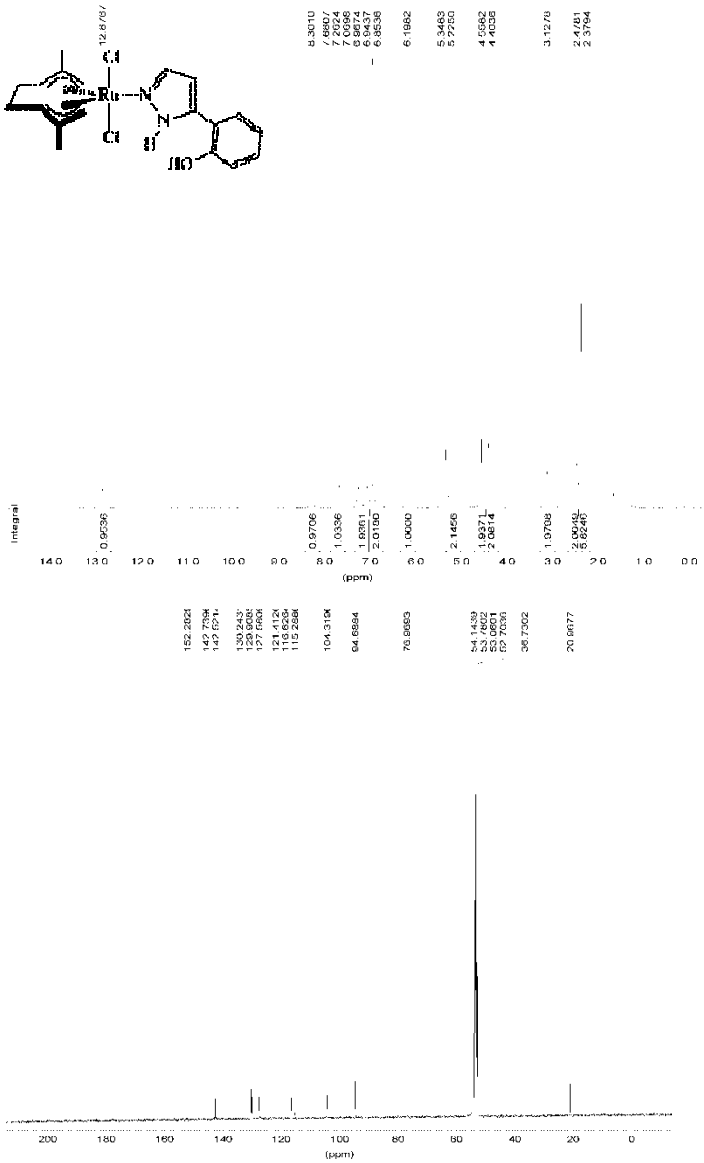


Figura S1.6. Espectros del complejo **1.2f**.

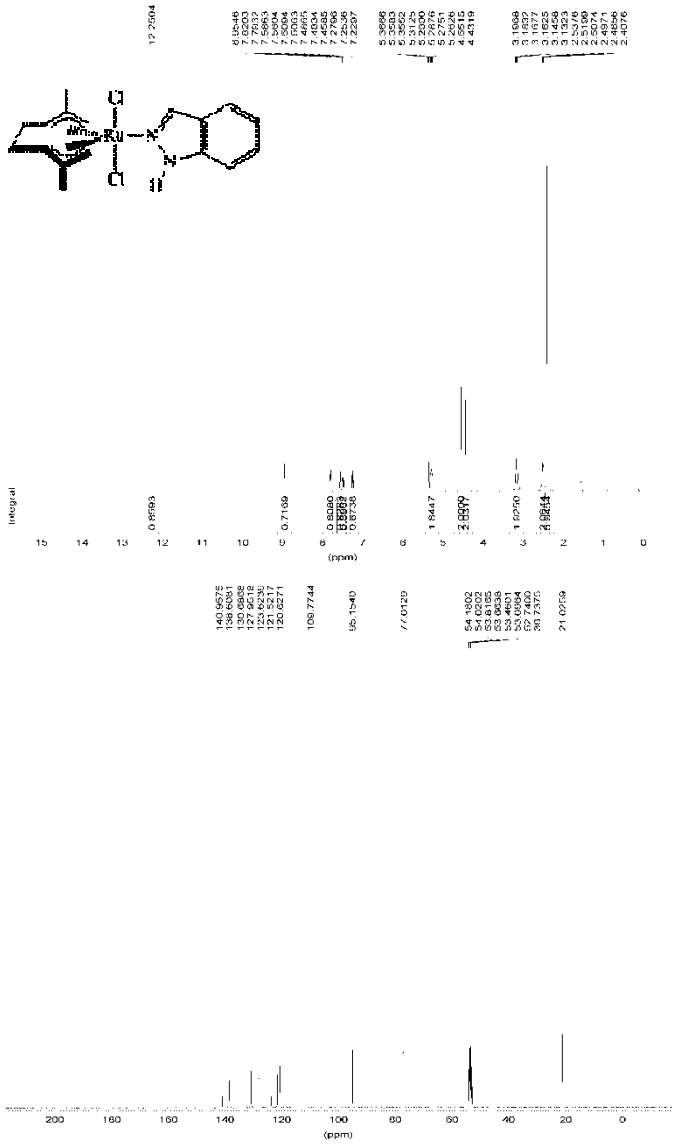


Figura S1.7. Espectros del complejo **1.2g**.

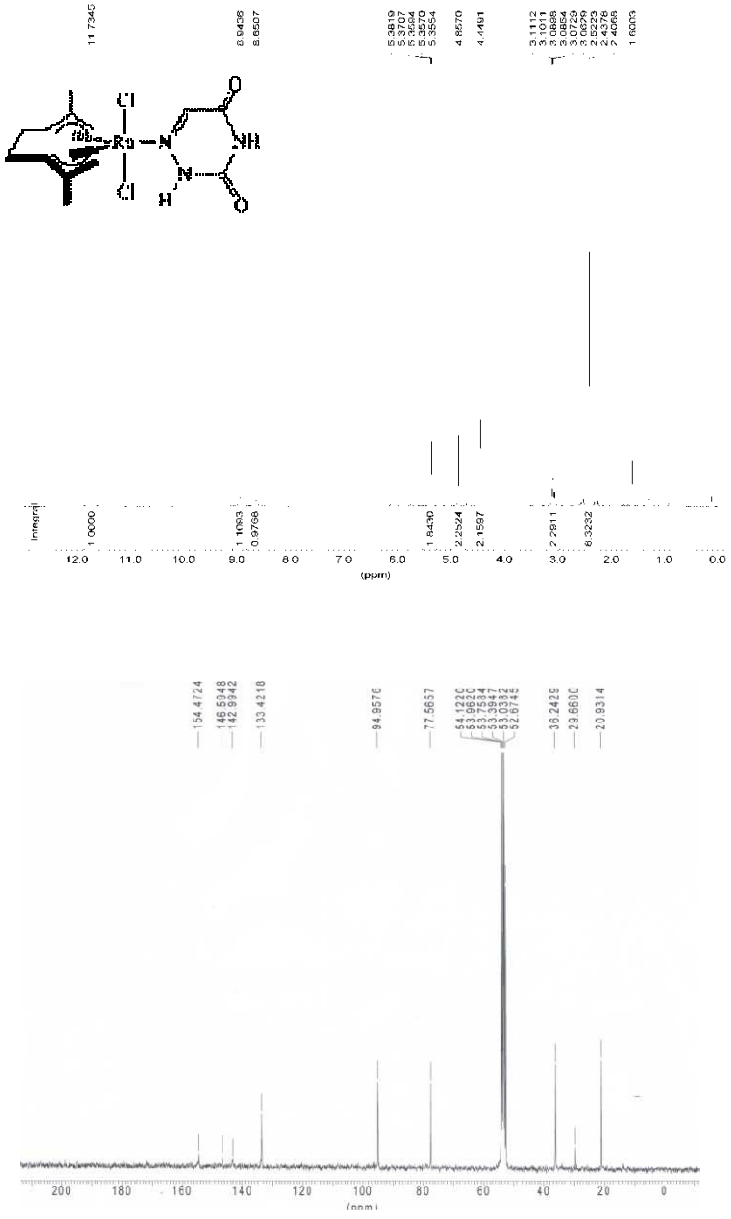


Figura S1.8. Espectros del complejo **1.2h**.

Figura S1.9. Espectros del complejo **1.2i**.

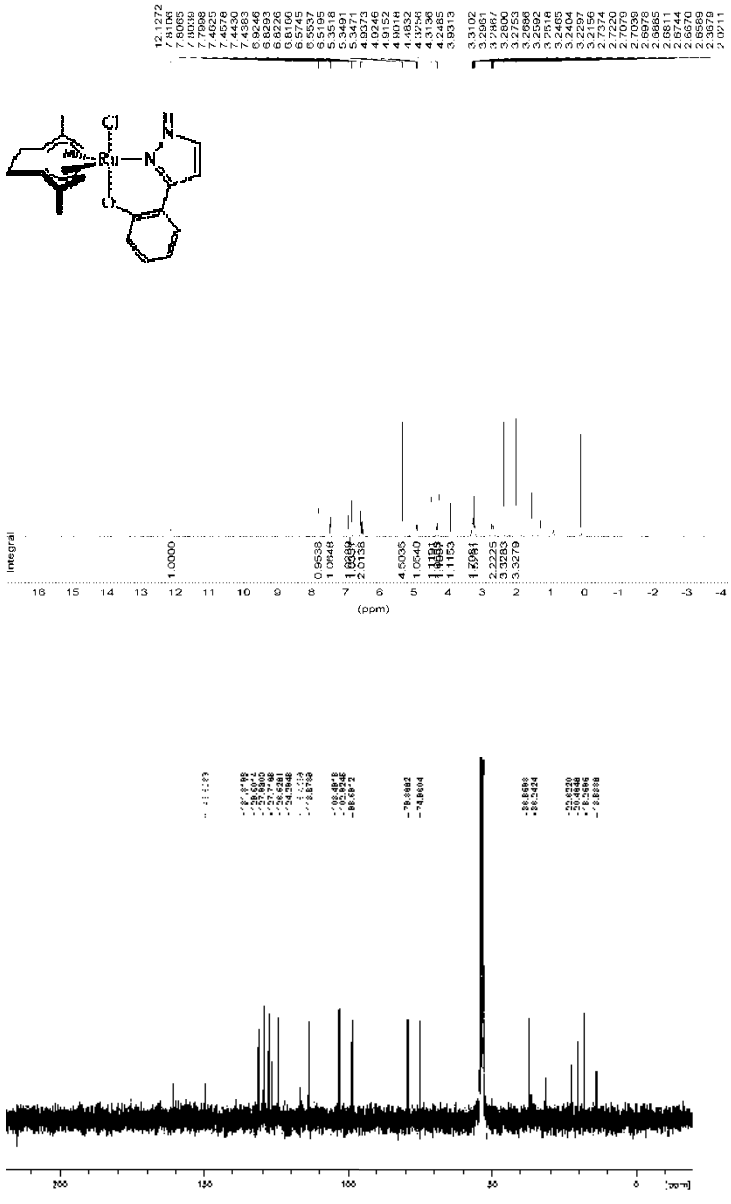


Figura S1.10. Espectros del complejo **1.2j**.

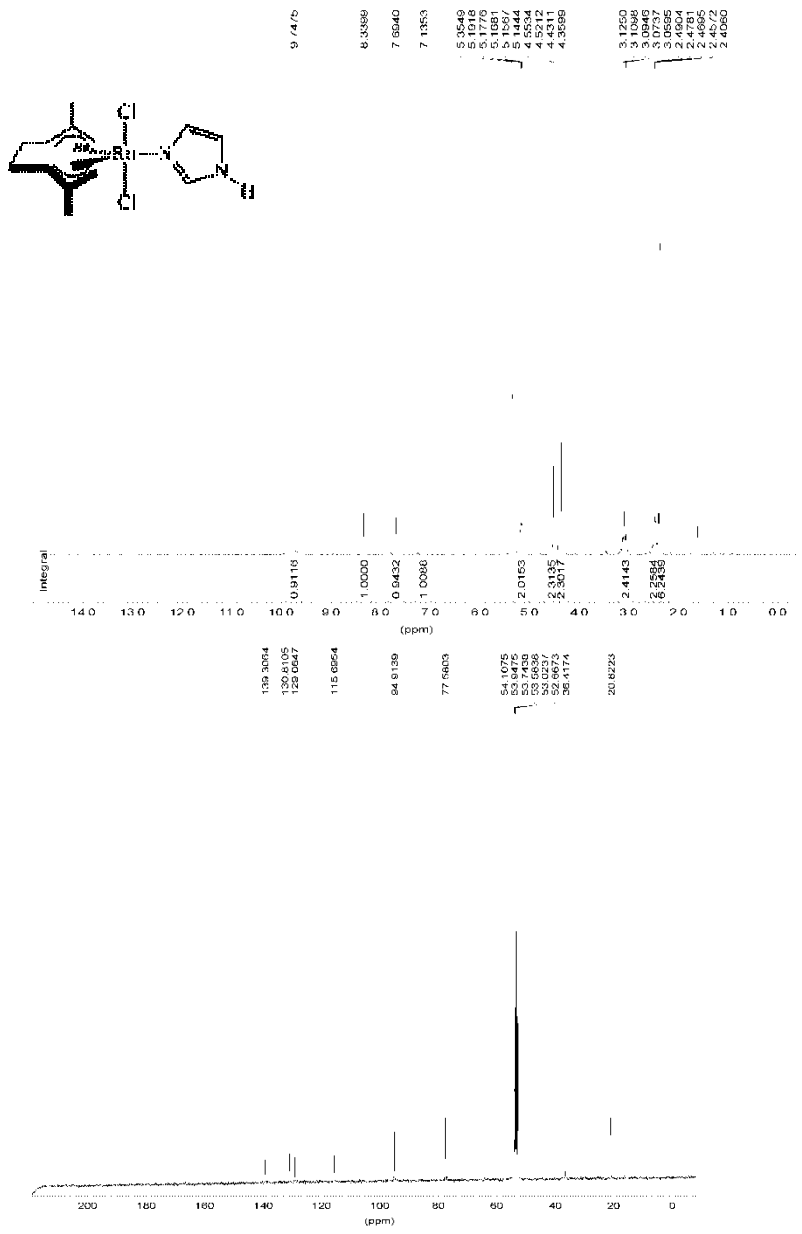


Figura S1.11. Espectros del complejo **1.2k**.

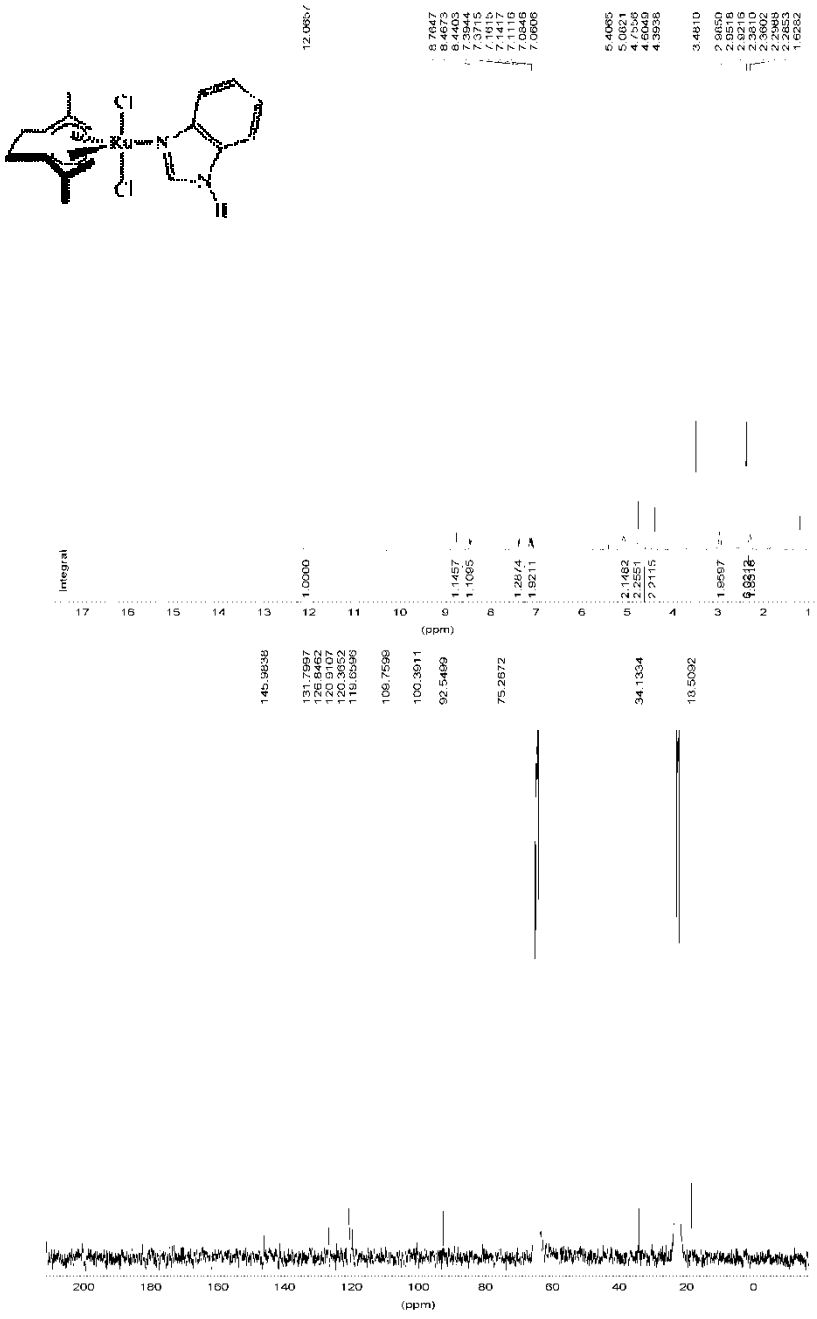
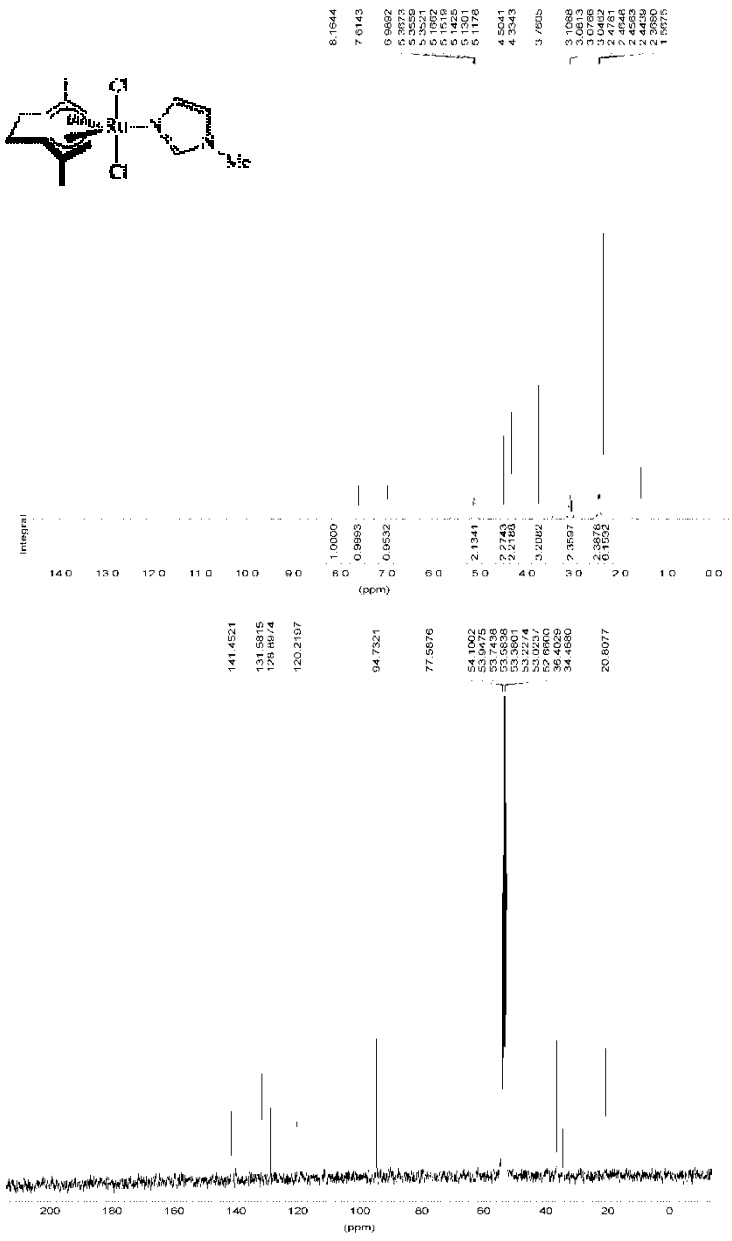


Figura S1.12. Espectros del complejo **1.2l**.



ESTRUCTURAS OPTIMIZADAS DE 1.2h Y 1.2h'

Estructura optimizada de 1.2h

E(gas) = -1860.09898787
$E(CH_2Cl_2)$ = -1860.415148;
$G(CH_2Cl_2)$ = -1860.10216513

C	-4.059091	-0.804589	0.032441
C	-3.604602	-0.159481	1.368063
H	-4.269306	-1.869487	0.160329
H	-3.061981	-0.890817	1.968849
H	-4.984388	-0.337534	-0.326057
H	-4.453006	0.211182	1.962882
C	-2.943665	-0.537081	-0.982904
C	-2.708118	0.984605	0.932065
C	-1.586023	1.634973	1.556517
H	-3.244151	1.674425	0.278514
C	-1.398867	3.127077	1.402310
C	-0.573149	0.870027	2.118678
C	-2.021012	-1.516177	-1.462012
H	-3.091864	0.328717	-1.624534
C	-2.183345	-2.995510	-1.229686
C	-0.856753	-1.013710	-2.077404
H	-2.7846	-3.374965	-2.069640
H	-1.222237	-3.512433	-1.240850
H	-2.693864	-3.244048	-0.300664
H	-0.342677	3.394696	1.301055
H	-1.941036	3.529182	0.545864
H	-1.782667	3.607469	2.313149
H	-0.029140	-1.699476	-2.240715
H	-0.877345	-0.133036	-2.708725
H	0.375582	1.348993	2.348285
H	-0.745807	-0.094256	2.574860
Ru	-0.963327	0.052450	-0.085711
Cl	-1.033335	2.054898	-1.582508
Cl	-0.751029	-2.071206	1.296489
C	3.280993	-0.880791	0.216708
C	3.478402	0.455155	-0.203678
C	4.773426	0.988787	-0.316481
C	5.842426	0.171494	0.011516
C	5.633250	-1.161817	0.443096
C	4.365403	-1.711813	0.549502
C	2.159587	0.965084	-0.421509
H	4.921198	2.011762	-0.648242
H	6.857175	0.551145	-0.061364
H	6.495285	-1.772926	0.696904
H	4.215655	-2.736123	0.876546
N	1.251692	0.030686	-0.156049
N	1.938951	-1.119564	0.178470
H	1.386803	-1.819835	0.670856
O	1.890947	2.205907	-0.816887
H	0.937727	2.274294	-1.088872

Estructura optimizada de 1.2h'

E(gas) = -1860.07571716
$E(CH_2Cl_2)$ = -1860.393524;
$G(CH_2Cl_2)$ = -1860.08196284

C	-4.065642	0.212406	-1.033436
C	-3.532274	1.530526	-0.427468
H	-4.865048	-0.213744	-0.420603
H	-3.573840	1.475061	0.663300
H	-4.483542	0.389042	-2.031403
H	-4.122011	2.406184	-0.739084
C	-2.858206	-0.707668	-1.159494
C	-2.097915	1.645184	-0.911424
C	-0.993707	2.287541	-0.251651
H	-2.014251	1.643280	-1.998373
C	0.091612	2.985506	-1.035130
C	-0.897469	2.106229	1.116688
C	-2.533708	-1.763536	-0.272926
H	-2.394278	-0.7403	-2.142784
C	-3.486551	-2.272296	0.776885
C	-1.202644	-2.249888	-0.383389
H	-4.170465	-2.969464	0.269786
H	-2.964206	-2.812785	1.565626
H	-4.083164	-1.486681	1.242390
H	1.032425	3.001248	-0.477066
H	0.263367	2.516158	-2.005432
H	-0.215068	4.027089	-1.201608
H	-0.842585	-2.917052	0.396500
H	-0.751741	-2.370694	-1.363651
H	0.019802	2.339543	1.646854
H	-1.760386	1.892416	1.729838
Ru	-0.995381	-0.064932	-0.022489
Cl	0.155032	-0.125184	-2.215793
Cl	-1.568195	-0.515483	2.394198
C	3.168336	-0.989929	-0.094124
C	3.401738	0.203376	0.590666
C	4.640970	0.850707	0.534662
C	5.635780	0.281211	-0.249949
C	5.384535	-0.909319	-0.962481
C	4.156673	-1.563192	-0.899970
C	2.178365	0.560856	1.296131
H	4.801013	1.771189	1.087800
H	6.611758	0.751314	-0.321304
H	6.175132	-1.333989	-1.575284
H	3.977707	-2.484070	-1.446115
N	1.194421	-0.460130	0.920398
H	0.760780	-0.857179	1.761823
N	1.878831	-1.482882	0.163896
H	1.353246	-1.621838	-0.701832
O	1.951720	1.462304	2.078206

MATERIAL SUPLEMENTARIO

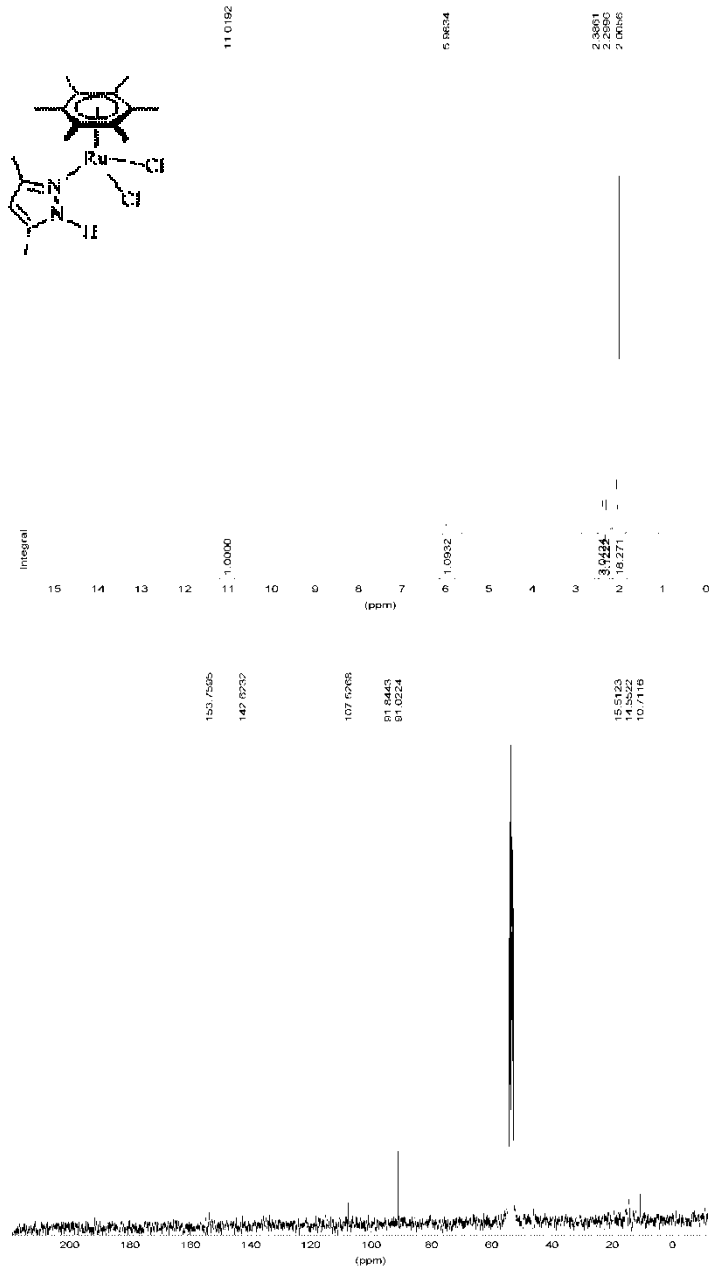
CAPÍTULO 2

Tabla S2.1. Datos cristalográficos para el compuesto **2.3a**.

	2.3a
Chem formula	$C_{17}H_{26}Cl_2N_2Ru$
fw	430.37
T (K)	293(2)
wavelength (Å)	0.71073
space group	C2/c
a, Å	13.5926(5)
b, Å	10.9068(5)
c, Å	25.1496(8)
α, deg	90
β, deg	90.842(2)
γ, deg	90
Z	8
V, Å^3	3728.1(2)
ρ_{calcd}, gcm^{-3}	1.534
μ, mm^{-1}	1.126
goodness of fit on F^2	1.141
weight function (*a*,*b*)	0.0670,0.0
R1[a] ($I > 2\sigma(I)$)	0.0339
wR2[a] ($I > 2\sigma(I)$)	0.0948
R1[a] (all data)	0.0485
wR2[a] (all data)	0.1250
F(0)	1760

[a] $R1 = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|$; $wR2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/ \Sigma[w(F_o^2)^2]\}^{1/2}$.

Figura S2.1. Espectros del complejo **2.3a**.



MATERIAL SUPLEMENTARIO

CAPÍTULO 3

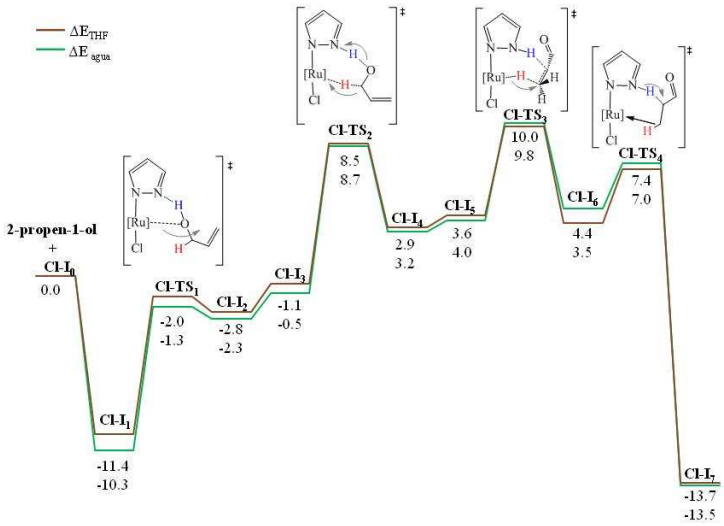


Figura S3.1. Perfil de energía en disolución ((ΔE_{sol}, sol=THF y agua) para la isomerización de 2-propen-1-ol a propanal tomando como especie active el complejo [Ru(η^3:η^3-$C_{10}H_{16}$)Cl(pirazolato)] (**Cl-I$_0$)** (*ruta cloruro*). Los valores están en kcal mol^{-1} y referidos a los reactivos separados. En cada paso el valor de la parte de arriba corresponde a THF y el de abajo a agua.

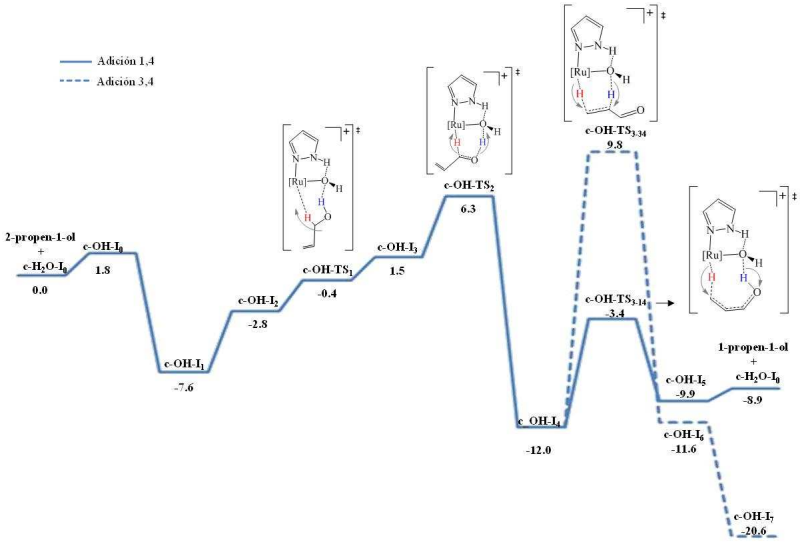
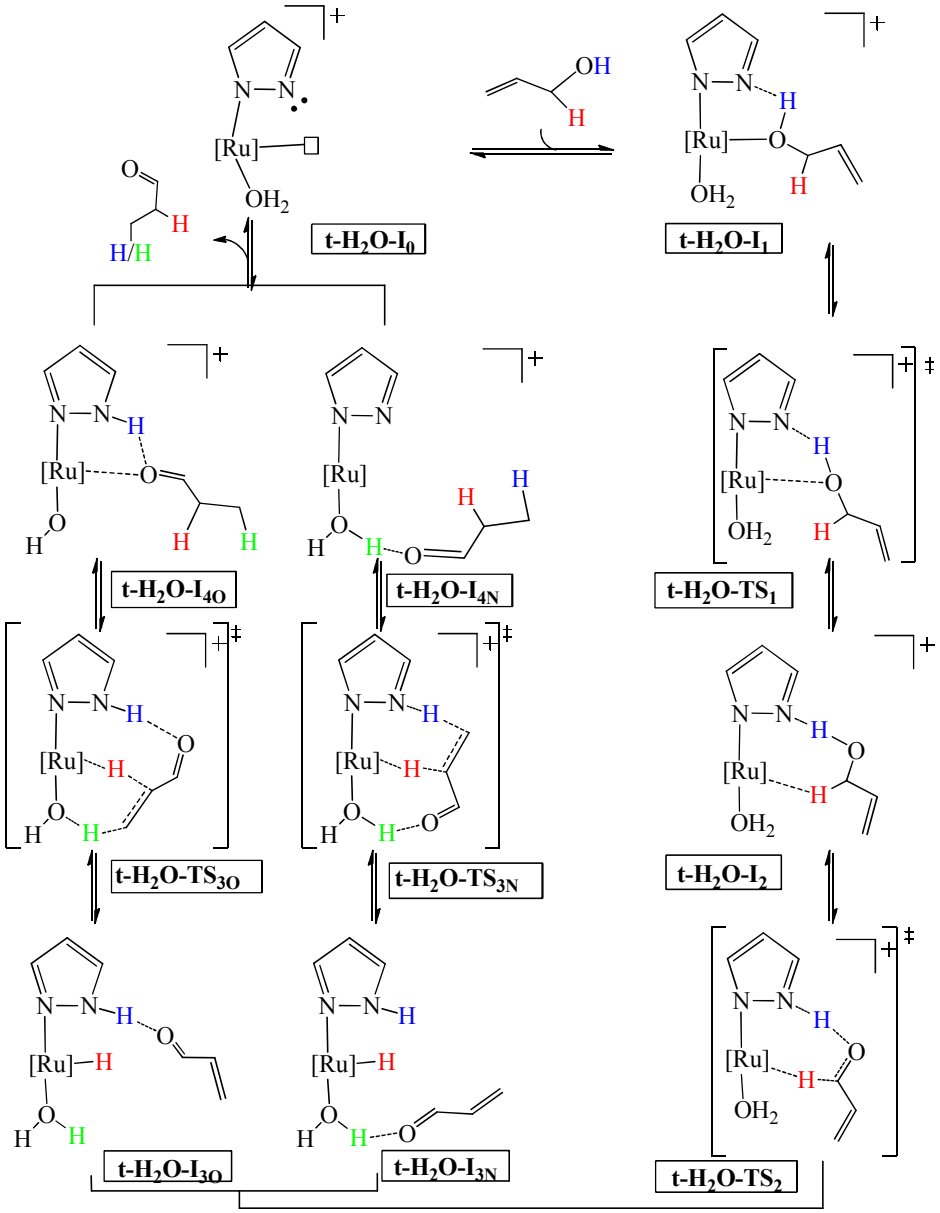
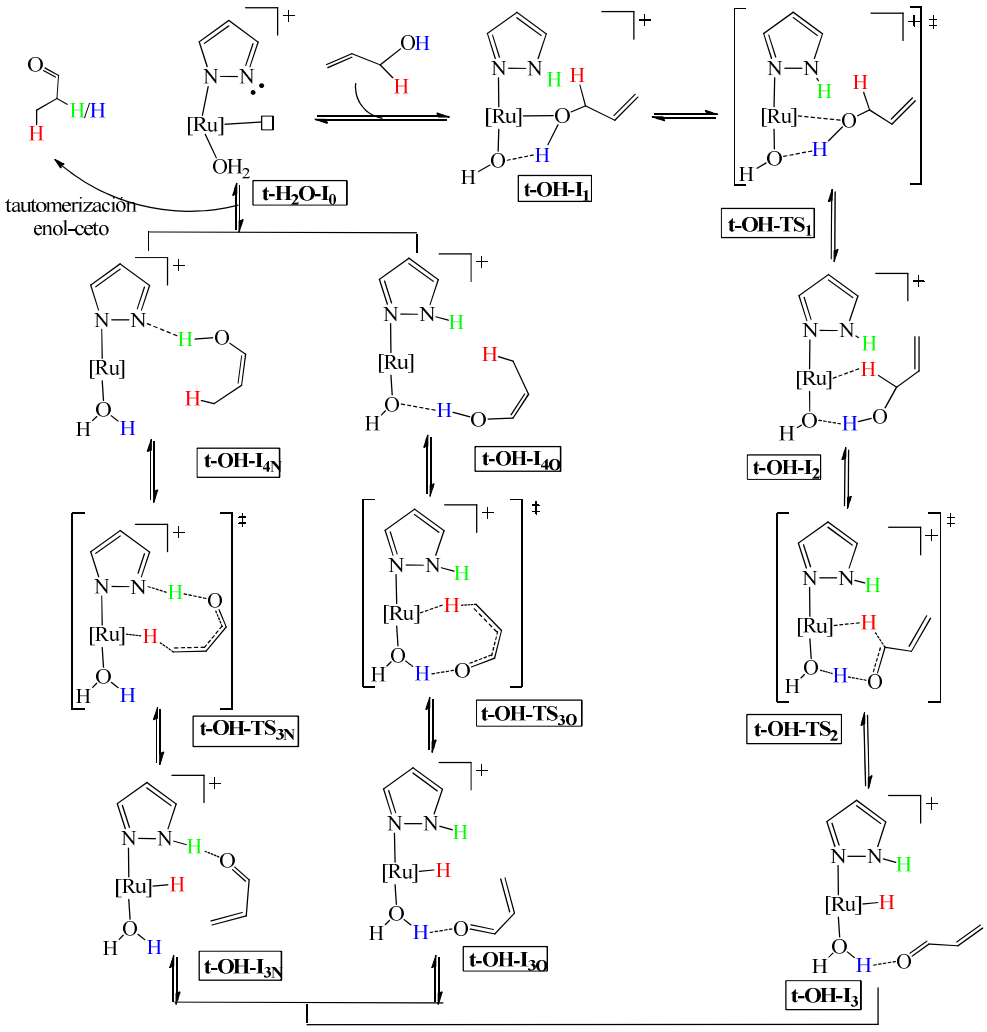


Figura S3.2. Perfil de energía en agua (ΔE_{H2O}) para la isomerización de 2-propen-1-ol a propanal tomando como especie active el complejo *cis*-[Ru(η^3:η^3-$C_{10}H_{16}$)(pirazol)(OH)]$^+$ (**c-OH-I$_0$)** (*ruta cis-hidroxo*). Los valores están en kcal mol^{-1} y referidos a los reactivos separados.



Esquema S3.1. Ciclo catalítico propuesto para la isomerización de 2-propen-1-ol a propanal en agua (*ruta trans-acuo).*



Esquema S3.2. Ciclo catalítico propuesto para la isomerización de 2-propen-1-ol a propanal en agua (*ruta trans-hidroxo)*.

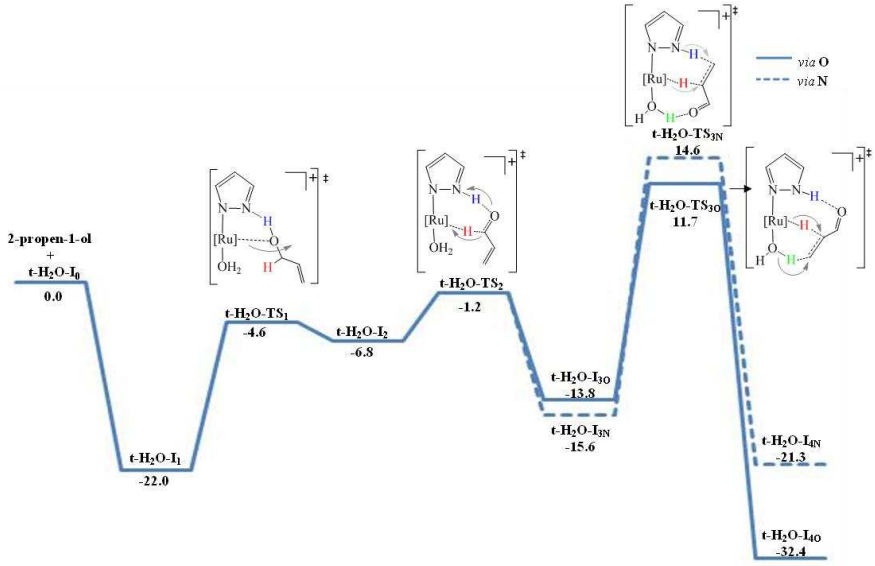


Figura S3.3. Perfil de energía en agua (ΔE_{H2O}) para la isomerización de 2-propen-1-ol a propanal tomando como especie active el complejo *trans*-[Ru(η^3:η^3-$C_{10}H_{16}$)(pirazolato)(H_2O)]$^+$ (**t-H_2O-I_0)** (*ruta trans-acuo*). Los valores están en kcal mol^{-1} y referidos a los reactivos separados.

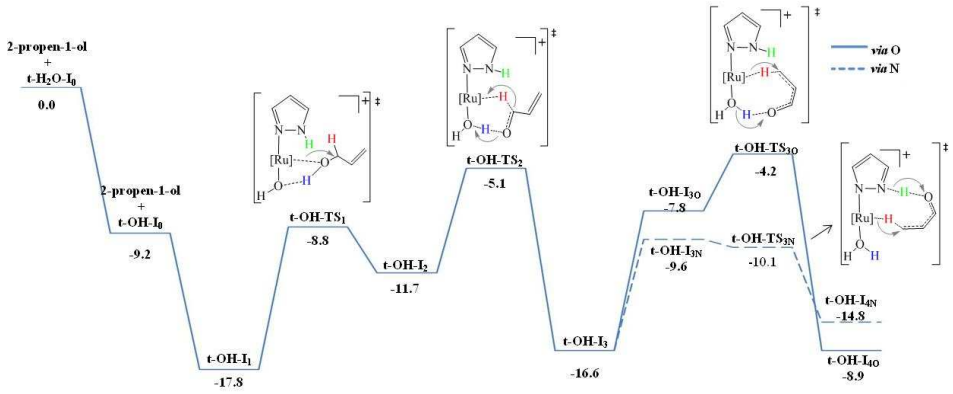
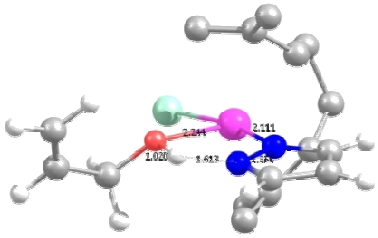
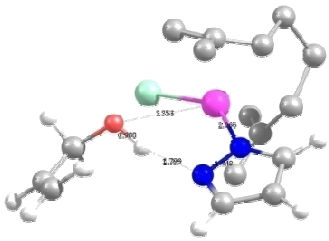


Figura S3.4. Perfil de energía en agua (ΔE_{H2O}) para la isomerización de 2-propen-1-ol a propanal tomando como especie active el complejo *trans*-[Ru(η^3:η^3-$C_{10}H_{16}$)(pirazol)(OH)]$^+$ (**t-OH-I_0)** (*ruta trans-hidroxo*). Los valores están en kcal mol^{-1} y referidos a los reactivos separados.

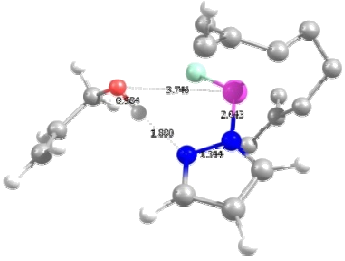
Figura S3.5. Estructuras relevantes en la *ruta cloruro.*



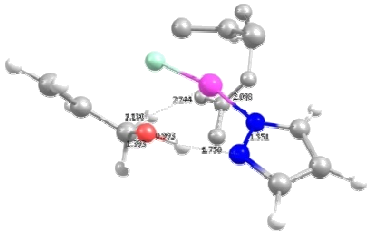
Cl-I$_1$



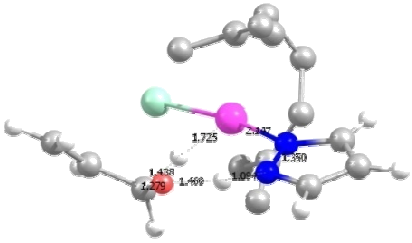
Cl-TS$_1$



Cl-I$_2$



Cl-I$_3$



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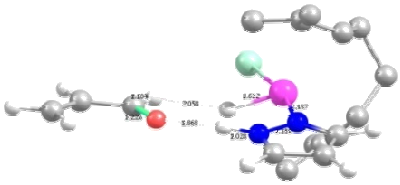
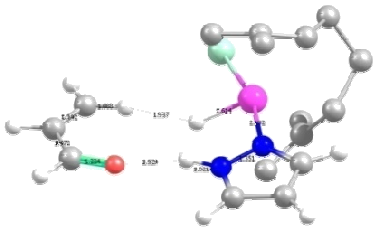
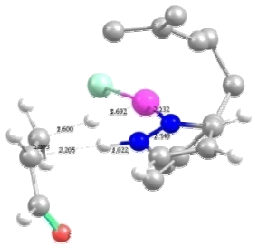


Cl-I$_4$



Cl-I$_5$



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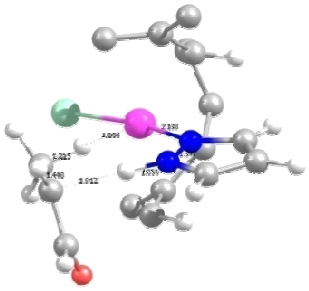
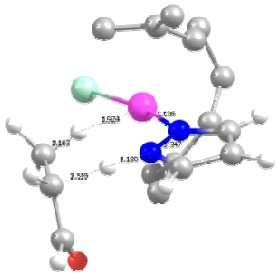
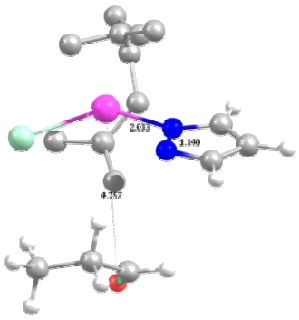


Cl-I$_6$



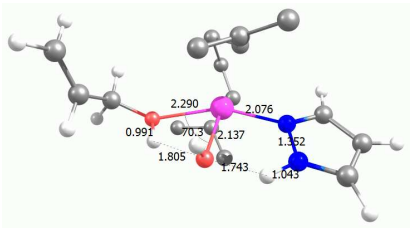
Cl-TS$_4$



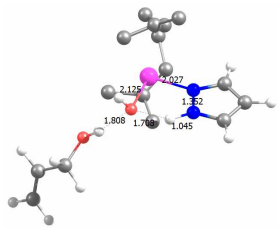
Cl-I$_7$

Figura S3.5. Geometrías optimizadas de los mínimos y estados de transición en la *ruta cloruro*. Los átomos de hidrógeno del ligandos bisalilo se han omitido para mayor claridad.

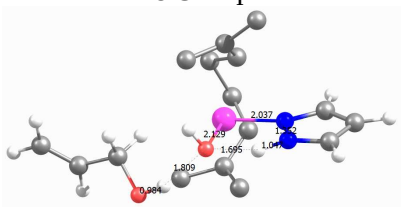
Figura S3.6. Estructuras relevantes en la *ruta cis-hidroxo.*



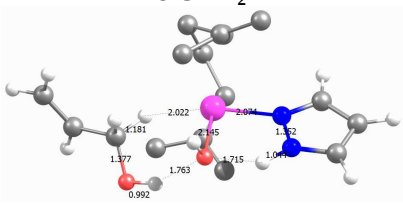
c-OH-I$_1$



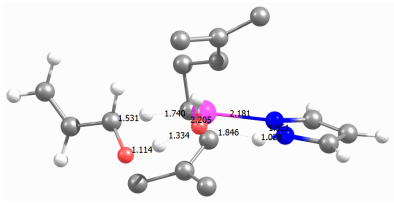
c-OH-I$_2$



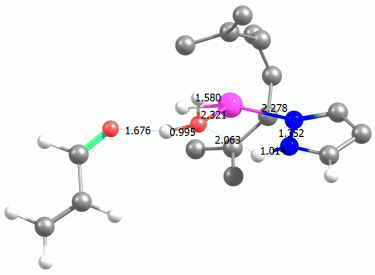
c-OH-TS$_1$



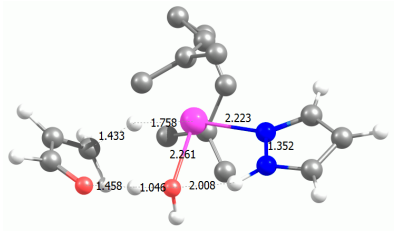
c-OH-I$_3$



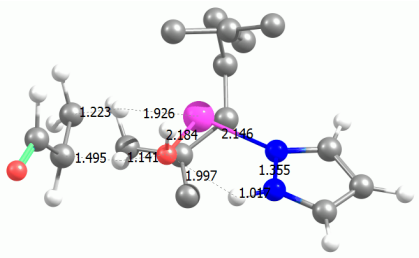
c-OH-TS$_2$



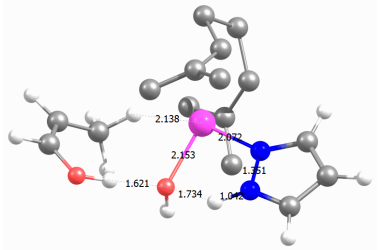
c-OH-I$_4$



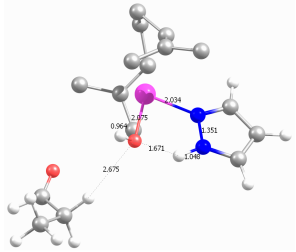
c-OH-TS$_{3\text{-}14}$ (adición 1,4)



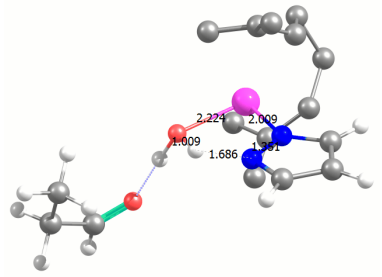
c-OH-TS$_{3\text{-}34}$ (adición 3,4)



c-OH-I$_5$



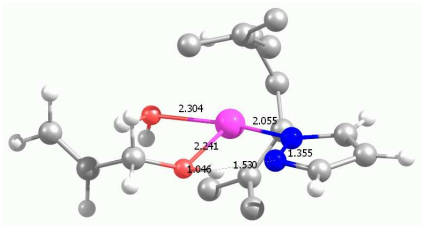
c-OH –I$_6$



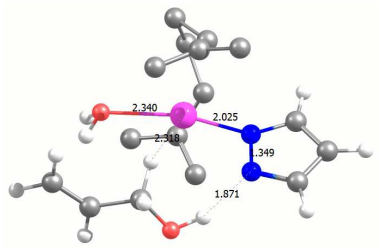
c-OH-I$_7$

Figura S3.6. Geometrías optimizadas de los mínimos y estados de transición en la *ruta cis-hidroxo*. Los átomos de hidrógeno del ligandos bisalilo se han omitido para mayor claridad.

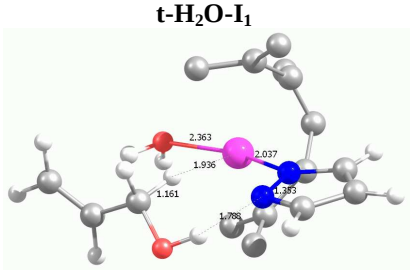
Figura S3.7. Estructuras relevantes en la *ruta trans-acuo*.



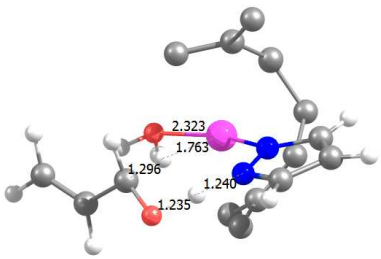
t-H_2O-I_1



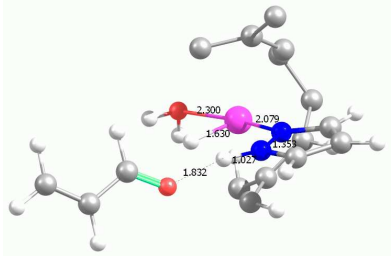
t-H_2O-TS_1



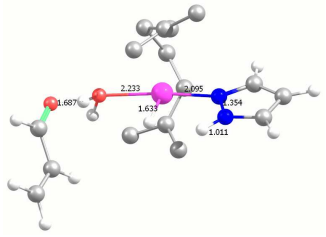
t-H_2O-I_2



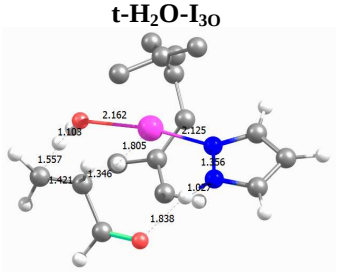
t-H_2O-TS_2



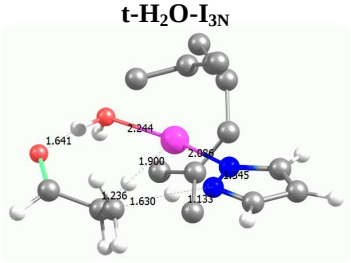
t-H_2O-I_{3O}



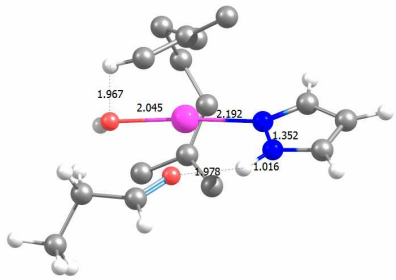
t-H_2O-I_{3N}



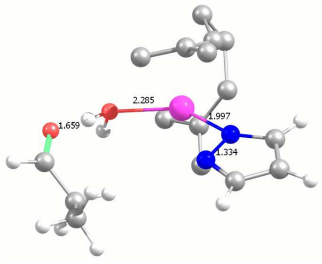
t-H_2O-TS_{3O}



t-H_2O-TS_{3N}



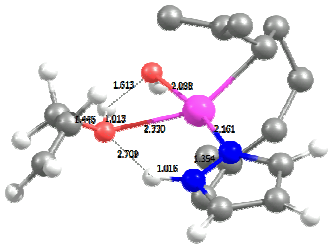
t-H_2O-I_{4O}



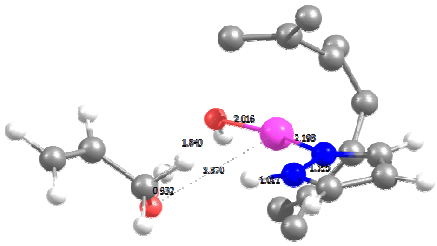
t-H_2O-I_{4N}

Figura S3.7. Geometrías optimizadas de los mínimos y estados de transición en la *ruta trans-acuo*. Los átomos de hidrógeno del ligandos bisalilo se han omitido para mayor claridad.

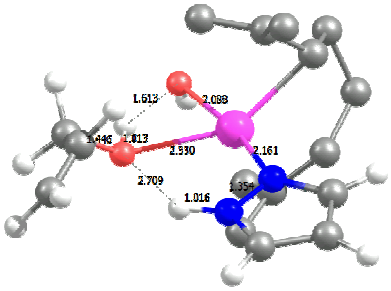
Figura S3.8. Estructuras relevantes en la *ruta trans-hidroxo.*



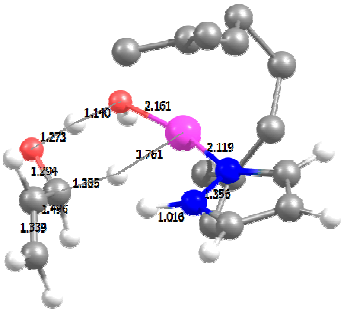
t-OH-I_1



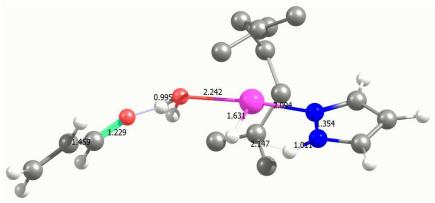
t-OH-TS_1



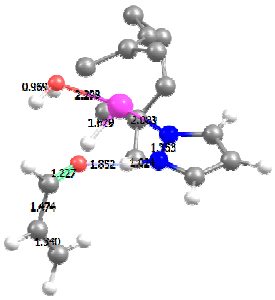
t-OH-I_2



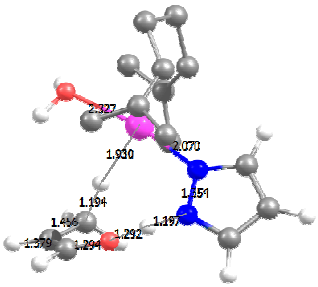
t-OH-TS_2



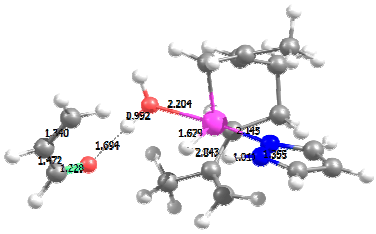
t-OH-I_3



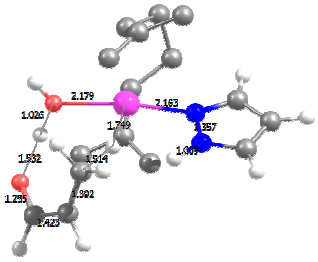
t-OH-I_{3N}



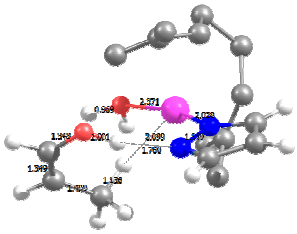
t-OH-TS_{3N}



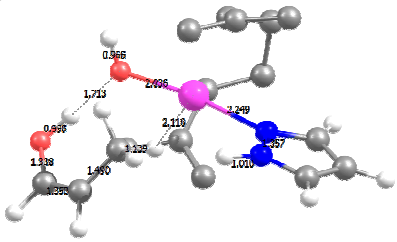
t-OH-I_{3O}



t-OH-TS_{3O}



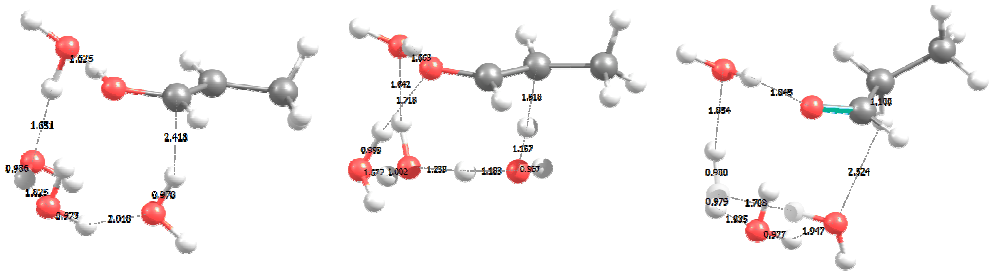
t-OH-I_{4O}



t-OH-I_{4N}

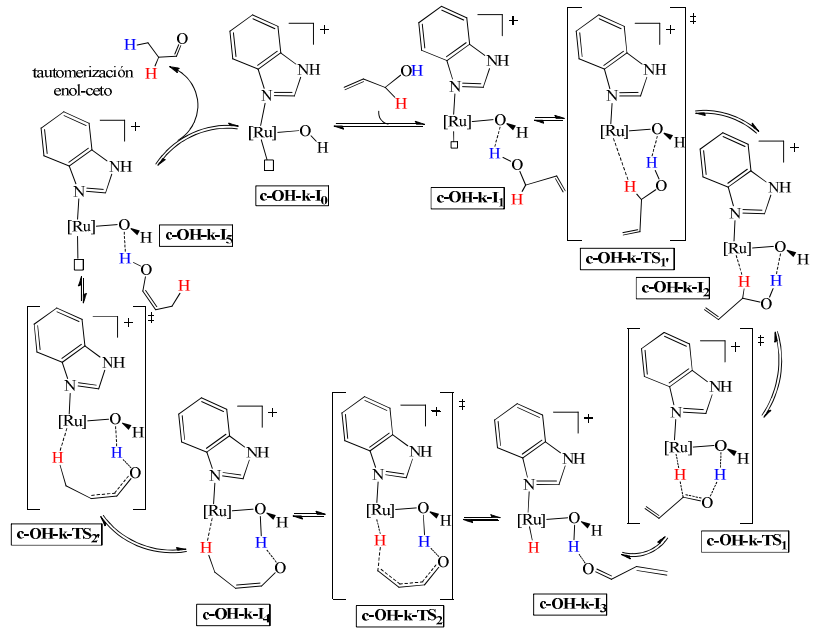
Figura S3.8. Geometrías optimizadas de los mínimos y estados de transición en la *ruta trans-hidroxo*. Los átomos de hidrógeno del ligandos bisalilo se han omitido para mayor claridad.

Figura S3.9. Estructuras relevantes en la tautomería enol-ceto.

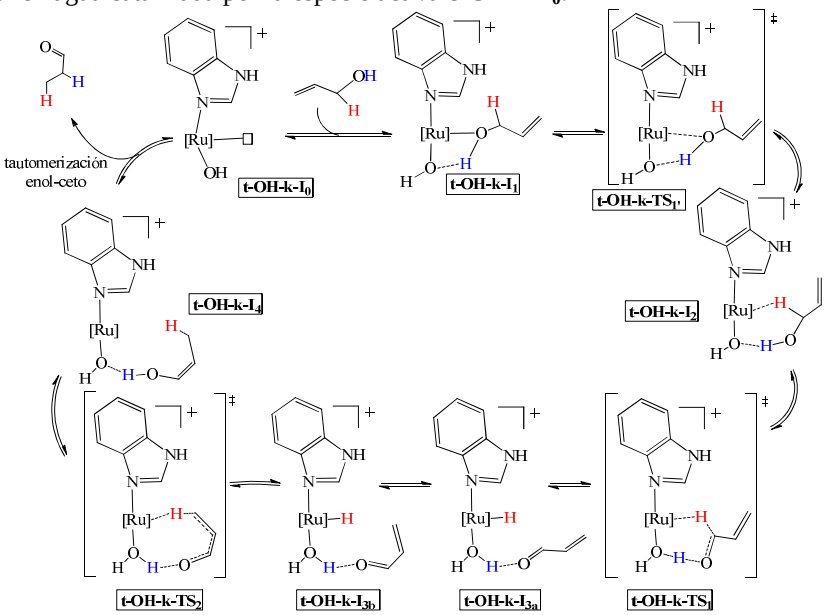


enol-4H2O **TSenol-ceto-4H2O** **enol-4H2O**

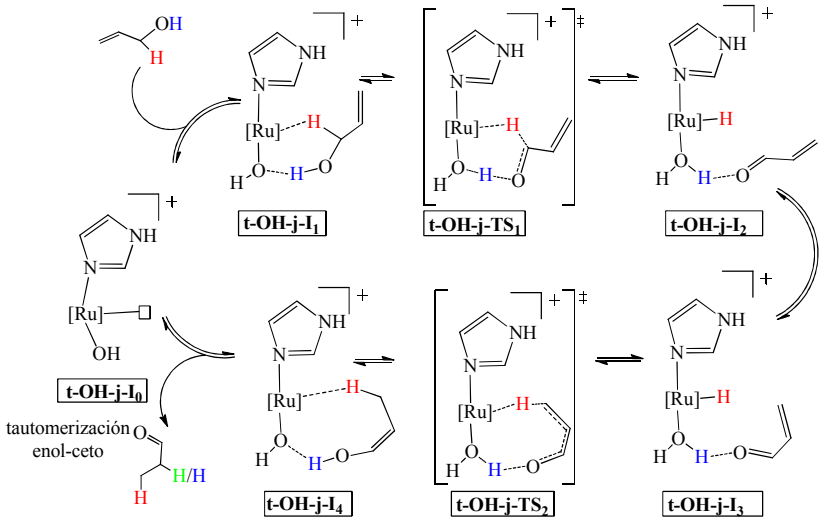
Figura S3.9. Geometrías optimizadas de los mínimos y el estados de transición en la tautomería enol-ceto.



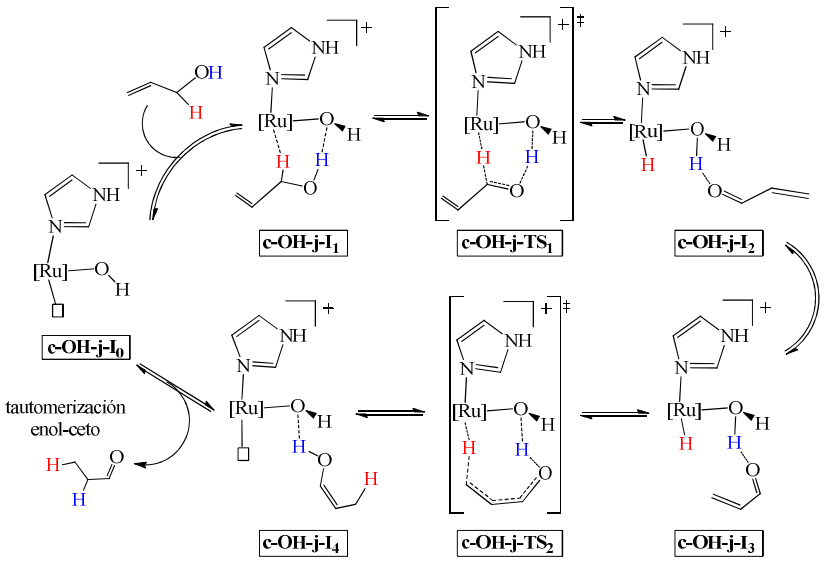
Esquema S3.3. Ciclo catalítico propuesto para la isomerización de 2-propen-1-ol a propanal en agua catalizada por la especie activa **c-OH-k-I$_0$**.



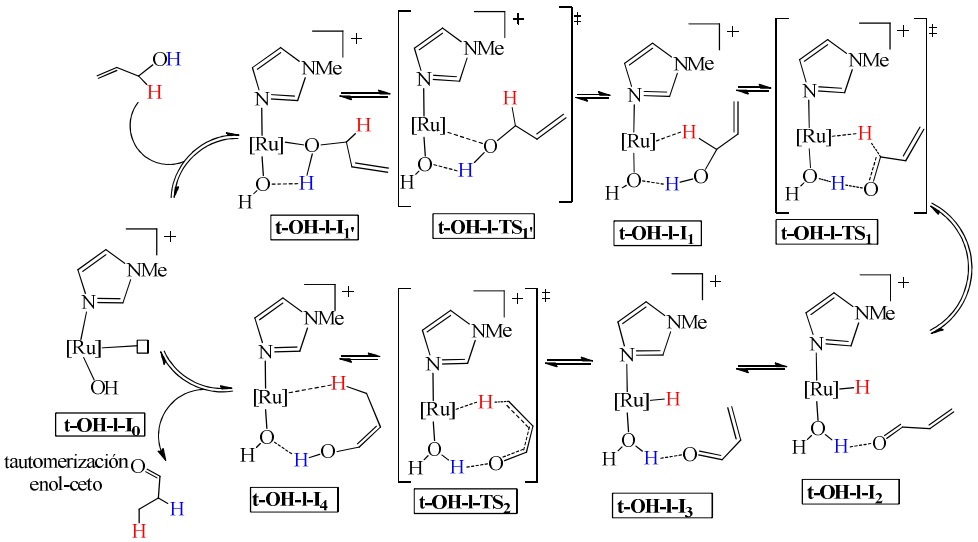
Esquema S3.4. Ciclo catalítico propuesto para la isomerización de 2-propen-1-ol a propanal en agua catalizada por la especie activa **t-OH-k-I$_0$**.



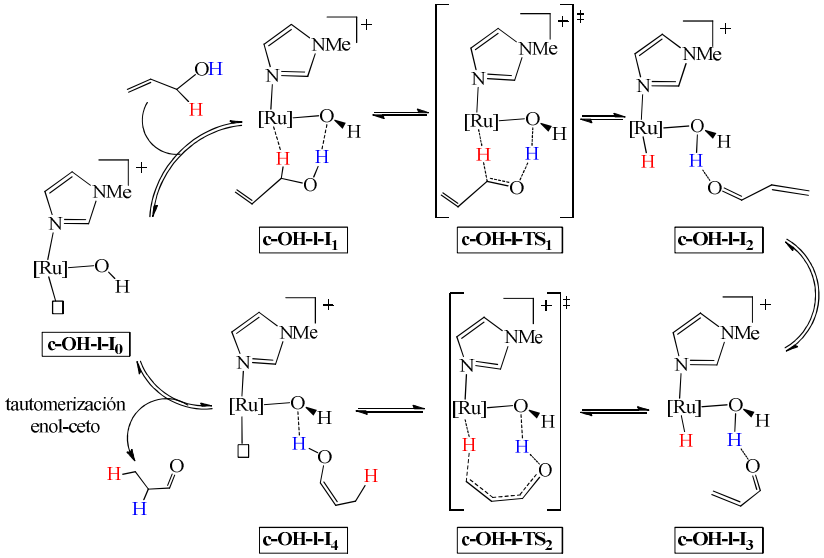
Esquema S3.5. Etapas de transferencia de hidrógeno en la isomerización de 2-propen-1-ol a propanal en agua catalizada por la especie activa **t-OH-j-I$_0$**.



Esquema S3.6. Etapas de transferencia de hidrógeno en la isomerización de 2-propen-1-ol a propanal en agua catalizada por la especie activa **c-OH-j-I$_0$**.

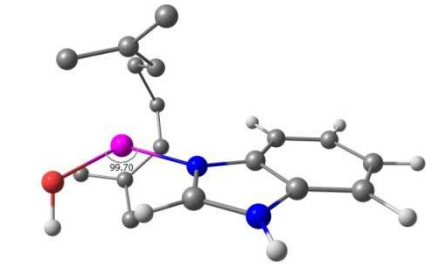


Esquema S3.7. Etapas de transferencia de hidrógeno en la isomerización de 2-propen-1-ol a propanal en agua catalizada por la especie activa **t-OH-l-I$_0$**.

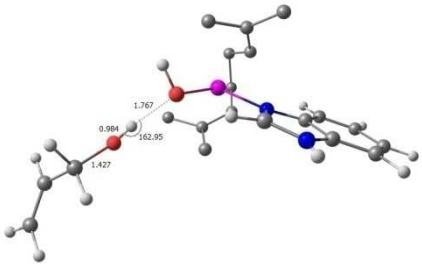


Esquema S3.8. Etapas de transferencia de hidrógeno en la isomerización de 2-propen-1-ol a propanal en agua catalizada por la especie activa **c-OH-l-I$_0$**.

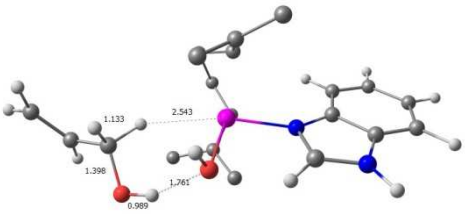
Figura S3.10. Estructuras relevantes en la *ruta cis-hidroxo* con el ligando benzimidazol.



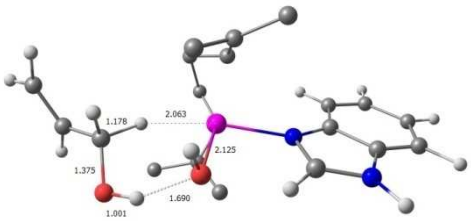
c-OH-k-I_0



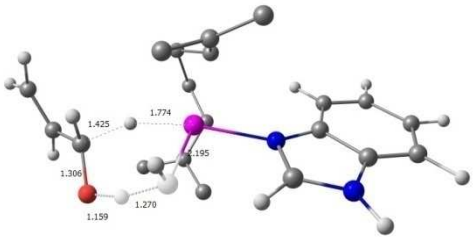
c-OH-k-I_1



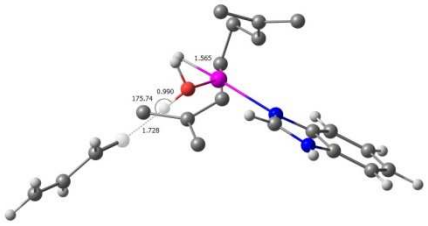
c-OH-k-TS_1,



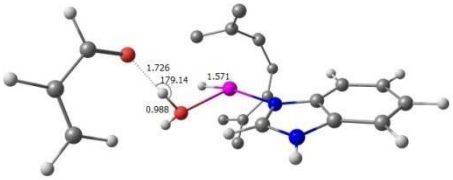
c-OH-k-I_2



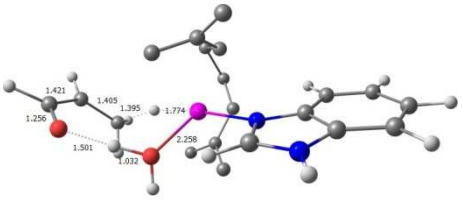
c-OH-k-TS_1



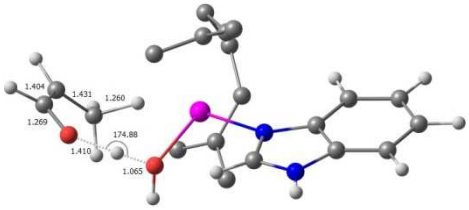
c-OH-k-I_{3a}



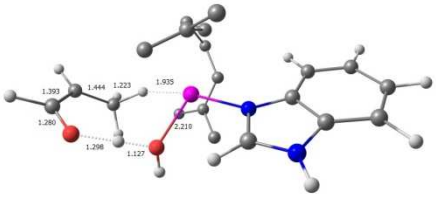
c-OH-k-I_{3b}



c-OH-k-TS_2



c-OH-k-I_2,



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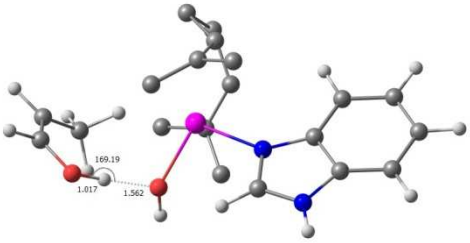
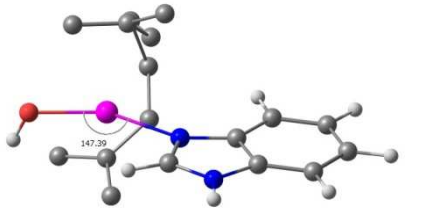


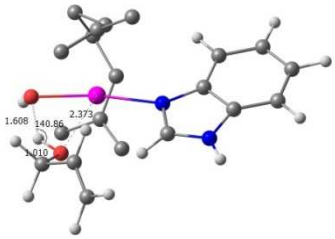
c-OH-k-I_5

Figura S3.10. Geometrías optimizadas de los mínimos y estados de transición en la *ruta cis-hidroxo* con el ligando benzimidazol. Los átomos de hidrógeno del ligandos bisalilo se han omitido para mayor claridad.

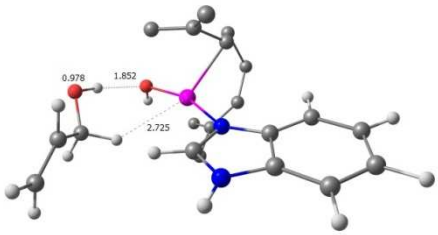
Figura S3.11. Estructuras relevantes en la *ruta trans-hidroxo* con el ligando benzimidazol.



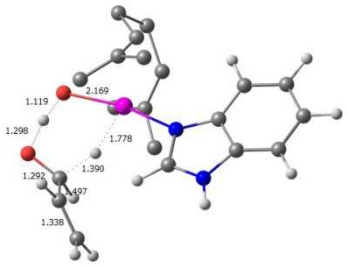
t-OH-k-I_0



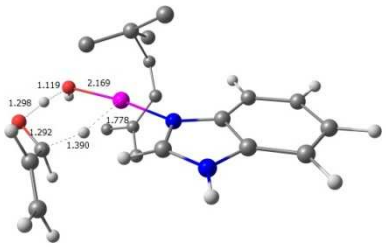
t-OH-k-I_1

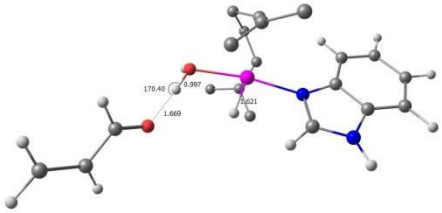


t-OH-k-TS_1'

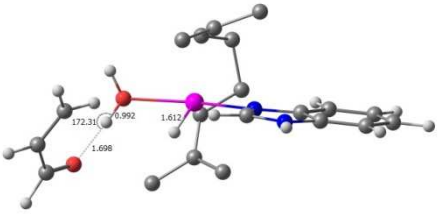


t-OH-k-I_2

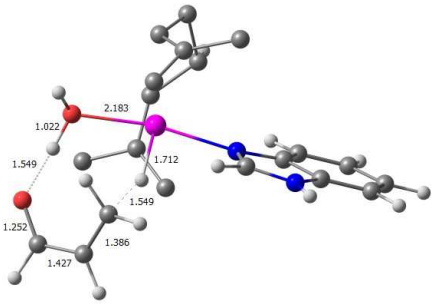




t-OH-k-TS$_1$

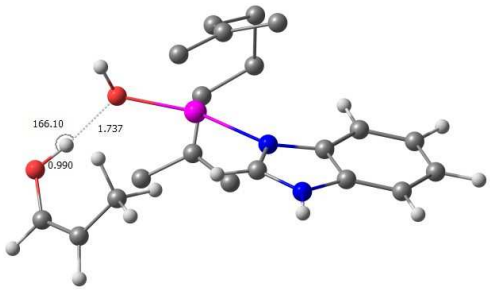


t-OH-k-I$_{3a}$



t-OH-k-I$_{3b}$

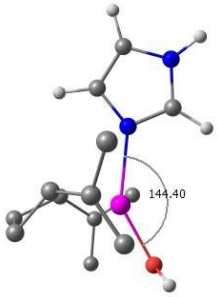
t-OH-k-TS$_2$



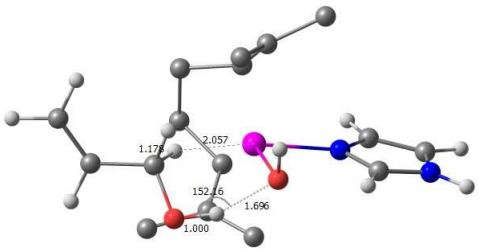
t-OH-k-I$_5$

Figura S3.11. Geometrías optimizadas de los mínimos y estados de transición en la *ruta trans-hidroxo* con el ligando benzimidazol. Los átomos de hidrógeno del ligandos bisalilo se han omitido para mayor claridad.

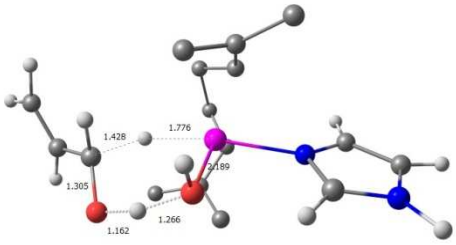
Figura S3.12. Estructuras relevantes en la *ruta cis-hidroxo* con el ligando imidazol.



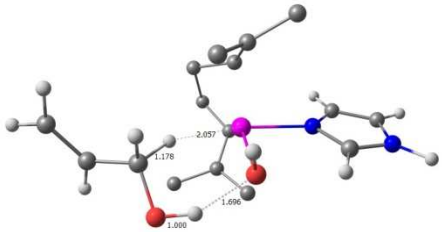
c-OH-j-I$_0$



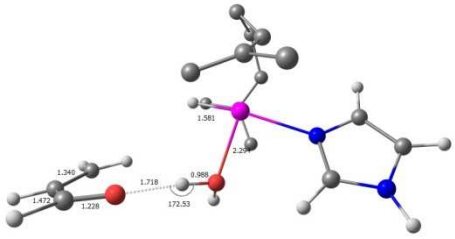
c-OH-j-I$_1$



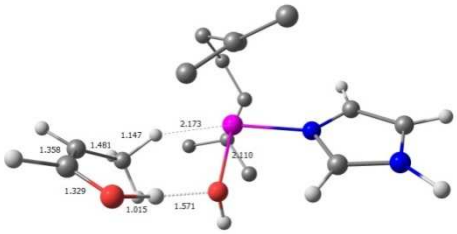
c-OH-j-TS$_1$



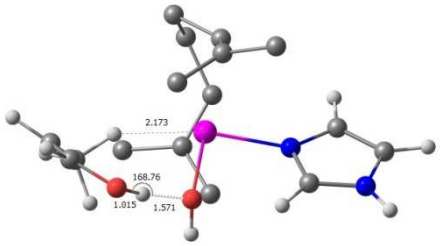
t-OH-j-I$_2$



c-OH-j-I$_3$



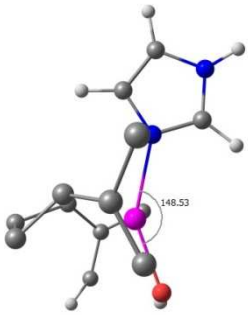
t-OH-j-TS$_2$



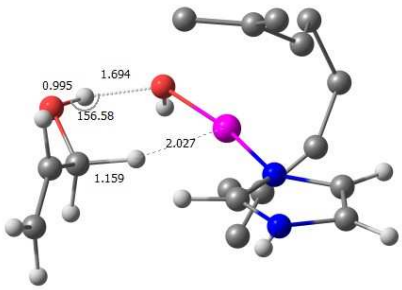
c-OH-j-I$_4$

Figura S3.12. Geometrías optimizadas de los mínimos y estados de transición en la *ruta cis-hidroxo* con el ligando imidazol. Los átomos de hidrógeno del ligandos bisalilo se han omitido para mayor claridad.

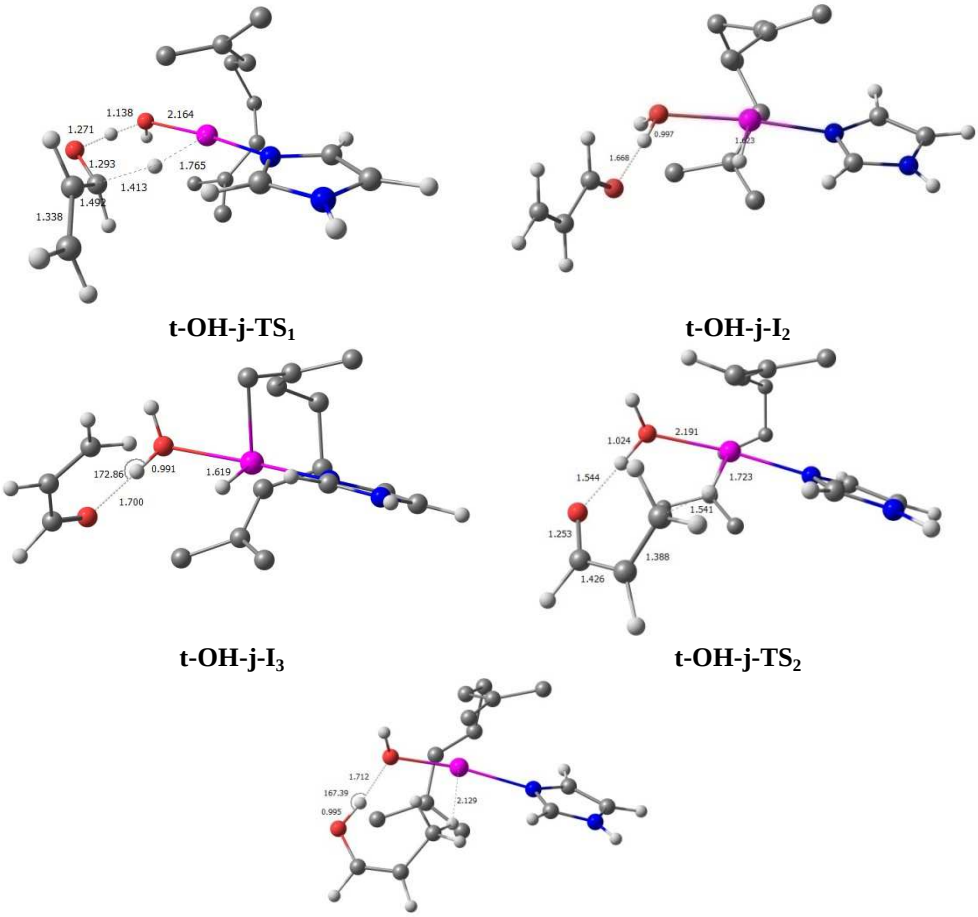
Figura S3.13. Estructuras relevantes en la *ruta trans-hidroxo* con el ligando imidazol.



t-OH-j-I$_0$



t-OH-j-I$_1$



t-OH-j-TS$_1$ **t-OH-j-I$_2$**

t-OH-j-I$_3$ **t-OH-j-TS$_2$**

t-OH-I$_4$

Figura S3.13. Geometrías optimizadas de los mínimos y estados de transición en la *ruta trans-hidroxo* con el ligando imidazol. Los átomos de hidrógeno del ligandos bisalilo se han omitido para mayor claridad.

Figura S3.14. Estructuras relevantes en la *ruta cis-hidroxo* con el ligando *N*-metilimidazol.

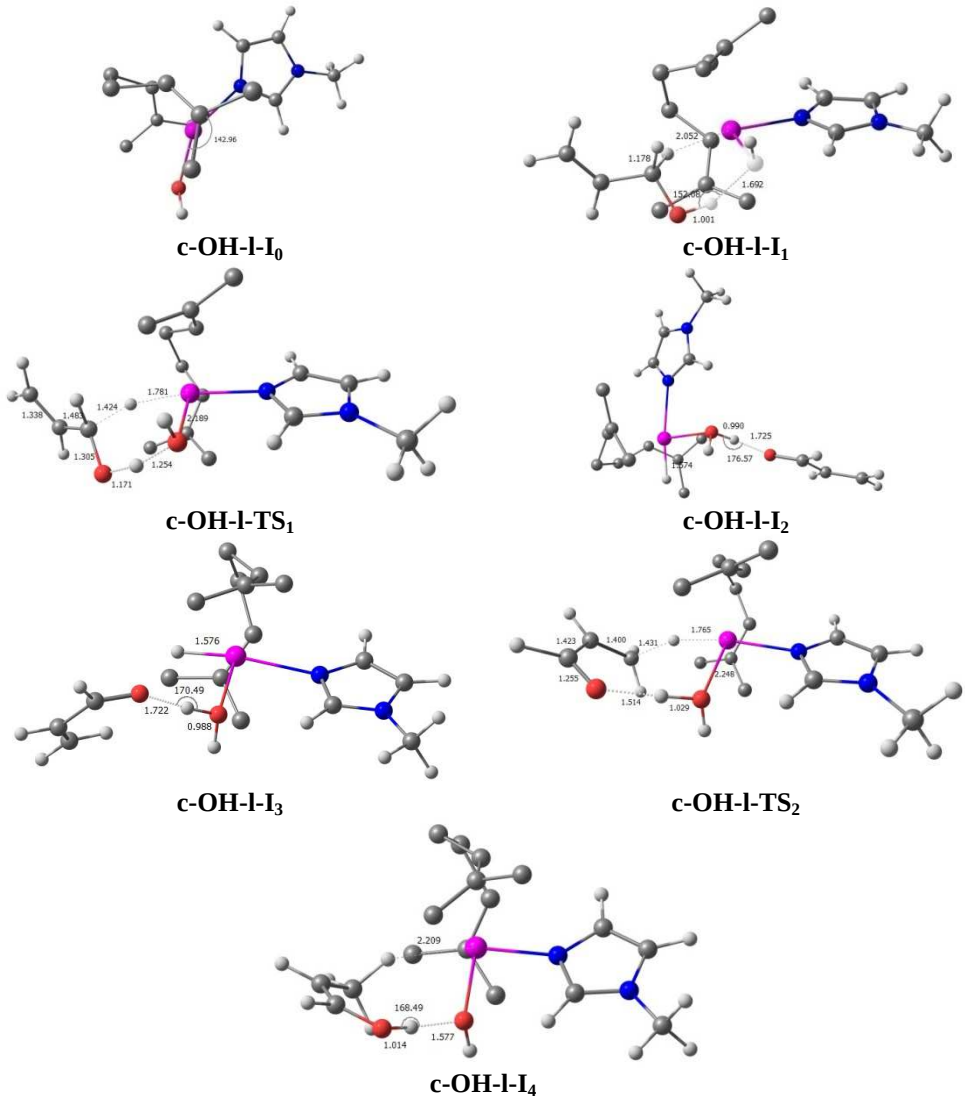
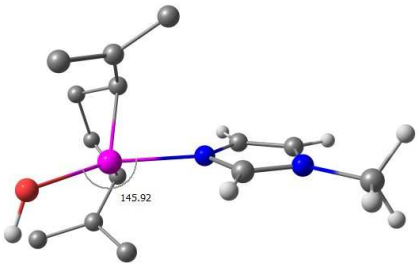
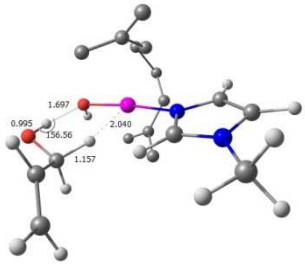


Figura S3.14. Geometrías optimizadas de los mínimos y estados de transición en la *ruta cis-hidroxo* con el ligando imidazol. Los átomos de hidrógeno del ligandos bisalilo se han omitido para mayor claridad.

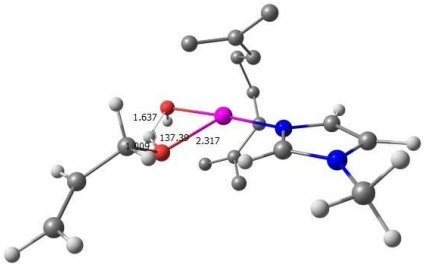
Figura S3.15. Estructuras relevantes en la *ruta trans-hidroxo* con el ligando *N*-metilimidazol.



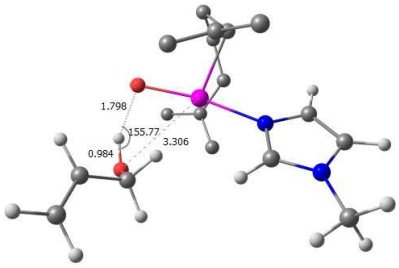
t-OH-l-I$_0$



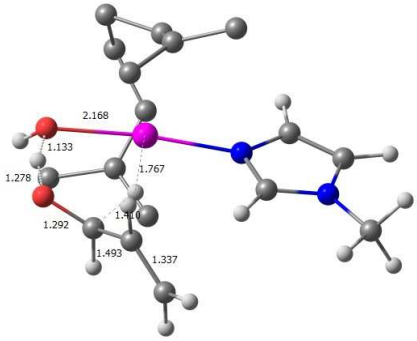
t-OH-l-I$_1$



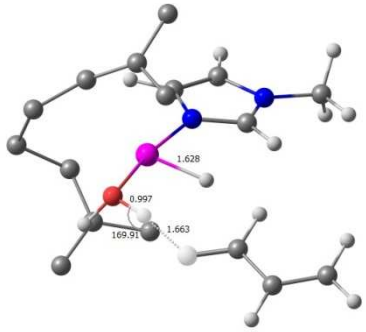
t-OH-l-I$_1$'



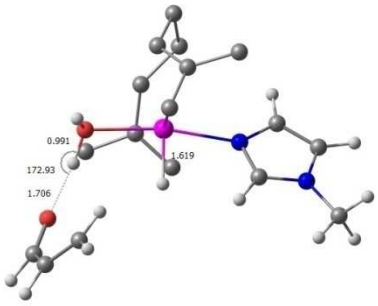
t-OH-l-TS$_1$'



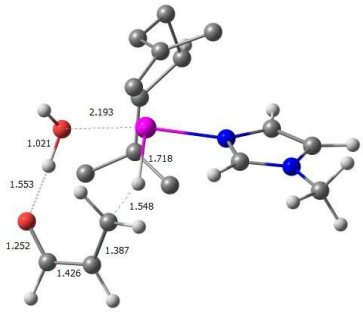
t-OH-l-TS$_1$



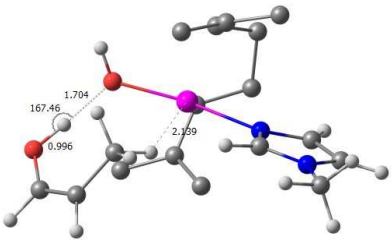
t-OH-l-I$_2$



t-OH-l-I_3



t-OH-l-TS_2



t-OH-I_4

Figura S3.15. Geometrías optimizadas de los mínimos y estados de transición en la *ruta trans-hidroxo* con el ligando *N*-metilimidazol. Los átomos de hidrógeno del ligandos bisalilo se han omitido para mayor claridad.

COORDINADAS CARTESIANAS Y ENERGÍAS ABSOLUTAS Y DE GIBBS (EN HARTREES) DE TODAS LAS ESPECIES CALCULADAS

Reactivos y productos

2-propen-1-ol (alcohol alílico)
E(gas): -193.11697
E(H_2O): -193.18212; G(H_2O): -193.12450
E(THF): -193.18296; G(THF): -193.12534

C 0.669103 -0.361788 0.24346100
C 1.843258 0.074515 -0.20918800
H 0.572627 -1.369778 0.64487900
H 2.734185 -0.545545 -0.178870
H 1.959331 1.072640 -0.625490
C -0.588359 0.456125 0.27296900
H -0.425412 1.411506 -0.25116300
O -1.635434 -0.304928 -0.32378200
H -0.834809 0.697924 1.32187200
H -2.466457 0.159561 -0.16442200

propanal
E(gas): -193.14805
E(H_2O): -193.20740; G(H_2O): -193.15049
E(THF): -193.20821; G(THF): -193.15130

O -1.827001 -0.027948 -0.288280
C -0.784964 -0.247442 0.28773800
H -0.690268 -1.118222 0.98010900
C 0.471585 0.584281 0.15698300
H 0.631914 1.082392 1.12480200
C 1.701266 -0.274175 -0.17978400
H 0.294930 1.360561 -0.59314200
H 2.607797 0.336994 -0.192900
H 1.846143 -1.069112 0.560060
H 1.598168 -0.745008 -1.16230600

***s-cis*-acroleína**
E(gas): -191.91146
E(THF): -191.97294; G(THF): -191.93778
E(H_2O): -191.97216; G(H_2O): -191.93700

O -1.402145 -0.597943 -0.0528
C -0.811242 0.465502 0.0516
C 0.667434 0.603178 -0.0555
H -1.373202 1.424563 0.002662
C 1.466768 -0.469477 0.0311
H 1.069684 1.614145 -0.001586
H 2.548700 -0.384243 -0.0091
H 1.034224 -1.466135 0.001602

***s-trans*-acroleína**
E(gas): -191.91406
E(THF): -191.97716; G(THF): -191.94193
E(H_2O): -191.97652; G(H_2O): -191.94130

O 1.796514 -0.122538 -0.0067
C 0.677191 0.351256 0.0054
C -0.562771 -0.448326 0.0064
H 0.515604 1.453724 0.0174
C -1.764163 0.140213 -0.0047
H -0.443513 -1.529041 0.0111
H -2.689009 -0.427672 -0.0101
H -1.856740 1.224436 -0.0078

H_2O
E(gas): -76.41816
E(H_2O): -76.46886; G(H_2O): -76.46513

O 0.00 0.00 0.118849
H 0.00 0.760074 -0.475396
H 0.00 -0.760074 -0.475396

Cl^-
E(gas): -460.24873
E(THF): -460.40354; G(THF): -460.43185
E(H_2O): -460.41683; G(H_2O): -460.41857

Cl 0.00 0.00 0.00

***trans*-1-propen-1-ol**
E(gas): -193.132484
E(THF):-193.197018; G(THF): -191.13670
E(H_2O):-193.196314; G(H_2O): -193.13600

H -1.422659 1.444943 -0.0062
C -0.774050 0.574068 -0.0012
C 0.558931 0.688909 0.0018
O -1.520103 -0.569209 -0.0030
H 0.955617 1.700197 0.0175
H -0.928616 -1.333943 0.0401
C 1.556780 -0.436248 -0.0011
H 2.206983 -0.396546 0.882820
H 1.088881 -1.428439 -0.003132
H 2.210648 -0.392912 -0.879929

***cis*-1-propen-1-ol**
E(gas):-193.13205
E(THF):-193.19375; G(THF): -191.13626
E(H_2O):-193.19299; G(H_2O): -193.13550

H 0.515233 1.466914 -0.0097
C 0.597136 0.382827 0.0016
C -0.473654 -0.415853 0.0035
O 1.908769 0.002771 0.0049
H -0.327088 -1.497466 0.0201
H 1.952458 -0.963639 -0.0535
C -1.889903 0.085915 -0.0026
H -2.444148 -0.262066 0.881206
H -1.923530 1.180194 -0.0860
H -2.444549 -0.263430 -0.880452

tBuO$^-$
E(gas):-233.04727
E(THF):-233.22172; G(THF): -233.13081

C -0.0212 -0.0167 0.161346
C 0.499829 1.375794 -0.435927
H -0.149949 2.175995 -0.056561
H 1.511191 1.572766 -0.055409
H 0.524485 1.442001 -1.538863
C 0.941815 -1.119583 -0.438014
H 1.958795 -0.958447 -0.055629
H 0.605497 -2.095099 -0.061547
H 0.989507 -1.1706 -1.541009
C -1.440777 -0.254593 -0.438326
H -1.808601 -1.218499 -0.061482
H -2.117549 0.521571 -0.056294
H -1.509993 -0.263570 -1.541347
O -0.0915 -0.001853 1.484208

tBuOH
E(gas):-233.68494
E(THF):-233.74833; G(THF): -233.64152

C -0.005288 -0.0002 0.014885
C -1.490072 -0.0307 -0.358233
H -1.983028 -0.886098 0.053040
H -1.983454 0.885103 0.053348
H -1.620693 -0.0151 -1.444635
C 0.690673 1.265481 -0.509504
H 0.210176 2.158852 -0.099827
H 1.746707 1.279644 -0.212252
H 0.654742 1.321138 -1.602782
C 0.691214 -1.265166 -0.509551
H 1.747297 -1.278810 -0.212445
H 0.211203 -2.158754 -0.099776
H 0.655162 -1.320882 -1.602822
O 0.013025 -0.0023 1.451480
H 0.938523 0.0106 1.730730

HCl
E(gas):-460.79227
E(THF):-460.83906; G(THF): -460.45028
E(H_2O):-460.83910; G(H_2O): 460.85032

H 0.00 0.00 -1.217808
Cl 0.00 0.00 0.071636

H_3O^+
E(gas):-76.70478
E(H_2O):-76.87279; G(H_2O): -76.85646

O 0.00 0.00 0.070279
H 0.00 0.947328 -0.187411
H 0.820410 -0.473664 -0.187411
H -0.820410 -0.473664 -0.187411

1.2a, *trans*-cloruro
E(gas):-1631.23316
E(THF):-1631.47926; G(THF): -1631.21320
E(H_2O):-1631.47533; G(H_2O): -1631.20927

C 3.339069 -0.433705 0.072612
C 2.870303 0.346935 -1.181599
H 3.687957 -1.436007 -0.189533
H 2.426934 -0.340068 -1.905300
H 4.179537 0.081139 0.553600
H 3.696426 0.879390 -1.677387
C 2.150073 -0.450116 1.036558
C 1.841820 1.319513 -0.633809
C 0.697557 1.952370 -1.235147
H 2.266993 1.945963 0.151660
C 0.353842 3.377187 -0.870909
C -0.190213 1.191047 -1.980377
C 1.312956 -1.578373 1.277603
H 2.158924 0.312234 1.812774
C 1.645575 -2.972541 0.813143
C 0.072058 -1.3016 1.888883
H 2.240790 -3.433284 1.615883
H 0.746641 -3.573552 0.667865
H 2.227112 -3.004417 -0.107201
H -0.726861 3.545463 -0.871840
H 0.746039 3.659569 0.106560
H 0.7999 4.0340 -1.631137
H -0.681136 -2.085911 1.888245
H -0.030647 -0.540447 2.654119
H -1.168638 1.605935 -2.210741
H 0.113389 0.327244 -2.554391
Ru 0.157827 0.072801 0.107906
Cl 0.157280 -1.844788 -1.607786
N -2.031356 -0.140936 0.059925
N -2.643597 -1.028899 -0.747940
C -3.004535 0.487935 0.728050
C -3.984647 -0.983078 -0.610258
C -4.261047 -0.009067 0.337851
H -2.740360 1.252125 1.443895
H -4.629087 -1.633692 -1.183776
H -5.231728 0.297596 0.697877
H -2.031492 -1.609752 -1.325970
Cl -0.117709 1.787320 1.859400

1.2a, *cis*-cloruro

E(gas): -1631.22412
E(H_2O): -1631.475550; G(H_2O): -1631.210102
E(THF): -1631.476559; G(THF): -1631.211111

C 2.092290 1.795799 1.484059
C 1.787016 2.390897 0.081885
H 3.135565 1.477921 1.546276
H 2.452138 1.942667 -0.656933
H 1.939649 2.546622 2.269793
H 1.927266 3.482021 0.055537
C 1.118577 0.635438 1.703352
C 0.338671 2.028974 -0.195649
C -0.357334 1.730512 -1.420919
H -0.326308 2.489377 0.538799
C -1.795150 2.170807 -1.595270
C 0.202098 0.858012 -2.342310
C 1.463835 -0.753839 1.725691
H 0.219748 0.896345 2.258608
C 2.870433 -1.280836 1.806050
C 0.381572 -1.637414 1.548834
H 3.065679 -1.466413 2.873632
H 2.975119 -2.224135 1.268172
H 3.621150 -0.588350 1.429962
H -2.388473 1.416214 -2.120609
H -2.284549 2.407303 -0.647976
H -1.801788 3.082450 -2.207452
H -0.583888 -1.442985 2.00173600
H -0.432374 0.417663 -3.10568400
H 1.267572 0.741654 -2.48023800
Ru 0.246111 -0.180162 -0.18357800
Cl 2.502886 -0.664856 -1.11368500
N -1.777029 0.003581 0.57010700
N -2.699547 -0.859944 0.103690
C -2.406639 0.745919 1.493590
C -3.892724 -0.688423 0.70415900
C -3.749213 0.349789 1.613280
H -1.882390 1.528414 2.02230600
H -4.741360 -1.304879 0.44534900
H -4.503415 0.761565 2.26701600
Cl -0.603870 -2.164091 -1.51905500
H -2.344878 -1.548604 -0.58627900

[**Ru**]***t*Cl**H_2**Opz**

E(gas):-1246.81649
E(H_2O):-1247.08600; G(H_2O): -1246.80757

C 3.282694 -0.712996 -0.200130
C 2.781294 0.212488 -1.337205
H 3.592645 -1.693756 -0.575653
H 2.225298 -0.363005 -2.082750
H 4.162518 -0.272518 0.282907
H 3.605937 0.722593 -1.858585
C 2.145780 -0.788922 0.824543
C 1.881715 1.197233 -0.609380
C 0.764737 1.991097 -1.051467
H 2.414164 1.686818 0.207295
C 0.564233 3.375056 -0.482014
C -0.231501 1.401823 -1.812686
C 1.202762 -1.848935 0.902211
H 2.251862 -0.169419 1.711855
C 1.358268 -3.131734 0.115553
C 0.021951 -1.607306 1.638879
H 1.984273 -3.812265 0.707693
H 0.398757 -3.640727 -0.0280
H 1.859541 -3.004935 -0.848429
H -0.496498 3.631519 -0.413939
H 1.007155 3.479625 0.509153
H 1.046563 4.093375 -1.159903
H -0.797764 -2.315390 1.548510
H 0.025831 -0.995650 2.534090
H -1.183615 1.911270 -1.928130
H -0.036773 0.581732 -2.490388
Ru 0.141926 -0.005128 0.086500
N -1.982823 -0.136864 0.018906
N -2.491997 -0.871441 -1.002298
C -2.990492 0.362853 0.757019
C -3.830314 -0.832114 -0.902223
C -4.202582 -0.057795 0.203238
H -2.778101 0.978613 1.619322
H -4.448710 -1.355141 -1.620897
H -5.200895 0.165818 0.552110
O -0.147344 -1.337936 -1.697600
H 0.075515 -2.262204 -1.512349
H -1.219709 -1.289143 -1.640492
Cl 0.075205 1.443857 2.051004

C 3.355747 -0.528191 -0.080068
C 2.880536 0.428280 -1.201523
H 3.727424 -1.475938 -0.480189
H 2.431670 -0.135534 -2.027748
H 4.188499 -0.076537 0.468919
H 3.703311 1.013278 -1.635296
C 2.170720 -0.694329 0.875974
C 1.876053 1.329414 -0.504985
C 0.726041 2.046945 -0.979409
H 2.329624 1.824865 0.353385
C 0.387709 3.400201 -0.410703
C -0.186145 1.381022 -1.793533
C 1.307076 -1.826023 0.914881
H 2.194191 -0.083887 1.776046
C 1.586431 -3.091130 0.135788
C 0.088019 -1.672021 1.602456
H 2.232881 -3.723441 0.758400
H 0.677860 -3.681818 -0.037331
H 2.125185 -2.936061 -0.803035
H -0.691838 3.557369 -0.342637
H 0.827527 3.561071 0.573801
H 0.795684 4.153112 -1.099317
H -0.675033 -2.438906 1.493576
H 0.012183 -1.053448 2.489843
H -1.163884 1.822138 -1.964520
H 0.131252 0.661651 -2.539050
Ru 0.161960 -0.009730 0.054189
N -2.015287 -0.210866 -0.020631
N -2.677719 -0.772589 -1.060770
C -2.959193 0.179542 0.844048
C -4.017052 -0.746064 -0.870217
C -4.237337 -0.137577 0.353022
H -2.667906 0.670484 1.760556
H -4.697614 -1.153719 -1.603960
H -5.188355 0.053422 0.826660
O 0.007262 -1.492547 -1.785168
H 0.1226 -2.413343 -1.491886
H 0.648113 -1.375784 -2.508592
Cl -0.066406 1.364596 2.001193
H -2.139384 -1.134848 -1.835469

[**Ru]*t*Cl**H2OpzH
E(gas):-1247.20824
E(H_2O):-1247.51582; G(H_2O): -1247.22539

[**Ru]*t*H2O*Cl*pzH**
E(gas):-1247.21583
E(H_2O):-1247.52071; G(H_2O): -1247.23064

C 3.398930 -0.368950 0.097699
C 2.943909 0.610394 -1.012068
H 3.871305 -1.265783 -0.313551
H 2.583859 0.068331 -1.893646
H 4.148597 0.109995 0.735841
H 3.757133 1.265125 -1.355092
C 2.157147 -0.668546 0.941485
C 1.840209 1.414474 -0.349907
C 0.701299 2.106809 -0.889863
H 2.191084 1.879288 0.571550
C 0.252882 3.411525 -0.282703
C -0.094196 1.451746 -1.820419
C 1.358624 -1.839513 0.829637
H 2.069828 -0.120046 1.876531
C 1.767191 -3.033341 -0.0803
C 0.079159 -1.791764 1.423831
H 2.335707 -3.703728 0.657329
H 0.908256 -3.609147 -0.358455
H 2.436465 -2.799526 -0.835303
H -0.834398 3.522459 -0.309797
H 0.591903 3.531598 0.746966
H 0.688719 4.221423 -0.883503
H -0.622612 -2.594772 1.208438
H -0.082649 -1.262807 2.356850
H -1.074960 1.856353 -2.053981
H 0.302958 0.732948 -2.525075
Ru 0.168573 -0.037566 0.006927
N -2.003660 -0.285977 -0.252173
N -2.826652 -0.061112 0.791853
C -2.8066 -0.668544 -1.264033
C -4.117182 -0.279962 0.468625
C -4.142450 -0.686602 -0.857330
H -2.384776 -0.880796 -2.239677
H -4.908737 -0.130054 1.188603
H -5.008197 -0.947175 -1.447155
O 0.256685 -1.357682 -1.881512
H -0.444177 -2.025037 -1.781201
H 1.072081 -1.863314 -2.036069
Cl -0.289360 1.216182 2.018964
H -2.4095 0.337209 1.632638

Ciclo con Cl como ligando (*ruta cloruro*)

Cl-I_0

E(gas): -1170.37047;
E(H_2O): -1170.58097; G(H_2O): -1170.32751
E(THF): -1170.58283; G(THF): -1170.32937

C	-1.652359	1.085440	-2.259491
C	-1.262686	2.209822	-1.269651
H	-2.739521	0.988587	-2.341324
H	-2.008412	2.282808	-0.472546
H	-1.278990	1.316691	-3.263789
H	-1.222512	3.193570	-1.760788
C	-0.984747	-0.198468	-1.773274
C	0.096955	1.833405	-0.707773
C	0.586179	2.038114	0.625204
H	0.880192	1.800748	-1.465142
C	2.060769	2.230867	0.882964
C	-0.306580	1.813042	1.668343
C	-1.630111	-1.246146	-1.042085
H	-0.103709	-0.496948	-2.335857
C	-3.111892	-1.270428	-0.767042
C	-0.735887	-2.171855	-0.469040
H	-3.611016	-1.716053	-1.639509
H	-3.339520	-1.873405	0.112099
H	-3.531853	-0.273390	-0.612629
H	2.362590	1.781097	1.832084
H	2.675004	1.803706	0.087041
H	2.266058	3.308687	0.932374
H	-1.096780	-2.865591	0.283229
H	0.199512	-2.424866	-0.955913
H	0.058350	1.693364	2.683585
H	-1.371889	1.984382	1.573852
Ru	-0.276060	-0.094649	0.306844
Cl	-1.743674	-0.746360	2.175041
N	1.603046	-0.573265	-0.298968
N	2.279818	-1.020996	0.763428
C	2.385770	-0.562863	-1.408479
C	3.521360	-1.301014	0.332636
C	3.646330	-1.030703	-1.0404
H	2.022406	-0.226530	-2.369878
H	4.258169	-1.684846	1.026532
H	4.512358	-1.154792	-1.675347

Cl-I_1

E(gas): -1363.52501;
E(H_2O): -1363.77958; G(H_2O): -1363.44561
E(THF): -1363.78392; G(THF): -1363.44995

C	-3.448368	0.462299	0.018217
C	-2.899600	0.427582	1.469231
H	-4.075265	-0.410046	-0.182134
H	-2.796096	-0.608876	1.797654
H	-4.074577	1.348867	-0.141047
H	-3.563253	0.944252	2.178902
C	-2.231183	0.534429	-0.905916
C	-1.547770	1.114866	1.389996
C	-0.339701	0.893500	2.140201
H	-1.639543	2.149321	1.055291
C	0.591037	2.040581	2.459805
C	0.052909	-0.413954	2.378651
C	-1.762299	-0.522781	-1.746075
H	-1.963692	1.536191	-1.232883
C	-2.546555	-1.771778	-2.042258
C	-0.440619	-0.370758	-2.209094
H	-3.143574	-1.552291	-2.940846
H	-1.891359	-2.615430	-2.262868
H	-3.221352	-2.067071	-1.240750
H	1.639015	1.746224	2.352778
H	0.412900	2.912814	1.828411
H	0.427940	2.335994	3.504900
H	0.043588	-1.233132	-2.661232
H	-0.045267	0.597388	-2.493755
H	1.077915	-0.617984	2.675124
H	-0.645652	-1.231436	2.481947
Ru	-0.322473	-0.126099	0.038517
Cl	-1.084826	-2.495175	0.516623
N	0.674561	1.641944	-0.542508
N	2.007936	1.497555	-0.735821
C	0.317110	2.905559	-0.865217
C	2.485932	2.675325	-1.166635
C	1.451215	3.611955	-1.268433
H	-0.706548	3.245331	-0.783969
H	3.541300	2.787105	-1.380465

H 1.509346 4.644430 -1.582731
H 2.204313 -0.057090 -0.352515
O 1.783406 -0.902110 0.032838
C 2.234957 -2.102667 -0.585926
C 3.618018 -2.499316 -0.147917
H 1.509602 -2.880280 -0.322222
H 2.211531 -1.999466 -1.682930
C 4.366701 -1.852980 0.744099
H 3.998387 -3.400671 -0.629749
H 5.359032 -2.203243 1.009905
H 4.006703 -0.955375 1.237070

Cl-I_2
E(gas): -1363.50931;
E(H_2O): -1363.76674; G(H_2O): -1363.43606
E(THF): -1363.77022; G(THF): -1363.43954

C -3.686064 0.646245 0.409180
C -2.963272 0.427056 1.760544
H -4.470134 -0.101485 0.253095
H -2.926355 -0.640072 1.998499
H -4.176663 1.626372 0.395747
H -3.488077 0.922320 2.590975
C -2.621995 0.617113 -0.685571
C -1.564454 0.993496 1.595423
C -0.338679 0.491545 2.144864
H -1.556097 2.066480 1.401611
C 0.805740 1.423182 2.462512
C -0.164400 -0.890434 2.152456
C -2.342373 -0.496672 -1.542037
H -2.354130 1.590031 -1.088641
C -3.166063 -1.759008 -1.544796
C -1.141584 -0.371439 -2.264495
H -4.038035 -1.590763 -2.193036
H -2.596862 -2.602256 -1.935989
H -3.532839 -2.029117 -0.551487
H 1.769439 0.931388 2.310916
H 0.769150 2.337916 1.865454
H 0.727493 1.708016 3.520714
H -0.724360 -1.241651 -2.760580
H -0.781815 0.596830 -2.594202
H 0.833115 -1.302169 2.264539
H -0.991020 -1.582330 2.260863
Ru -0.712656 -0.243635 -0.029712
Cl -0.310927 -2.662890 -0.234893
N 0.256876 1.463976 -0.593930
N 1.562087 1.215460 -0.799163
C -0.022797 2.761996 -0.866986
C 2.120121 2.370943 -1.199023
C 1.158364 3.388187 -1.262911
H -1.018138 3.170371 -0.761583
H 3.179932 2.406339 -1.415242
H 1.290348 4.422168 -1.548818
H 2.494424 -0.059563 0.220415
O 2.890887 -0.630766 0.915997
C 3.528970 -1.725137 0.287768
C 4.835762 -1.378567 -0.381411
H 3.716701 -2.478459 1.066847
H 2.858977 -2.209475 -0.440524
C 5.422379 -0.183307 -0.331758
H 5.304488 -2.196050 -0.931552
H 6.366061 0.012091 -0.831941
H 4.969243 0.631001 0.225559

Cl-I_3
E(gas): -1363.50224;
E(H_2O): -1363.76386; G(H_2O): -1363.42939
E(THF): -1363.76749; G(THF): -1363.43302

C -3.309343 -0.092029 0.938107
C -2.331514 -0.302831 2.129847
H -3.834788 -1.022641 0.711875
H -2.038415 -1.353332 2.177426
H -4.070152 0.658317 1.186060
H -2.798383 -0.037946 3.089928
C -2.478521 0.407281 -0.239580
C -1.129239 0.583585 1.866337
C 0.264513 0.333513 2.104439
H -1.376351 1.645765 1.860760
C 1.218514 1.460894 2.418483
C 0.748396 -0.943612 1.833306
C -2.229424 -0.304718 -1.463396
H -2.426955 1.489321 -0.323287
C -2.972390 -1.542306 -1.883563

C -1.146127 0.185769 -2.208756
H -3.847219 -1.195451 -2.454508
H -2.366243 -2.173252 -2.535401
H -3.319778 -2.149678 -1.049373
H 2.191599 1.290288 1.951253
H 0.837917 2.434304 2.103259
H 1.363521 1.485031 3.507108
H -0.739650 -0.437654 -3.002113
H -0.916978 1.242601 -2.265611
H 1.819329 -1.088698 1.707648
H 0.156013 -1.837296 1.967025
Ru -0.371647 -0.146298 -0.071473
Cl -0.740524 -2.626099 -0.139840
N 0.271653 1.826087 -0.381918
N 1.536812 1.971027 -0.832692
C -0.320908 3.043794 -0.313461
C 1.740684 3.283541 -1.036822
C 0.589755 4.015671 -0.724589
H -1.340320 3.167663 0.025709
H 2.702556 3.630103 -1.392927
H 0.434115 5.083573 -0.783560
H 2.780223 0.779510 -0.523006
H 1.535598 -1.031755 -0.854462
H 2.774538 -0.969120 -2.097474
C 2.655487 -1.067252 -1.002350
C 3.107073 -2.427039 -0.566575
O 3.289224 -0.043962 -0.300584
C 4.074461 -2.641039 0.326497
H 2.586357 -3.259231 -1.036477
H 4.375587 -3.646839 0.603359
H 4.597719 -1.810213 0.788284

Cl-I_4
E(gas): -1363.49795;
E(H_2O): -1363.75798; G(H_2O): -1363.42998
E(THF): -1363.76125; G(THF): -1363.43325

C -3.748744 -0.021865 0.094744
C -3.131165 -0.351468 1.479748
H -4.398359 -0.832105 -0.252095
H -2.798454 -1.389556 1.506125
H -4.382222 0.871463 0.173412
H -3.860450 -0.201587 2.292911
C -2.602024 0.281922 -0.884930
C -1.969727 0.620126 1.615830
C -0.653351 0.619559 2.136525
H -2.330171 1.643729 1.479170
C -0.069277 1.963099 2.540635
C 0.250521 -0.471286 2.054633
C -2.010255 -0.679369 -1.747167
H -2.469338 1.328112 -1.147513
C -2.654581 -2.012339 -2.040788
C -0.709362 -0.397857 -2.250733
H -3.336579 -1.851784 -2.890090
H -1.914322 -2.759723 -2.328418
H -3.226966 -2.416417 -1.206906
H 0.983659 2.053936 2.257715
H -0.617677 2.809072 2.117494
H -0.125457 2.045043 3.634423
H -0.199495 -1.193113 -2.785909
H -0.436425 0.607883 -2.557033
H 1.287411 -0.254251 2.302814
H -0.060792 -1.493903 2.222931
Ru -0.538028 -0.225492 -0.032338
Cl -0.966665 -2.682720 0.388869
N 0.256417 1.708669 -0.473697
N 1.593374 1.851894 -0.607508
C -0.261459 2.918594 -0.725603
C 1.928863 3.118189 -0.933061
C 0.753361 3.845754 -1.020415
H -1.328609 3.073988 -0.674364
H 2.962228 3.398578 -1.075988
H 0.642539 4.892479 -1.260811
H 2.214759 1.046504 -0.461255
H 0.921151 -0.801096 -0.403501
H 2.711871 -1.728532 0.006155
C 3.690793 -1.219991 -0.041551
C 4.892580 -2.065029 0.121716
O 3.739133 -0.006728 -0.224142
C 6.127491 -1.550142 0.073572
H 4.723070 -3.126837 0.281963
H 7.013036 -2.166203 0.192118
H 6.268533 -0.485296 -0.088622

Cl-I_5
E(gas): -1363.49685;

E(H_2O): -1363.75676; G(H_2O): -1363.43003
E(THF): -1363.760047; G(THF): -1363.43331

C	-3.669034	0.327845	0.100647
C	-3.080307	-0.076117	1.478842
H	-4.390150	-0.414852	-0.255720
H	-2.855306	-1.143194	1.493743
H	-4.218172	1.273971	0.193889
H	-3.785777	0.138607	2.298354
C	-2.500760	0.538917	-0.878204
C	-1.826126	0.773692	1.613865
C	-0.517420	0.640572	2.141418
H	-2.084540	1.829098	1.489114
C	0.191019	1.915266	2.567208
C	0.271754	-0.532082	2.045852
C	-2.002159	-0.459991	-1.756512
H	-2.270254	1.572325	-1.124850
C	-2.769365	-1.720787	-2.071443
C	-0.680976	-0.292858	-2.260155
H	-2.103772	-2.531768	-2.368643
H	-3.382244	-2.079357	-1.245847
H	-3.429084	-1.482149	-2.919990
H	1.252443	1.903478	2.302145
H	-0.263771	2.815079	2.144372
H	0.124936	1.992723	3.660764
H	-0.247297	-1.123950	-2.807852
H	-0.318683	0.687862	-2.555379
H	1.325563	-0.429189	2.295443
H	-0.143394	-1.520943	2.189921
Ru	-0.490057	-0.172819	-0.042985
Cl	-1.133556	-2.591255	0.332272
N	0.482373	1.679426	-0.452704
N	1.827270	1.677917	-0.575804
C	0.102785	2.942883	-0.686730
C	2.305156	2.903342	-0.877225
C	1.217072	3.756835	-0.958760
H	-0.941392	3.214092	-0.639650
H	3.364896	3.065190	-1.007507
H	1.224322	4.813423	-1.180671
H	2.349300	0.810305	-0.448225
H	0.921856	-0.855353	-0.424654
H	5.205004	-3.147780	0.261694
C	4.389292	-2.438829	0.134858
C	4.790467	-1.046726	-0.126890
C	3.108886	-2.833270	0.211744
H	5.886829	-0.881646	-0.178345
O	4.041338	-0.091783	-0.285851
H	2.851097	-3.870423	0.403576
H	2.280650	-2.139490	0.082306

Cl-I_6
E(gas): -1363.48402;
E(H_2O): -1363.75750; G(H_2O): -1363.42621
E(THF): -1363.75884; G(THF): -1363.42755

C	-3.145520	0.356159	-1.399014
C	-3.253671	0.925016	0.043342
H	-3.778502	-0.527719	-1.510698
H	-3.416487	0.110343	0.749936
H	-3.497605	1.094510	-2.130509
H	-4.086840	1.638096	0.139166
C	-1.669195	0.051594	-1.673718
C	-1.927036	1.618330	0.294341
C	-1.100530	1.785819	1.449527
H	-1.763632	2.417250	-0.432964
C	-0.266538	3.042962	1.582647
C	-0.861451	0.726794	2.332901
C	-1.083293	-1.254762	-1.703976
H	-1.132745	0.818850	-2.228794
C	-1.877363	-2.532498	-1.756307
C	0.319207	-1.289818	-1.583550
H	-1.336549	-3.356594	-1.288914
H	-2.859295	-2.461838	-1.291489
H	-2.008017	-2.769527	-2.823136
H	0.730928	2.831454	1.979647
H	-0.159884	3.585998	0.641321
H	-0.772423	3.708734	2.294411
H	0.835680	-2.223251	-1.379022
H	0.935109	-0.525398	-2.042518
H	-0.039486	0.830493	3.038335
H	-1.608725	-0.014023	2.582430
Ru	-0.445252	-0.071396	0.198858
Cl	-1.813231	-1.904141	1.205068
N	1.062626	1.261151	-0.524314

N	2.345382	1.039056	-0.179235
C	1.084113	2.294801	-1.379125
C	3.176069	1.903182	-0.795872
C	2.399516	2.742267	-1.580039
H	0.164543	2.672550	-1.802120
H	4.243512	1.849151	-0.637331
H	2.732674	3.554803	-2.207995
H	2.630739	0.216067	0.412725
H	0.938354	-0.937237	1.103583
H	3.683041	-0.884722	2.178944
C	3.106200	-1.358966	1.387729
C	3.783906	-1.835036	0.229988
C	1.720288	-1.713084	1.615379
H	4.887321	-1.667311	0.230138
O	3.253467	-2.376747	-0.756309
H	1.380606	-1.678516	2.651334
H	1.401724	-2.634365	1.127400

Cl-I_7
E(gas): -1363.52720;
E(H_2O): -1363.78460; G(H_2O): -1363.45788
E(THF): -1363.78767; G(THF): -1363.46094

C	-3.229623	-0.865177	-1.438106
C	-3.576027	-0.376622	-0.010908
H	-3.510615	-1.913979	-1.577080
H	-3.471786	-1.200410	0.701477
H	-3.787849	-0.286923	-2.183443
H	-4.614866	-0.021424	0.061237
C	-1.736321	-0.625632	-1.651264
C	-2.599736	0.742831	0.305176
C	-1.991308	1.051731	1.567442
H	-2.704018	1.601915	-0.357623
C	-1.600443	2.468933	1.908659
C	-1.567263	-0.021429	2.345211
C	-0.711727	-1.621822	-1.554460
H	-1.495640	0.227544	-2.280763
C	-1.001446	-3.084636	-1.332906
C	0.591710	-1.096235	-1.524332
H	-0.148348	-3.589196	-0.878859
H	-1.876022	-3.254811	-0.699528
H	-1.200758	-3.542199	-2.312446
H	-0.691540	2.498243	2.514780
H	-1.440589	3.077267	1.015484
H	-2.414754	2.922570	2.489469
H	1.429773	-1.721581	-1.237908
H	0.841889	-0.184583	-2.054656
H	-0.880568	0.137971	3.170559
H	-2.065454	-0.983514	2.335477
Ru	-0.632685	-0.256840	0.213173
Cl	0.407700	-2.089056	1.490778
N	0.045972	1.516186	-0.514024
N	1.122909	1.901444	0.183243
C	-0.285087	2.443821	-1.447931
C	1.485476	3.098575	-0.311243
C	0.628521	3.491979	-1.350788
H	-1.131982	2.320905	-2.108608
H	2.342321	3.615125	0.102767
H	0.660772	4.393456	-1.946698
H	3.492883	0.604147	1.240191
H	3.455773	-1.900910	1.067731
H	5.214516	0.640902	0.925141
C	4.298253	0.067010	0.717988
C	4.0524	0.220361	-0.751494
C	4.407768	-1.379627	1.193143
H	3.988608	1.271441	-1.115987
O	3.776038	-0.695600	-1.517716
H	4.676405	-1.416797	2.252955
H	5.168997	-1.923234	0.625566

Cl-TS_1
E(gas): -1363.50896;
Frecuencia imaginaria: -39.7 cm^{-1}
E(H_2O): -1363.76524; G(H_2O): -1363.43241
E(THF): -1363.76893; G(THF): -1363.43609

C	-3.628859	0.570231	0.34720600
C	-2.939076	0.413835	1.72670300
H	-4.364548	-0.223407	0.18608600
H	-2.900644	-0.642439	2.00620300
H	-4.172265	1.521148	0.29631300
H	-3.493077	0.936158	2.52068500
C	-2.531661	0.574993	-0.71267100
C	-1.540027	0.988105	1.59127900

C -0.327725 0.490045 2.17336200
H -1.532191 2.059425 1.39274900
C 0.823595 1.409859 2.50184800
C -0.176157 -0.893091 2.20609400
C -2.211105 -0.508992 -1.59197600
H -2.262263 1.561200 -1.08048500
C -3.036162 -1.765713 -1.68039700
C -0.979953 -0.357876 -2.25728800
H -3.887589 -1.555578 -2.34402700
H -2.461167 -2.590459 -2.10068300
H -3.429372 -2.085586 -0.71343100
H 1.780523 0.923724 2.29604900
H 0.771415 2.348277 1.94477800
H 0.780695 1.648119 3.57320900
H -0.540369 -1.217100 -2.75468600
H -0.618168 0.617506 -2.56166600
H 0.809191 -1.323461 2.34410900
H -1.016876 -1.567619 2.30255500
Ru -0.623384 -0.233132 -0.00922700
Cl -0.431004 -2.690450 -0.11814400
N 0.282793 1.540099 -0.55772600
N 1.580766 1.357902 -0.87083100
C -0.059547 2.837855 -0.75221700
C 2.065399 2.551444 -1.25165500
C 1.064481 3.530122 -1.19954600
H -1.058210 3.204740 -0.559390
H 3.105192 2.641596 -1.53837800
H 1.136585 4.580515 -1.44393300
H 2.395683 0.019409 0.01183400
O 2.629895 -0.677961 0.67121900
C 3.259185 -1.754683 0.00530800
C 4.701731 -1.501079 -0.354580
H 3.201967 -2.626758 0.67201600
H 2.701313 -2.042103 -0.90039800
C 5.383231 -0.398480 -0.04735200
H 5.186996 -2.308611 -0.90523600
H 6.422697 -0.270764 -0.33387200
H 4.912291 0.405771 0.50948300

Cl-TS$_2$
E(gas): -1363.48737;
Frecuencia imaginaria: -259.7 cm^{-1}
E(H$_2$O): -1363.74920; G(H$_2$O): -1363.41921
E(THF): -1363.75225; G(THF): -1363.42226

C 3.222306 -1.180874 0.475016
C 2.609793 -0.597440 1.778227
H 4.094661 -0.600466 0.162615
H 2.706373 0.488963 1.778690
H 3.571518 -2.207384 0.644825
H 3.112392 -0.988852 2.676584
C 2.118521 -1.206578 -0.591177
C 1.153418 -1.027633 1.750010
C -0.074864 -0.440084 2.181105
H 1.073996 -2.116482 1.697330
C -1.201026 -1.348692 2.629098
C -0.354572 0.917559 1.963353
C 1.976635 -0.266138 -1.655311
H 1.646261 -2.171975 -0.748117
C 3.068070 0.682089 -2.078007
C 0.696125 -0.184729 -2.254114
H 3.642281 0.158606 -2.858002
H 2.661744 1.598537 -2.507739
H 3.7480 0.958678 -1.274178
H -2.177080 -0.977710 2.304125
H -1.080935 -2.377293 2.281001
H -1.201524 -1.366399 3.727318
H 0.507729 0.642323 -2.934212
H 0.1061 -1.074150 -2.428651
H -1.387259 1.247795 2.048390
H 0.398088 1.690256 2.039793
Ru 0.332152 0.077285 -0.049039
Cl 1.673473 2.201212 0.126080
N -1.054147 -1.527734 -0.381993
N -2.346157 -1.266266 -0.673756
C -0.919663 -2.864469 -0.437277
C -3.024702 -2.406281 -0.900889
C -2.141794 -3.468875 -0.761704
H 0.032032 -3.331562 -0.232735
H -4.077472 -2.379230 -1.143969
H -2.348608 -4.522554 -0.875731
H -2.733555 -0.243425 -0.658855
H -0.896951 1.190088 -0.525809
H -1.816201 1.808059 -1.967752
C -2.114109 1.857060 -0.900917
C -1.828797 3.184108 -0.279933

O	-3.112414	1.158515	-0.510397
C	-2.677802	3.751663	0.581156
H	-0.901126	3.665018	-0.578389
H	-2.486182	4.730692	1.009310
H	-3.595783	3.243105	0.860117

Cl-TS$_3$
E(gas): -1363.47948;
Frecuencia imaginaria: -270.3 cm^{-1}
E(H_2O): -1363.74746; G(H_2O): -1363.41846
E(THF): -1363.74982; G(THF): -1363.42082

C	-3.254890	0.331859	-1.301742
C	-3.347150	0.650106	0.215155
H	-3.877315	-0.529931	-1.560157
H	-3.368652	-0.275642	0.7910
H	-3.634812	1.178925	-1.887394
H	-4.254714	1.227113	0.454553
C	-1.775301	0.116931	-1.655718
C	-2.1083	1.466923	0.509370
C	-1.187724	1.600634	1.590992
H	-2.068153	2.346693	-0.139563
C	-0.472732	2.928273	1.757146
C	-0.721137	0.508354	2.351104
C	-1.144513	-1.155668	-1.763458
H	-1.286261	0.943057	-2.167130
C	-1.911438	-2.449807	-1.861917
C	0.269783	-1.175017	-1.668300
H	-1.328079	-3.290079	-1.483733
H	-2.865282	-2.438990	-1.336889
H	-2.102152	-2.615923	-2.933272
H	0.573621	2.796643	2.048787
H	-0.510381	3.548001	0.857825
H	-0.972326	3.483738	2.561971
H	0.772846	-2.132606	-1.575968
H	0.867320	-0.395026	-2.128784
H	0.138135	0.687602	2.994127
H	-1.361711	-0.312792	2.643974
Ru	-0.445510	-0.100828	0.179799
Cl	-1.621732	-2.105504	1.135812
N	0.933408	1.375291	-0.502476
N	2.238450	1.199577	-0.210490
C	0.882252	2.464515	-1.279722
C	3.013283	2.144856	-0.785146
C	2.170119	2.991578	-1.484468
H	-0.067553	2.823195	-1.648166
H	4.085992	2.139386	-0.658473
H	2.443588	3.862204	-2.061194
H	2.523028	0.379379	0.329135
H	0.901396	-0.883083	0.841300
H	3.741125	-0.906401	2.205194
C	3.287521	-1.415654	1.357153
C	4.100428	-1.629477	0.174512
C	1.991836	-1.895228	1.429453
H	5.178030	-1.370637	0.293800
O	3.689568	-2.052237	-0.905515
H	1.458749	-1.918796	2.373911
H	1.664386	-2.621269	0.693587

Cl-TS$_4$
E(gas): -1363.48216;
Frecuencia imaginaria: -846.3 cm^{-1}
E(H_2O): -1363.75197; G(H_2O): -1363.42364
E(THF): -1363.75396; G(THF): -1363.42564

C	-3.128196	0.2509	-1.40553300
C	-3.227301	0.997808	-0.04486900
H	-3.734584	-0.658192	-1.381770
H	-3.451499	0.286001	0.75063300
H	-3.512980	0.873926	-2.22202900
H	-4.019523	1.761205	-0.05576900
C	-1.651772	-0.053724	-1.66112200
C	-1.872744	1.647834	0.16680600
C	-1.087783	1.872249	1.346860
H	-1.662392	2.389699	-0.60605800
C	-0.217584	3.105433	1.44846800
C	-0.950249	0.860894	2.29676700
C	-1.047321	-1.356400	-1.64341300
H	-1.128342	0.688753	-2.26102100
C	-1.810793	-2.652323	-1.64420900
C	0.351901	-1.348300	-1.52862700
H	-1.266808	-3.434543	-1.11235600
H	-2.809500	-2.577693	-1.21750800
H	-1.899307	-2.954072	-2.69888500

H 0.750731 2.882697 1.90627600
H -0.044259 3.5840 0.48308900
H -0.733852 3.828763 2.09358700
H 0.901375 -2.248581 -1.26344700
H 0.943947 -0.577614 -2.00743400
H -0.156897 0.953636 3.03546900
H -1.733952 0.152351 2.52662500
Ru -0.451223 -0.058623 0.20393900
Cl -1.869976 -1.821337 1.26817100
N 1.067256 1.219932 -0.55645700
N 2.330236 1.049922 -0.12101500
C 1.096836 2.195162 -1.48303300
C 3.156445 1.898115 -0.76202800
C 2.405762 2.666042 -1.64498800
H 0.190873 2.516204 -1.97809500
H 4.216927 1.889488 -0.550630
H 2.751108 3.444091 -2.30969800
H 2.701662 0.122322 0.50701300
H 0.920870 -0.890475 1.26633700
H 3.761713 -0.751423 2.06266300
C 3.104888 -1.161337 1.29483200
C 3.738906 -1.873921 0.222450
C 1.746878 -1.581902 1.70531800
H 4.840049 -1.709154 0.14149200
O 3.173504 -2.579937 -0.62354300
H 1.545597 -1.507988 2.77659700
H 1.454758 -2.564571 1.33126600

Ciclo con *cis*-H_2O como ligando (*ruta cis-hidroxo*)

c-H_2O-I_0
E(gas): -786.38195;
E(H_2O): -786.63006; G(H_2O): -786.35240

C	-2.614500	0.491556	-1.66012700
C	-2.343300	1.680433	-0.71195300
H	-3.620554	0.082544	-1.522180
H	-2.822339	1.513222	0.25980400
H	-2.547731	0.817396	-2.70282700
H	-2.746767	2.626812	-1.09676900
C	-1.524024	-0.548205	-1.40367100
C	-0.828272	1.750734	-0.58699200
C	-0.032111	2.155793	0.53386500
H	-0.340033	1.910311	-1.54874800
C	1.301791	2.825358	0.33535700
C	-0.412353	1.651657	1.783120
C	-1.642008	-1.640231	-0.48789900
H	-0.786379	-0.674588	-2.193280
C	-2.874024	-1.845929	0.36136300
C	-0.449477	-2.325504	-0.21544500
H	-3.641126	-2.347188	-0.24415800
H	-2.664869	-2.480209	1.22625300
H	-3.319910	-0.905486	0.70752400
H	2.004673	2.582758	1.13667500
H	1.754680	2.556943	-0.62184500
H	1.145074	3.911768	0.34087600
H	-0.401785	-3.021558	0.61642300
H	0.340013	-2.398595	-0.95656800
H	0.253257	1.766804	2.634710
H	-1.461452	1.482147	2.03941200
Ru	-0.291397	-0.145126	0.44948800
N	1.514660	-0.262579	-0.42430200
N	2.497976	-0.723291	0.38270100
C	1.989002	-0.054544	-1.67711900
C	3.611103	-0.784814	-0.36304100
C	3.345312	-0.370302	-1.67497600
H	1.360543	0.313571	-2.47503100
H	4.540104	-1.119771	0.07834800
H	4.033866	-0.299783	-2.50429600
H	0.820497	-0.670614	2.99543400
O	0.750276	-1.145908	2.15738100
H	1.668193	-1.108609	1.690050

c-OH-I_0
E(gas): -786.38184;
E(H_2O): -786.62720; G(H_2O): -786.34918

C	2.445291	-0.066855	1.97515400
C	2.327016	1.279520	1.23650100
H	3.464611	-0.466213	1.93918500
H	2.932498	1.262174	0.32398600
H	2.197011	0.059528	3.03364500
H	2.694305	2.125288	1.834710
C	1.428714	-1.006726	1.34536500
C	0.846867	1.452250	0.91189300
C	0.310448	2.249611	-0.17028600
H	0.227587	1.464603	1.81015100
C	-0.956937	3.043069	0.01989100
C	0.867326	2.049084	-1.41782100
C	1.599805	-1.718708	0.14627500
H	0.592404	-1.312233	1.96858800
C	2.884031	-1.737293	-0.64781400
C	0.397513	-2.253519	-0.42754900
H	3.349615	-2.724784	-0.52338100
H	2.699518	-1.619929	-1.72279300
H	3.608007	-0.987026	-0.32332400
H	-1.445961	3.270327	-0.931090
H	-1.666004	2.518668	0.66813200
H	-0.712223	3.994735	0.50838100
H	0.446262	-2.708067	-1.41388200
H	-0.382584	-2.644049	0.22146100
H	0.405384	2.463939	-2.30898400
H	1.884942	1.675497	-1.54275600
Ru	0.250164	-0.117842	-0.54339300
N	-1.559837	-0.359437	0.37347600
N	-2.607710	-0.569759	-0.45319400
C	-2.043147	-0.381794	1.62707300
C	-3.746772	-0.714620	0.24691600
C	-3.427116	-0.601681	1.594030
H	-1.392588	-0.242734	2.47713700
H	-4.690853	-0.881849	-0.25122200
H	-4.099159	-0.667709	2.43618600
H	-0.538816	0.271529	-2.98292800
O	-0.830771	-0.272141	-2.24163900
H	-2.360409	-0.539166	-1.45853800

c-OH-I_1
E(gas): -979.531298;
E(H_2O): -979.824252; G(H_2O): -979,461945

C	-0.336732	2.729051	1.62285100
C	-0.840460	1.452162	2.33403600
H	-1.153560	3.418569	1.39200700
H	-1.810927	1.149426	1.92762300
H	0.359406	3.273344	2.26991800
H	-0.971784	1.591737	3.41651100
C	0.410670	2.258230	0.37466200
C	0.232260	0.416608	2.03666300
C	0.153036	-1.015682	1.95255700
H	1.211723	0.758935	2.374650
C	1.305470	-1.876440	2.40693200
C	-0.909880	-1.567241	1.25196400
C	-0.153808	2.184876	-0.92564300
H	1.496347	2.290815	0.425050
C	-1.505734	2.761735	-1.253520
C	0.559421	1.397951	-1.86250500
H	-1.357879	3.833075	-1.44915400
H	-1.929633	2.310875	-2.15066500
H	-2.227242	2.674338	-0.43860100
H	1.393002	-2.790337	1.81216900
H	2.260392	-1.347358	2.38484100
H	1.118051	-2.174973	3.44649400
H	0.083137	1.144386	-2.80548600
H	1.644796	1.403590	-1.87349300
H	-0.900371	-2.625302	1.00174900
H	-1.879364	-1.090483	1.21455400
Ru	0.094152	0.026941	-0.16867200
N	2.141694	-0.312295	-0.226050
N	2.496550	-1.169103	-1.20994700
C	3.283527	0.128456	0.32550700
C	3.835397	-1.286957	-1.28829300
C	4.383430	-0.467329	-0.31056200
H	3.269927	0.836311	1.14137200
H	4.298365	-1.935299	-2.01817700
H	5.429364	-0.321479	-0.08676200
H	-1.692968	-0.701962	-1.61968900
O	-2.035197	-0.0058	-1.00972800
C	-3.443527	-0.149537	-0.69894500
C	-3.907816	-1.576024	-0.72396800
H	-3.608163	0.303742	0.28315200
H	-3.997325	0.444676	-1.43748100
C	-4.544151	-2.176015	0.28287400
H	-3.750986	-2.110551	-1.661670
H	-4.911435	-3.193772	0.19744400
H	-4.746068	-1.664638	1.22153700
H	-0.295047	-2.314653	-1.29538700
O	-0.058673	-1.464652	-1.69081200
H	1.682168	-1.544026	-1.742280

c-OH-I_2
E(gas): -979.51926;
E(H_2O): -979.81668; G(H_2O): -979.46148

C	-1.285320	-2.955737	-1.343506
C	-1.622804	-2.985522	0.160246
H	-0.569797	-3.736698	-1.620553
H	-0.726695	-3.206546	0.751049
H	-2.189573	-3.135393	-1.933888
H	-2.360640	-3.759252	0.414492
C	-0.765791	-1.554694	-1.660090
C	-2.168914	-1.597769	0.467459
C	-2.106917	-0.862174	1.698523
H	-3.049718	-1.365015	-0.133330
C	-3.230902	0.054672	2.109069
C	-0.871691	-0.818890	2.344419
C	0.588460	-1.147327	-1.531561
H	-1.391449	-0.936421	-2.300257
C	1.684217	-2.070302	-1.056135
C	0.823095	0.247216	-1.591833
H	2.171244	-2.496728	-1.945237
H	2.446687	-1.517631	-0.497831
H	1.315012	-2.913021	-0.464106
H	-2.876256	0.887703	2.722491
H	-3.768848	0.454971	1.245178
H	-3.950317	-0.518456	2.707485
H	1.802883	0.619201	-1.306564
H	0.208577	0.881804	-2.224008
H	-0.718755	-0.147342	3.184743
H	-0.156649	-1.643460	2.280373
Ru	-0.433779	-0.202558	0.198149
N	-1.602616	1.297795	-0.502279
N	-1.201899	2.542483	-0.159870

C -2.689946 1.432208 -1.279706
C -2.018963 3.466095 -0.697154
C -2.992998 2.793357 -1.424964
H -3.193519 0.568524 -1.687466
H -1.857371 4.520868 -0.527461
H -3.810563 3.224875 -1.982386
H 2.418060 0.898168 0.795486
O 3.185521 0.360038 0.506671
C 4.403737 1.081972 0.710604
C 5.565396 0.167424 0.459491
H 4.465238 1.956347 0.045334
H 4.448961 1.453904 1.747281
C 6.550314 0.422477 -0.400722
H 5.577381 -0.746478 1.052800
H 7.389043 -0.255173 -0.527275
H 6.561540 1.327688 -1.003593
H 0.664187 1.303439 2.061596
O 0.695438 1.356638 1.098296
H -0.344278 2.5393 0.437560

c-OH-I_3
E(gas): -979.51217;
E(H_2O): -979.80981; G(H_2O): -979.44916

C 0.726329 2.498965 1.748072
C 0.873896 2.763118 0.232180
H 1.689690 2.529251 2.264604
H 1.787095 2.291854 -0.146274
H 0.099708 3.270809 2.207425
H 0.937875 3.833444 -0.009091
C 0.024240 1.146907 1.884419
C -0.372050 2.135211 -0.372552
C -0.601610 1.568311 -1.669991
H -1.278834 2.552451 0.067802
C -1.956632 1.664328 -2.325417
C 0.385236 0.745722 -2.204508
C 0.688641 -0.093706 2.090362
H -1.024280 1.176401 2.170450
C 2.162173 -0.201860 2.381417
C -0.085065 -1.250861 1.847435
H 2.282017 -0.116060 3.470262
H 2.551398 -1.175839 2.079928
H 2.760779 0.589386 1.924659
H -2.194352 0.769108 -2.907490
H -2.759346 1.841998 -1.607066
H -1.938945 2.515226 -3.018567
H 0.416891 -2.211884 1.791074
H -1.138055 -1.278513 2.108401
H 0.166152 0.152408 -3.089150
H 1.436543 0.931083 -2.012529
Ru -0.102884 -0.077543 -0.064119
N -2.152445 -0.330789 0.127109
N -2.594006 -1.543363 -0.274669
C -3.213057 0.314725 0.639616
C -3.911756 -1.677229 -0.037262
C -4.352594 -0.497857 0.549670
H -3.118376 1.314320 1.037569
H -4.438004 -2.583735 -0.299709
H -5.356143 -0.257120 0.866418
H 1.438526 -2.578781 -0.420203
O 2.372730 -2.370699 -0.157543
C 2.634260 -1.144302 -0.725879
C 4.014316 -0.6532 -0.429061
H 2.429821 -1.106880 -1.804511
H 1.8894 -0.341811 -0.283123
C 4.753919 0.017782 -1.315189
H 4.404036 -0.885656 0.558166
H 5.755471 0.358986 -1.074520
H 4.398273 0.231198 -2.320762
H -0.024773 -1.967901 -1.910504
O -0.148865 -2.028102 -0.954132
H -1.832919 -2.148703 -0.655588

c-OH-I_4
E(gas): -979.54502
E(H_2O): -979.83133; G(H_2O): -979.47953

C -2.618548 -2.471350 -0.717060
C -2.402589 -2.445053 0.812302
H -2.382869 -3.459177 -1.127285
H -1.575133 -3.108091 1.076801
H -3.670161 -2.279673 -0.957550
H -3.285387 -2.815453 1.352932
C -1.772944 -1.362146 -1.333734
C -2.100118 -1.014912 1.242373
C -1.065382 -0.591014 2.124383
H -2.959564 -0.345637 1.178863
C -1.204748 0.606788 3.032802

C 0.148004 -1.316194 1.965594
C -0.466583 -1.490406 -1.885433
H -2.343768 -0.508241 -1.694572
C 0.233369 -2.813821 -2.073219
C 0.178913 -0.245697 -2.141987
H -0.038015 -3.208542 -3.061518
H 1.320392 -2.698579 -2.048136
H -0.056599 -3.558023 -1.327857
H -0.240929 1.094559 3.226727
H -1.900478 1.348186 2.627784
H -1.588938 0.287332 4.009965
H 1.226956 -0.255142 -2.432251
H -0.399828 0.587878 -2.530967
H 1.058769 -0.934466 2.423075
H 0.144021 -2.393429 1.851698
Ru -0.363350 -0.313157 0.030522
N -1.525419 1.610193 -0.340768
N -0.781374 2.724457 -0.522784
C -2.793620 2.002591 -0.517175
C -1.544909 3.805362 -0.798843
C -2.861361 3.377217 -0.806106
H -3.601191 1.289008 -0.434045
H -1.105839 4.778391 -0.965946
H -3.743103 3.971166 -0.993317
H 2.173879 0.770135 0.636014
O 3.550459 -0.090670 1.053583
C 4.720516 -0.152923 0.680361
C 5.296468 0.626415 -0.410791
H 5.411416 -0.844950 1.196121
H 0.728116 -1.455280 0.051253
C 6.590134 0.479496 -0.734886
H 4.644448 1.319186 -0.936969
H 7.050034 1.044350 -1.539106
H 7.231175 -0.216415 -0.198567
H 1.146642 1.480912 1.557030
O 1.280677 1.208291 0.638347
H 0.222207 2.639262 -0.405203

c-OH-I_5
E(gas): -979.52997;
E(H_2O): -979.82997; G(H_2O): -979.47325

C -1.003948 -2.976824 -1.444715
C -1.161807 -3.100712 0.083857
H -0.228865 -3.645638 -1.832804
H -0.184373 -3.242228 0.559072
H -1.937504 -3.255681 -1.943785
H -1.776986 -3.961504 0.380517
C -0.707904 -1.508147 -1.747876
C -1.811857 -1.794719 0.520379
C -1.664456 -1.096192 1.764436
H -2.781163 -1.640504 0.043753
C -2.811186 -0.315420 2.353982
C -0.367220 -0.953162 2.260720
C 0.597158 -0.939886 -1.807243
H -1.490038 -0.953536 -2.262316
C 1.844265 -1.750753 -1.543103
C 0.652689 0.466747 -1.845973
H 2.137343 -2.246563 -2.479241
H 2.681503 -1.122051 -1.226487
H 1.691924 -2.548585 -0.806956
H -2.467872 0.541783 2.939951
H -3.508440 0.034557 1.588164
H -3.369408 -0.977331 3.028333
H 1.600564 0.980446 -1.702299
H -0.146707 1.028720 -2.320041
H -0.177646 -0.295850 3.104790
H 0.402069 -1.709225 2.086297
Ru -0.258061 -0.225574 0.113705
N -1.615483 1.219454 -0.296240
N -1.232817 2.474436 0.030656
C -2.814207 1.315740 -0.894664
C -2.168601 3.366273 -0.341408
C -3.206669 2.661038 -0.938120
H -3.328016 0.437404 -1.255564
H -2.037381 4.422760 -0.156734
H -4.122088 3.061709 -1.346513
H -0.294760 2.514054 0.479694
H 4.993598 1.341459 -1.309238
C 4.363024 1.1205 -0.452344
C 4.784156 0.273494 0.498386
O 3.192389 1.814564 -0.536718
H 5.772454 -0.151131 0.343503
H 1.032883 1.253116 1.875991
O 0.922938 1.340381 0.921455
H 2.555453 1.610521 0.184596
C 4.083206 -0.104067 1.773810
H 4.650184 0.232416 2.650905

H 3.082519 0.332056 1.843881
H 3.981069 -1.193221 1.869974

c-OH-I_6
E(gas): -979.54208;
E(H_2O): -979.83061; G(H_2O): -979.47754

C -2.139777 -2.803311 -0.930452
C -2.336466 -2.555937 0.577418
H -1.705932 -3.789369 -1.130864
H -1.488268 -2.958841 1.141054
H -3.105460 -2.776595 -1.445320
H -3.235750 -3.047633 0.974205
C -1.272247 -1.669051 -1.463822
C -2.434852 -1.042239 0.723100
C -2.079832 -0.242323 1.865472
H -3.261330 -0.628957 0.142878
C -2.863874 0.998333 2.209874
C -0.858314 -0.515313 2.468944
C 0.139818 -1.620606 -1.400363
H -1.739206 -0.987997 -2.171928
C 0.956580 -2.692567 -0.711119
C 0.739828 -0.359979 -1.665851
H 1.997491 -2.646085 -1.037082
H 0.978245 -2.546091 0.385612
H 0.546077 -3.690697 -0.886661
H -2.253431 1.734848 2.739828
H -3.293996 1.468132 1.320916
H -3.695615 0.717617 2.868383
H 1.803198 -0.244756 -1.477002
H 0.283585 0.319359 -2.381190
H -0.449144 0.164788 3.210398
H -0.425965 -1.516522 2.465224
Ru -0.423788 -0.228232 0.191180
N -1.223259 1.458966 -0.614681
N -0.531609 2.593149 -0.370863
C -2.274389 1.793425 -1.380933
C -1.125122 3.644725 -0.962278
C -2.254083 3.174463 -1.622634
H -2.979685 1.047054 -1.714161
H -0.714027 4.640043 -0.874526
H -2.964416 3.748150 -2.198498
H 5.129151 1.553841 -0.642748
O 3.834209 -1.120367 -0.900177
C 4.791455 -0.513061 -0.457127
C 4.732261 0.874751 0.127768
H 5.799662 -0.982161 -0.474588
H 5.571572 2.046871 1.757789
C 5.578988 1.013204 1.402940
H 3.681433 1.136796 0.291373
H 5.196134 0.378563 2.208701
H 6.621904 0.732522 1.223382
H 1.322823 0.932618 1.761342
O 1.064445 1.063333 0.841936
H 0.322629 2.421088 0.210661

c-OH-I_7
E(gas): -979.55842;
E(H_2O): -979.84507; G(H_2O): -979.49214

C -2.853801 -2.361043 -0.534910
C -2.890280 -1.933239 0.948509
H -2.647034 -3.430589 -0.645820
H -2.136738 -2.481694 1.525770
H -3.826909 -2.180541 -1.2574
H -3.858089 -2.145257 1.423361
C -1.808117 -1.489876 -1.233724
C -2.610273 -0.437540 0.937166
C -1.916503 0.363548 1.902411
H -3.350545 0.117270 0.359650
C -2.285322 1.807487 2.121605
C -0.717478 -0.159848 2.394958
C -0.434412 -1.848635 -1.394267
H -2.190179 -0.759706 -1.943405
C 0.130449 -3.136671 -0.839902
C 0.418951 -0.822577 -1.831036
H -0.099281 -3.953256 -1.537446
H 1.216823 -3.081045 -0.734118
H -0.309472 -3.419659 0.123937
H -1.416056 2.409725 2.397809
H -2.749629 2.247891 1.235701
H -3.9983 1.859766 2.944270
H 1.493845 -0.972274 -1.796475
H 0.054549 -0.025968 -2.471925
H -0.019584 0.468628 2.938357
H -0.569409 -1.235544 2.525832
Ru -0.517595 -0.289135 0.176184
N -0.849760 1.486951 -0.702223

N	0.140272	2.392871	-0.547121
C	-1.858904	2.4491	-1.446745
C	-0.255164	3.502553	-1.188575
C	-1.513503	3.312361	-1.776133
H	-2.748253	1.438597	-1.682704
H	0.380972	4.377590	-1.195076
H	-2.096049	4.017261	-2.351271
H	1.283829	1.458814	0.267025
H	5.187441	-1.706145	-1.147958
C	4.703383	-0.952867	-0.496490
C	5.630162	-0.164389	0.377577
O	3.486034	-0.834110	-0.538554
H	6.170624	-0.903126	0.990505
H	6.406110	0.249778	-0.283951
O	1.464326	0.569356	0.708138
H	2.242019	0.150808	0.276963
C	4.975774	0.915508	1.235191
H	5.724645	1.405039	1.861964
H	4.506262	1.683450	0.613691
H	4.208018	0.495836	1.890688

c-OH-TS$_1$
E(gas): -979.51037;
Frecuencia imaginaria: -46.4 cm^{-1}
E(H_2O): -979.81276; G(H_2O): -979.45265

C	-0.130969	3.001561	-1.198308
C	-0.326177	2.953040	0.331871
H	-1.036149	3.327672	-1.719280
H	-1.319603	2.558385	0.573734
H	0.655434	3.718965	-1.454473
H	-0.254180	3.942439	0.804615
C	0.318234	1.603674	-1.623284
C	0.779217	2.027778	0.819384
C	0.831417	1.178117	1.973723
H	1.763017	2.380308	0.506020
C	2.138771	0.922649	2.680221
C	-0.297253	0.412737	2.261157
C	-0.567454	0.564045	-2.017953
H	1.351698	1.500745	-1.945574
C	-2.054455	0.763088	-2.165924
C	-0.016944	-0.735772	-2.065427
H	-2.235443	1.112220	-3.192488
H	-2.586130	-0.181206	-2.035054
H	-2.469242	1.518520	-1.493116
H	2.176862	-0.075203	3.126376
H	2.999695	1.048374	2.019118
H	2.238548	1.653576	3.492895
H	-0.689086	-1.582773	-2.161979
H	1.011094	-0.894291	-2.376478
H	-0.240041	-0.373868	3.008999
H	-1.301605	0.769496	2.039474
Ru	0.186099	0.006344	0.044783
N	2.123276	-0.573946	-0.202380
N	2.342946	-1.897155	-0.035731
C	3.294750	-0.023799	-0.564409
C	3.632047	-2.197490	-0.273863
C	4.282160	-1.017611	-0.615260
H	3.377280	1.034268	-0.763026
H	3.994952	-3.211254	-0.183657
H	5.324813	-0.891151	-0.864786
H	-1.782260	-2.344257	-0.222646
O	-2.704589	-2.104754	-0.467195
C	-3.102456	-1.141338	0.474635
C	-4.503096	-0.679902	0.208388
H	-3.015483	-1.501746	1.512485
H	-2.415451	-0.248208	0.408653
C	-5.417146	-0.489315	1.160105
H	-4.749894	-0.496956	-0.835940
H	-6.417229	-0.138678	0.926345
H	-5.205736	-0.689712	2.208037
H	-0.383546	-2.163795	1.440827
O	-0.155528	-2.043301	0.510071
H	1.472826	-2.417624	0.223935

c-OH-TS$_2$
E(gas): -979.50420;
Frecuencia imaginaria: -816.9 cm^{-1}
E(H_2O): -979.796860; G(H_2O): -979.44114

C	-0.742779	2.678949	-1.495260
C	-0.811564	2.859402	0.038888
H	-1.731902	2.750855	-1.956246
H	-1.748851	2.447144	0.423674
H	-0.128178	3.465171	-1.946941
H	-0.769699	3.914688	0.343643
C	-0.074605	1.326843	-1.740188
C	0.388645	2.090063	0.567172

C 0.557230 1.395016 1.812211
H 1.325578 2.487004 0.173699
C 1.889750 1.357807 2.517893
C -0.511295 0.615960 2.246674
C -0.755242 0.120519 -2.068137
H 0.974211 1.365491 -2.025899
C -2.219894 0.063599 -2.414279
C 0.016773 -1.056599 -1.939236
H -2.315781 0.318908 -3.478362
H -2.613550 -0.946151 -2.284869
H -2.832751 0.768119 -1.848464
H 2.034694 0.426588 3.074145
H 2.729767 1.494179 1.834349
H 1.914214 2.181027 3.243729
H -0.486120 -2.018665 -1.987387
H 1.068179 -1.058716 -2.207367
H -0.362341 -0.076519 3.072929
H -1.535327 0.915528 2.060715
Ru 0.049241 -0.054949 0.068765
N 2.202668 -0.293832 -0.177397
N 2.638332 -1.552089 0.051157
C 3.269618 0.389750 -0.616517
C 3.952175 -1.679207 -0.225289
C 4.401607 -0.440906 -0.658872
H 3.186455 1.435221 -0.877625
H 4.465173 -2.621206 -0.095101
H 5.403133 -0.175092 -0.961635
H -1.084714 -2.508545 0.480261
O -2.145381 -2.452006 0.142920
C -2.601867 -1.363208 0.685643
C -3.934455 -0.886417 0.284523
H -2.339084 -1.167095 1.731029
H -1.675195 -0.242535 0.207256
C -4.691172 -0.142395 1.101117
H -4.301117 -1.220641 -0.680852
H -5.695590 0.160447 0.824399
H -4.342539 0.171024 2.082452
H 0.157930 -2.134552 1.811482
O 0.137302 -2.117159 0.845037
H 1.916897 -2.214238 0.363285

c-OH-TS$_{3\text{-}14}$
E(gas): -979.51790;
Frecuencia imaginaria: -519.7 cm^{-1}
E(H_2O): -979.81760; G(H_2O): -979.45993

C -0.338275 3.167818 0.994546
C -0.610584 2.125498 2.104381
H -1.243625 3.721756 0.731849
H -1.629214 1.736124 2.021294
H 0.393374 3.909087 1.334015
H -0.504987 2.548698 3.113182
C 0.250438 2.397424 -0.187178
C 0.415193 1.031273 1.869188
C 0.311812 -0.381395 2.085951
H 1.438101 1.402048 1.954486
C 1.503833 -1.188511 2.537390
C -0.870284 -1.003047 1.688244
C -0.450667 2.047328 -1.379447
H 1.332021 2.466112 -0.287387
C -1.809009 2.586953 -1.740742
C 0.1997 1.081833 -2.180177
H -1.647917 3.527384 -2.285070
H -2.350885 1.917902 -2.413504
H -2.435212 2.815842 -0.876486
H 1.494607 -2.201814 2.125301
H 2.453381 -0.709127 2.290049
H 1.454229 -1.280376 3.630222
H -0.346647 0.659468 -3.022458
H 1.280109 1.081377 -2.283876
H -0.895466 -2.086546 1.608292
H -1.838504 -0.522929 1.759804
Ru -0.044569 0.168556 -0.138113
N 2.116309 -0.299945 -0.368059
N 2.409370 -1.558896 -0.762892
C 3.296941 0.316315 -0.226794
C 3.742081 -1.751970 -0.875048
C 4.354683 -0.557743 -0.533613
H 3.342479 1.348917 0.089943
H 4.148760 -2.704438 -1.183190
H 5.413141 -0.346742 -0.510461
H 1.625803 -2.179861 -0.949909
H -4.086334 -3.173014 0.698170
C -3.397406 -2.491182 0.176531
C -3.715772 -1.107023 0.200727
O -2.390753 -3.006651 -0.373996
H -4.481551 -0.775359 0.895166
H -1.211908 -2.296425 -0.856627

O -0.336557 -1.819434 -1.174630
H -0.428050 -1.699771 -2.129146
C -3.077725 -0.183550 -0.637460
H -3.521132 0.805018 -0.708904
H -1.800612 0.258091 -0.161703
H -2.683961 -0.557463 -1.579414

c-OH-TS$_{3\text{-}34}$
E(gas): -979.48080;
Frecuencia imaginaria: -930.4 cm^{-1}
E(H_2O): -979.79652; G(H_2O): -979.44445

C 1.577017 3.091474 -0.160469
C 1.161624 2.736768 1.283700
H 1.052592 3.979437 -0.525763
H 0.1069 2.955880 1.432325
H 2.647730 3.316347 -0.206229
H 1.717420 3.311320 2.038088
C 1.294798 1.852670 -1.003779
C 1.443305 1.249359 1.424037
C 0.771160 0.284373 2.250663
H 2.4967 1.019038 1.259233
C 1.512370 -0.866385 2.884426
C -0.614132 0.378297 2.289967
C 0.117022 1.625433 -1.755997
H 2.163816 1.268137 -1.295381
C -0.919118 2.694607 -1.987433
C -0.062701 0.276741 -2.181305
H -0.524202 3.376901 -2.752318
H -1.848939 2.278599 -2.379056
H -1.138270 3.294393 -1.099865
H 0.869940 -1.741854 3.021559
H 2.392962 -1.160874 2.308865
H 1.855752 -0.554893 3.879136
H -1.018887 -0.007343 -2.616630
H 0.788535 -0.296630 -2.537960
H -1.203301 -0.420976 2.734079
H -1.121921 1.329318 2.184940
Ru 0.081449 0.176368 0.015755
N 1.669448 -1.212829 -0.375288
N 1.287592 -2.451323 -0.771202
C 3.009296 -1.207601 -0.449410
C 2.349765 -3.223834 -1.081187
C 3.484993 -2.454578 -0.885171
H 3.573867 -0.323392 -0.192791
H 2.223138 -4.245327 -1.410020
H 4.512144 -2.750425 -1.035507
H -2.263279 -1.207308 -0.280998
O -5.112690 -2.011312 0.114902
C -4.372557 -1.104045 0.447545
C -3.484221 -0.362740 -0.454531
H -4.304890 -0.786479 1.519313
H -1.699035 0.911243 0.019086
C -2.921086 0.905728 -0.016735
H -3.700196 -0.490441 -1.515675
H -3.078219 1.757791 -0.678683
H -3.169782 1.172881 1.014705
H -1.342961 -1.981686 0.851864
O -1.217077 -1.579498 -0.020632
H 0.289084 -2.645921 -0.784192

Ciclo con *trans*-H_2O como ligando (*ruta trans-acuo)*

t-H_2O-I_0
E(gas): -786.35030;
E(H_2O): -786.61113; G(H_2O): -786.33348

C	-2.716005	0.572551	-1.435786
C	-2.234904	1.802542	-0.620345
H	-3.669637	0.193758	-1.058354
H	-2.565434	1.722438	0.419083
H	-2.879857	0.845750	-2.483659
H	-2.632490	2.746297	-1.018503
C	-1.593468	-0.462035	-1.366990
C	-0.721779	1.771501	-0.726337
C	0.296823	2.188771	0.194299
H	-0.385301	1.810389	-1.763387
C	1.612226	2.717830	-0.316364
C	0.127598	1.870516	1.538563
C	-1.585704	-1.644566	-0.573187
H	-0.912120	-0.463166	-2.215452
C	-2.799699	-2.139258	0.173878
C	-0.328198	-2.254536	-0.396619
H	-3.371328	-2.775184	-0.514808
H	-2.529263	-2.780857	1.020422
H	-3.479844	-1.345831	0.496394
H	2.447654	2.406589	0.315772
H	1.812583	2.407795	-1.344136
H	1.565903	3.814571	-0.297883
H	-0.216717	-3.036944	0.350368
H	0.413900	-2.259530	-1.188184
H	0.972685	1.954054	2.216560
H	-0.858135	1.840331	1.988395
Ru	-0.107616	-0.111622	0.300293
N	1.719656	-0.306124	-0.519883
N	2.092547	-0.583025	0.731306
C	2.705404	-0.595229	-1.392103
C	3.357864	-1.040366	0.690075
C	3.796830	-1.051962	-0.643232
H	2.595753	-0.440213	-2.456404
H	3.879641	-1.320286	1.594571
H	4.769017	-1.341319	-1.015590
H	-1.115570	-0.244516	2.885181
O	-1.638529	-0.245671	2.064668
H	-2.185434	-1.047910	2.104289

t-H_2O-I_1
E(gas): -979.53357;
E(H_2O): -979.82831; G(H_2O): -979.46829

C	0.281053	3.363745	0.27260400
C	0.043503	2.679767	1.64298200
H	-0.568405	3.989241	-0.01594500
H	-1.018588	2.461928	1.78094300
H	1.152121	4.026287	0.31835800
H	0.361855	3.308751	2.48554600
C	0.569514	2.241838	-0.72720200
C	0.867543	1.406967	1.57539300
C	0.668122	0.125041	2.18985800
H	1.922487	1.619228	1.4020
C	1.845091	-0.711658	2.62288800
C	-0.612395	-0.416255	2.176070
C	-0.333262	1.757918	-1.72444700
H	1.621480	2.069474	-0.93916300
C	-1.646422	2.425566	-2.05046600
C	0.005820	0.525225	-2.30101800
H	-1.457360	3.139360	-2.86299600
H	-2.386231	1.714593	-2.43419200
H	-2.067744	3.011738	-1.22792600
H	1.679741	-1.775728	2.43371300
H	2.775170	-0.411473	2.13824900
H	1.968902	-0.577227	3.70560900
H	-0.731126	-0.005725	-2.89736900
H	1.039240	0.239443	-2.460270
H	-0.739574	-1.461770	2.442800
H	-1.495588	0.207211	2.24009700
Ru	-0.093320	0.197631	-0.03755800
N	1.724980	-0.683238	-0.41473900
N	1.635241	-2.007535	-0.689030
C	3.010273	-0.282216	-0.55462700
C	2.869155	-2.441006	-0.98977500
C	3.783486	-1.384329	-0.91637600
H	3.313516	0.740583	-0.37765800
H	3.035039	-3.480449	-1.23955200
H	4.848546	-1.410121	-1.09470100
H	0.119877	-2.216700	-0.73272700
O	-0.844684	-1.817170	-0.66818300
C	-1.802703	-2.716679	-0.098510

C	-3.191894	-2.192882	-0.32417400
H	-1.692856	-3.684243	-0.60641100
H	-1.619687	-2.878005	0.97139200
C	-4.090018	-1.987199	0.64739800
H	-3.463046	-2.016197	-1.36497300
H	-5.102624	-1.660557	0.429420
H	-3.858223	-2.188485	1.69116800
H	-2.810439	-0.051760	0.30547200
O	-2.296851	0.783386	0.29632700
H	-2.710869	1.337478	-0.37872300

t-H_2O-I_2
E(gas): -979.49886;
E(H_2O): -979.80408; G(H_2O): -979.44656

C	1.140905	3.155272	-0.563497
C	1.063304	2.890439	0.964891
H	0.440544	3.939119	-0.865102
H	0.039160	3.017721	1.326483
H	2.140632	3.509788	-0.836012
H	1.697739	3.585494	1.532180
C	0.886984	1.822028	-1.268433
C	1.545327	1.463555	1.141398
C	1.178255	0.442556	2.077061
H	2.554800	1.327896	0.752716
C	2.184646	-0.587531	2.521558
C	-0.175149	0.287896	2.383764
C	-0.338079	1.426611	-1.894972
H	1.773753	1.299126	-1.617900
C	-1.484491	2.373297	-2.145911
C	-0.467308	0.051015	-2.148813
H	-1.334882	2.804047	-3.144935
H	-2.448537	1.856101	-2.175190
H	-1.526060	3.222841	-1.456779
H	1.725021	-1.569040	2.664797
H	3.018173	-0.690779	1.825371
H	2.588620	-0.261267	3.489134
H	-1.438219	-0.362333	-2.412018
H	0.387526	-0.557332	-2.418996
H	-0.490676	-0.615490	2.901038
H	-0.851501	1.132044	2.441319
Ru	-0.025463	0.284710	0.076521
N	1.369433	-1.119552	-0.405463
N	0.908503	-2.390874	-0.433464
C	2.675192	-1.093913	-0.776998
C	1.940507	-3.169466	-0.802055
C	3.086236	-2.398492	-1.032607
H	3.243786	-0.175604	-0.819184
H	1.804551	-4.239680	-0.886511
H	4.067601	-2.730817	-1.338195
H	-0.796188	-2.840648	-0.731353
O	-1.784480	-2.726288	-0.785446
C	-2.115209	-1.959121	0.301646
C	-3.480976	-1.349799	0.170377
H	-1.981613	-2.459327	1.274708
H	-1.365817	-1.076904	0.386624
C	-4.258273	-1.008228	1.205880
H	-3.819481	-1.198924	-0.853898
H	-5.242096	-0.573623	1.058499
H	-3.961167	-1.200334	2.234789
H	-2.706665	0.800470	0.747272
O	-1.999826	1.466036	0.615086
H	-2.360965	2.108469	-0.010153

t-H_2O-I_{3O}
E(gas): -979.52383;
E(H_2O): -979.81523; G(H_2O): -979.46521

C	-3.855231	-0.235520	-0.30949200
C	-3.449970	-0.324404	1.18530100
H	-4.466979	-1.090921	-0.61544200
H	-3.123328	-1.333053	1.44759400
H	-4.478146	0.652164	-0.46622900
H	-4.292680	-0.077352	1.84795300
C	-2.574050	-0.079481	-1.14627400
C	-2.335084	0.700551	1.33854100
C	-1.126391	0.811365	2.06678600
H	-2.680407	1.676250	0.99084200
C	-0.588618	2.197490	2.35772100
C	-0.259702	-0.286803	2.31003100
C	-1.838867	-1.163952	-1.691450
H	-2.401150	0.896747	-1.58971600
C	-2.403052	-2.568051	-1.74158500
C	-0.483672	-0.950617	-2.05674700
H	-2.960641	-2.665659	-2.68215500
H	-1.615640	-3.329840	-1.77863500
H	-3.118047	-2.796902	-0.94471700
H	0.492473	2.259038	2.20359900

H -1.073452 2.976103 1.76471100
H -0.784434 2.417198 3.41518800
H 0.107528 -1.809008 -2.36081700
H -0.170765 -0.008031 -2.49378300
H 0.720210 -0.058076 2.71826700
H -0.662261 -1.248165 2.61081800
Ru -0.662017 -0.369119 0.11069300
N 0.153152 1.424158 -0.55366900
N 1.488193 1.554551 -0.73085700
C -0.382253 2.595175 -0.93815800
C 1.801340 2.773689 -1.21390600
C 0.618940 3.481424 -1.35926900
H -1.448266 2.753798 -0.88594800
H 2.828381 3.039946 -1.41675400
H 0.495192 4.492010 -1.71764900
H 2.134288 0.779103 -0.540410
O 3.726942 -0.124516 -0.59500800
C 4.519366 -0.571593 0.22691800
C 5.786412 -1.206617 -0.13174100
H 4.304951 -0.510324 1.31389200
H 0.849073 -0.980446 0.12528400
C 6.611360 -1.664492 0.82075700
H 6.018977 -1.279727 -1.19065500
H 7.559843 -2.135332 0.58412300
H 6.359891 -1.577950 1.87559200
H -0.2507 -2.800802 1.02951400
O -1.152205 -2.478152 0.88682300
H -1.546321 -3.078128 0.23758500

t-H_2O-I_{3N}
E(gas): -979.52811;
E(H_2O): -979.81806; G(H_2O): -979.46635

C -1.746535 -2.996240 0.01854500
C -1.108333 -2.610619 1.37853100
H -1.309458 -3.914059 -0.38794300
H -0.025355 -2.738466 1.34938800
H -2.813888 -3.202969 0.15659900
H -1.493295 -3.233187 2.19971700
C -1.605771 -1.793728 -0.92858800
C -1.508710 -1.156525 1.58079400
C -0.925379 0.003716 2.14953600
H -2.594159 -1.057817 1.507900
C -1.846178 1.087832 2.67102100
C 0.449284 0.317026 2.02351700
C -0.523506 -1.598761 -1.82380700
H -2.512741 -1.232474 -1.13303200
C 0.457984 -2.705797 -2.143310
C -0.276379 -0.290163 -2.31995700
H 0.041319 -3.281589 -2.97984700
H 1.419823 -2.315165 -2.495830
H 0.617327 -3.417117 -1.32861300
H -1.479185 2.089912 2.43009400
H -2.871213 0.989599 2.30635200
H -1.876421 1.004142 3.76505700
H 0.619061 -0.132398 -2.91376400
H -1.102548 0.370241 -2.56400700
H 0.763089 1.309839 2.33148100
H 1.206780 -0.448053 2.13828300
Ru -0.236148 -0.129971 -0.07849800
N -1.687593 1.346508 -0.39751700
N -1.281177 2.613588 -0.64944700
C -3.025381 1.381418 -0.47616400
C -2.324155 3.441169 -0.88326500
C -3.473837 2.678707 -0.77749900
H -3.606997 0.488444 -0.30515500
H -2.173068 4.488278 -1.10160300
H -4.493841 3.010459 -0.89853500
H -0.286403 2.791898 -0.66049700
O 3.699851 -0.224615 1.17929300
C 4.610439 0.522728 0.83278200
C 4.761441 1.098510 -0.50180600
H 5.391336 0.795796 1.566890
H 0.884018 1.012782 -0.40613200
C 5.808005 1.888631 -0.78311300
H 3.999723 0.861240 -1.24028900
H 5.950997 2.328895 -1.76451900
H 6.560576 2.116991 -0.03183900
H 2.326858 -0.911010 0.47989500
O 1.536272 -1.454534 0.22317400
H 1.802652 -1.950388 -0.56044500

t-H_2O-I_{4O}
E(gas): -979.55541;
E(H_2O): -979.84483; G(H_2O): -979.48691

C 0.856966 3.285985 -0.23439300
C 0.804997 2.831208 1.24828500

H 0.061031 4.002544 -0.455260
H -0.223677 2.845617 1.61156400
H 1.802629 3.794440 -0.45192800
H 1.409211 3.476250 1.900800
C 0.769318 2.022370 -1.08844600
C 1.346619 1.412348 1.24153300
C 1.062731 0.317721 2.14701900
H 2.377506 1.379563 0.88384100
C 2.190985 -0.594983 2.57183100
C -0.240688 0.007969 2.475020
C -0.378472 1.572680 -1.811610
H 1.723888 1.649792 -1.45556200
C -1.623136 2.384318 -2.053050
C -0.310134 0.219700 -2.20813700
H -1.564250 2.766682 -3.080590
H -2.527973 1.775599 -1.97896600
H -1.717689 3.255316 -1.39985500
H 1.836069 -1.601687 2.81066100
H 2.982460 -0.666758 1.82300500
H 2.639796 -0.178534 3.48312900
H -1.216715 -0.261780 -2.570010
H 0.620491 -0.214076 -2.55810400
H -0.440132 -0.934076 2.98164400
H -1.059252 0.710653 2.37600800
Ru -0.045323 0.262619 0.00283300
N 1.625258 -1.054751 -0.525100
N 1.382553 -2.382205 -0.60967900
C 2.909634 -0.905846 -0.878050
C 2.476534 -3.070836 -1.00337200
C 3.491942 -2.147645 -1.18571400
H 3.364714 0.074345 -0.89264900
H 2.453559 -4.144689 -1.120380
H 4.507642 -2.341793 -1.49535600
H 0.434506 -2.695378 -0.422040
O -1.277505 -1.803799 0.01114800
C -2.430717 -2.183939 0.22855500
C -3.556863 -1.350809 0.72958200
H -2.651592 -3.253090 0.04423800
H -3.253927 -0.298788 0.72221300
C -4.866346 -1.629005 -0.03233400
H -3.690537 -1.657307 1.781250
H -5.131050 -2.691397 -0.01869500
H -4.795524 -1.308766 -1.07602400
H -5.685972 -1.075853 0.431270
O -1.767203 1.186886 0.60394400
H -1.978250 2.004512 0.14355700

t-H_2O-I_{4N}
E(gas): -979.53658;
E(H_2O): -979.82720; G(H_2O): -979.47518

C -3.578459 -0.928742 0.24754700
C -2.888295 -0.806442 1.63016700
H -3.848237 -1.966629 0.03370700
H -2.344891 -1.726910 1.86139900
H -4.506473 -0.347556 0.22645800
H -3.615207 -0.649041 2.43921300
C -2.614091 -0.349601 -0.77877600
C -1.946197 0.377826 1.53555700
C -0.657171 0.547604 2.13976700
H -2.458953 1.318216 1.33061300
C -0.163627 1.911400 2.54539300
C 0.193407 -0.554604 2.11179100
C -1.808330 -1.097612 -1.68620400
H -2.806960 0.682522 -1.063880
C -1.928676 -2.595236 -1.82554200
C -0.783577 -0.359276 -2.31239300
H -2.838218 -2.812171 -2.40013300
H -1.095041 -3.015893 -2.39697700
H -2.015271 -3.116585 -0.86850600
H 0.911881 2.015924 2.38281900
H -0.677790 2.712879 2.01114200
H -0.360165 2.038063 3.61800400
H -0.009125 -0.887915 -2.864520
H -0.917748 0.683543 -2.57862400
H 1.251115 -0.423239 2.325920
H -0.176116 -1.572847 2.16246200
Ru -0.503669 -0.195352 -0.06972200
N -0.327084 1.746405 -0.50051600
N 1.002549 1.848063 -0.54644900
C -0.927306 2.920217 -0.80422500
C 1.277647 3.125857 -0.87186200
C 0.087231 3.848508 -1.04734800
H -2.002944 3.033402 -0.81943400
H 2.302507 3.458328 -0.96643500
H -0.028126 4.889362 -1.31357600
H 5.360107 0.943087 -1.14143400
O 2.906652 -2.277998 0.85623700

C	3.964495	-1.764810	0.51254200
C	4.134908	-0.761161	-0.59039800
H	4.888406	-2.067127	1.04268500
H	3.169479	-0.296244	-0.81675600
C	5.215470	0.286727	-0.28052300
H	4.437491	-1.341169	-1.47750400
H	6.177378	-0.184344	-0.05540800
H	4.932740	0.909895	0.57284800
H	1.353822	-2.267977	0.27367200
O	0.405998	-2.291071	-0.03574300
H	0.383750	-2.826732	-0.83813200

t-H_2O-TS_1
E(gas): -979.49695;
Frecuencia imaginaria: -166.2 cm^{-1}
E(H_2O): -979.80057; G(H_2O): -979.44298

C	1.141896	3.162957	-0.49804200
C	1.096026	2.852358	1.02413300
H	0.411504	3.932384	-0.76240100
H	0.082519	2.990862	1.41075100
H	2.125549	3.553949	-0.77893100
H	1.756368	3.519371	1.59514400
C	0.911883	1.845459	-1.23203300
C	1.550291	1.413096	1.16147700
C	1.155888	0.4030	2.10031200
H	2.559371	1.261193	0.778420
C	2.133112	-0.651337	2.55847200
C	-0.198623	0.295157	2.39982200
C	-0.288735	1.445810	-1.90243100
H	1.814208	1.337671	-1.56557400
C	-1.447194	2.373065	-2.16373800
C	-0.372220	0.074996	-2.18930800
H	-1.276917	2.833024	-3.14635200
H	-2.396646	1.833783	-2.23778800
H	-1.529782	3.202657	-1.45402900
H	1.643202	-1.613813	2.728360
H	2.954492	-0.796722	1.85529900
H	2.558763	-0.317653	3.51410600
H	-1.327851	-0.374878	-2.44696400
H	0.506252	-0.502013	-2.452440
H	-0.553540	-0.590749	2.92146200
H	-0.857159	1.154614	2.41296700
Ru	0.003423	0.278191	0.05740500
N	1.415474	-1.094871	-0.41229300
N	0.900580	-2.341664	-0.43582600
C	2.726894	-1.120376	-0.76022400
C	1.906780	-3.167335	-0.77488500
C	3.087160	-2.445117	-0.99337200
H	3.330555	-0.224287	-0.80386900
H	1.728895	-4.231856	-0.85143800
H	4.058797	-2.820984	-1.27913200
H	-0.885801	-2.646021	-0.89983600
O	-1.854210	-2.472774	-0.96840600
C	-2.253465	-2.057696	0.304850
C	-3.595333	-1.369747	0.23107500
H	-2.287020	-2.886390	1.03214700
H	-1.503747	-1.343316	0.74328700
C	-4.243799	-0.827831	1.27071900
H	-4.041572	-1.356630	-0.76254700
H	-5.224389	-0.377337	1.15327200
H	-3.851244	-0.873983	2.28540500
H	-2.722393	0.693289	0.67477500
O	-2.011777	1.362688	0.54505400
H	-2.370901	1.998931	-0.08725300

t-H_2O-TS_2
E(gas): -979.49228;
Frecuencia imaginaria: -1018.4 cm^{-1}
E(H_2O): -979.79510; G(H_2O): -979.44058

C	0.930425	3.243613	-0.60781900
C	0.761150	3.019312	0.91777200
H	0.239887	4.005138	-0.98259100
H	-0.292621	3.063960	1.20739800
H	1.939580	3.612644	-0.81993900
H	1.289646	3.783374	1.50557300
C	0.754616	1.884373	-1.29392900
C	1.360928	1.645793	1.16260500
C	1.075956	0.594404	2.08640400
H	2.390420	1.605533	0.80510100
C	2.184353	-0.316745	2.55589100
C	-0.255922	0.263761	2.37092500
C	-0.457216	1.420604	-1.88483800
H	1.663938	1.397218	-1.63574300
C	-1.646124	2.321585	-2.12062600
C	-0.559221	0.033098	-2.11922800
H	-1.514463	2.781608	-3.108940

H -2.585759 1.761730 -2.16674500
H -1.731007 3.153078 -1.41311800
H 1.851827 -1.354420 2.64740400
H 3.062493 -0.285755 1.90920800
H 2.492187 0.023179 3.55347600
H -1.520899 -0.385785 -2.40452200
H 0.303811 -0.550597 -2.417880
H -0.452847 -0.664885 2.90121700
H -1.026871 1.021599 2.44102100
Ru -0.103818 0.288755 0.08487400
N 1.409997 -1.040025 -0.39692600
N 1.094072 -2.348278 -0.55063500
C 2.723053 -0.899215 -0.68195900
C 2.196093 -3.024919 -0.91811800
C 3.268426 -2.140645 -1.01144300
H 3.210559 0.063138 -0.62515600
H 2.147133 -4.091057 -1.09198500
H 4.291085 -2.360834 -1.278990
H -0.074769 -2.762677 -0.54177400
O -1.289624 -2.981075 -0.57814600
C -1.824759 -2.211335 0.32944800
C -3.235924 -1.755726 0.09963100
H -1.624356 -2.447134 1.39228400
H -1.185970 -1.084237 0.31017600
C -4.081954 -1.428328 1.08586200
H -3.547642 -1.734285 -0.94335800
H -5.107911 -1.136014 0.88409100
H -3.794175 -1.501393 2.13296900
H -2.754476 0.577430 0.68611100
O -2.120786 1.318655 0.60011100
H -2.509273 1.923925 -0.04599700

t-H_2O-TS_{3O}
E(gas): -979.47905;
Frecuencia imaginaria: -951.3 cm^{-1}
E(H_2O): -979.77455; G(H_2O): -979.41986

C 3.016715 -1.3609 -0.91501500
C 2.921273 -1.311915 0.63330200
H 3.860175 -0.768149 -1.28298700
H 3.162084 -0.314934 1.00872500
H 3.195886 -2.388912 -1.24555300
H 3.616205 -2.020800 1.10636800
C 1.669089 -0.894642 -1.47799800
C 1.482044 -1.694731 0.93364900
C 0.553738 -1.350142 1.962800
H 1.247058 -2.664355 0.49130100
C -0.482711 -2.362201 2.39546900
C 0.433133 -0.029396 2.41099100
C 1.380251 0.429875 -1.90662900
H 1.011634 -1.675041 -1.85202900
C 2.450718 1.474110 -2.122330
C 0.012775 0.785558 -2.01196800
H 2.777587 1.391883 -3.16739100
H 2.068763 2.491788 -1.99646900
H 3.347598 1.333291 -1.51153400
H -1.454593 -1.898775 2.58758100
H -0.614499 -3.175261 1.67922700
H -0.137387 -2.806973 3.33787500
H -0.229657 1.828519 -2.202310
H -0.720367 0.071951 -2.37241300
H -0.421779 0.219268 3.03547900
H 1.286694 0.631809 2.48700200
Ru 0.329763 0.081775 0.10049100
N -1.319706 -1.167106 -0.38582300
N -2.581778 -0.670713 -0.39661700
C -1.431620 -2.438049 -0.80559400
C -3.471989 -1.594724 -0.81470800
C -2.768781 -2.757587 -1.08215100
H -0.559149 -3.069090 -0.88390900
H -4.523561 -1.358056 -0.88985600
H -3.163275 -3.701222 -1.42716400
H -2.748861 0.327175 -0.21952400
O -3.028421 2.131234 -0.43152900
C -2.169347 2.919267 -0.07861300
C -1.176211 2.636050 1.023500
H -2.098089 3.915786 -0.55414400
H -0.765583 1.440424 0.562340
C -0.119872 3.555265 1.26318600
H -1.679025 2.214380 1.898090
H 0.137810 3.796999 2.29034100
H 0.043523 4.352666 0.540310
H 1.031370 2.552147 0.95828700
O 1.656243 1.680370 0.70143300
H 2.312446 2.006910 0.07125200

t-H_2O-TS_{3N}
E(gas): -979.47228;

Frecuencia imaginaria: -628.0 cm^{-1}
E(H_2O): -979.77005; G(H_2O): -979.41516

C	2.956657	-1.779252	0.11307900
C	2.481602	-1.332871	1.52240600
H	3.926382	-1.340156	-0.13801100
H	2.763071	-0.295850	1.71517800
H	3.094410	-2.865740	0.08877800
H	2.926573	-1.950039	2.31572600
C	1.855989	-1.407171	-0.88658500
C	0.975638	-1.512968	1.49202600
C	-0.114204	-0.818357	2.09765800
H	0.705983	-2.538486	1.23308600
C	-1.370044	-1.582757	2.44300200
C	-0.119623	0.584033	2.15504500
C	1.859399	-0.256411	-1.72851100
H	1.220603	-2.226811	-1.20807300
C	3.075961	0.618324	-1.91563200
C	0.621884	0.127133	-2.28795500
H	3.635304	0.221097	-2.77276900
H	2.808659	1.648453	-2.176040
H	3.768306	0.610414	-1.06930900
H	-2.268348	-0.971651	2.32704900
H	-1.483373	-2.498538	1.85914600
H	-1.299662	-1.869370	3.50063400
H	0.560988	1.082217	-2.80410900
H	-0.113535	-0.610805	-2.58953500
H	-1.051465	1.081891	2.41213700
H	0.784723	1.142937	2.36063200
Ru	0.336351	0.052963	-0.03131500
N	-1.326628	-1.098132	-0.54011500
N	-2.535819	-0.514377	-0.46679900
C	-1.528974	-2.369810	-0.93309500
C	-3.500928	-1.388387	-0.81311300
C	-2.897162	-2.601296	-1.11905100
H	-0.702813	-3.055183	-1.054930
H	-4.539237	-1.087201	-0.81842900
H	-3.373584	-3.518577	-1.43116500
H	-2.701904	0.583677	-0.24238800
O	0.169750	3.615680	0.78428500
C	-0.850673	3.659395	0.11008500
C	-1.546869	2.501135	-0.55557800
H	-1.361433	4.628498	-0.03243200
H	-0.757398	1.566163	-0.38315500
C	-2.883341	2.197102	-0.09759400
H	-1.512673	2.653499	-1.64201200
H	-3.697786	2.324690	-0.80588300
H	-3.133072	2.411121	0.93995700
H	1.266767	2.397535	0.70236400
O	1.851945	1.601961	0.54972800
H	2.506765	1.865238	-0.10940600

Ruta trans-hidroxo

t-OH-I_0
E(gas):-786.37760
E(H_2O):-786.62574 ; G(H_2O): -786.34640

C	1.965301	0.205825	2.144859
C	1.678552	1.594084	1.519526
H	3.036090	-0.018357	2.137211
H	2.381185	1.801417	0.707273
H	1.647195	0.189356	3.192489
H	1.789636	2.403095	2.255218
C	1.149772	-0.825198	1.368288
C	0.251854	1.528675	1.004370
C	-0.321358	2.254393	-0.113678
H	-0.466041	1.343176	1.803459
C	-1.766950	2.691713	-0.053601
C	0.404777	2.386720	-1.274139
C	1.660202	-1.639227	0.302728
H	0.286998	-1.232826	1.891110
C	3.124119	-1.716040	-0.051281
C	0.6542	-2.262198	-0.467579
H	3.611533	-2.379614	0.675010
H	3.285163	-2.161711	-1.037310
H	3.630961	-0.749259	-0.009984
H	-2.199941	2.802592	-1.051966
H	-2.388621	2.010350	0.531470
H	-1.809420	3.673510	0.435091
H	0.924663	-2.753263	-1.399946
H	-0.264726	-2.609603	-0.006764
H	-0.079277	2.729116	-2.184825
H	1.480947	2.288551	-1.318706
Ru	0.378241	-0.030703	-0.528868
N	-1.630225	-0.527350	0.146436
N	-2.503791	-0.852776	-0.837249
C	-2.316261	-0.681805	1.288003
C	-3.714691	-1.201722	-0.345660
C	-3.632389	-1.102169	1.031555
H	-1.848514	-0.482995	2.241148
H	-4.525523	-1.487611	-1.0007
H	-4.411285	-1.304357	1.751111
H	-2.194569	-0.830388	-1.799331
O	1.668932	0.128163	-1.964852
H	2.234833	-0.642968	-2.107363

t-OH-I_1
E(gas): -979.53082
E(H_2O): -979.82163; G(H_2O): -979.46097

C	-3.442403	0.783999	0.031230
C	-2.909206	0.502581	1.458741
H	-4.226006	0.075093	-0.250111
H	-2.923578	-0.569381	1.664338
H	-3.889391	1.782516	-0.023213
H	-3.503520	1.008070	2.232219
C	-2.236274	0.733991	-0.906591
C	-1.485801	1.030822	1.433645
C	-0.335851	0.642523	2.218561
H	-1.464705	2.094662	1.188920
C	0.639498	1.701655	2.678535
C	-0.039068	-0.695277	2.387996
C	-1.889074	-0.365251	-1.751348
H	-1.847492	1.700692	-1.219998
C	-2.784726	-1.544464	-2.024783
C	-0.569733	-0.321328	-2.244540
H	-3.344593	-1.317316	-2.941978
H	-2.214056	-2.457123	-2.219481
H	-3.526277	-1.730619	-1.243727
H	1.658923	1.313155	2.761929
H	0.648696	2.579962	2.030056
H	0.331779	2.035375	3.678049
H	-0.147334	-1.212509	-2.702402
H	-0.115267	0.619527	-2.534720
H	0.929529	-0.967223	2.801302
H	-0.777128	-1.482546	2.300161
Ru	-0.434753	-0.254490	-0.008554
N	0.870453	1.397930	-0.492661
N	2.148420	1.128458	-0.849922
C	0.7214	2.716981	-0.684645
C	2.805367	2.241064	-1.246186
C	1.912496	3.294517	-1.154652
H	-0.223872	3.197301	-0.478183
H	3.839767	2.200805	-1.555452
H	2.094056	4.331809	-1.391779
H	2.500867	0.178111	-0.779022
O	1.019267	-2.045792	-0.334738
C	2.153196	-2.639477	0.337059
C	3.247944	-1.637226	0.553980

H	1.825649	-3.052019	1.3008
H	2.517178	-3.466837	-0.282451
C	4.407952	-1.646857	-0.109830
H	3.074415	-0.886613	1.325304
H	5.194381	-0.927776	0.100830
H	4.623168	-2.396745	-0.867185
H	0.160044	-2.494502	-0.040984
O	-1.311264	-2.086110	0.477595
H	-2.036524	-2.377316	-0.083875

t-OH-I_2
E(gas): -979.5109
E(H_2O): -979.81184; G(H_2O): -979.45232

C	-3.420621	0.783553	-0.060466
C	-2.894809	0.6089	1.388578
H	-4.175724	0.030489	-0.300912
H	-2.897718	-0.457683	1.656386
H	-3.901335	1.761079	-0.175469
H	-3.510538	1.142919	2.119021
C	-2.210777	0.720484	-0.988925
C	-1.481244	1.151001	1.370364
C	-0.327323	0.782916	2.154019
H	-1.457935	2.202409	1.077878
C	0.656396	1.850825	2.572989
C	-0.030650	-0.554892	2.352736
C	-1.826810	-0.4001	-1.790319
H	-1.834389	1.683944	-1.325609
C	-2.701987	-1.600425	-2.036543
C	-0.498126	-0.351143	-2.263169
H	-3.276269	-1.399455	-2.950824
H	-2.115935	-2.505126	-2.226140
H	-3.427838	-1.789723	-1.242215
H	1.678359	1.465656	2.633677
H	0.641883	2.723836	1.917357
H	0.374354	2.190167	3.578206
H	-0.071717	-1.244924	-2.714928
H	-0.046542	0.586410	-2.568625
H	0.945776	-0.830582	2.743017
H	-0.779995	-1.334528	2.331342
Ru	-0.420484	-0.195958	-0.023139
N	0.902921	1.464743	-0.507589
N	2.242551	1.256532	-0.553635
C	0.736430	2.750160	-0.851046
C	2.912743	2.374815	-0.912129
C	1.970532	3.367315	-1.113739
H	-0.252777	3.183152	-0.890145
H	3.990072	2.378806	-0.994457
H	2.147279	4.390839	-1.407591
H	2.634145	0.340646	-0.349162
O	1.089719	-3.165978	0.843148
C	1.740621	-2.375488	-0.077685
C	3.136341	-2.028559	0.354052
H	1.729742	-2.773139	-1.106602
H	1.194643	-1.361132	-0.184895
C	4.159113	-1.845264	-0.487778
H	3.272864	-1.927448	1.429775
H	5.151123	-1.588925	-0.129259
H	4.051434	-1.990893	-1.560642
H	0.117902	-2.971864	0.752774
O	-1.260898	-1.995248	0.508388
H	-1.847414	-2.394215	-0.143158

t-OH-I_3
E(gas): -979.52927
E(H_2O): -979.81973; G(H_2O): -979.46730

C	1.701208	2.966573	0.619217
C	0.934119	2.342734	1.814460
H	1.268453	3.926239	0.318323
H	-0.143908	2.441860	1.678576
H	2.734891	3.179366	0.914684
H	1.193457	2.834051	2.764076
C	1.727393	1.934434	-0.520408
C	1.377214	0.887207	1.829032
C	0.787601	-0.367489	2.125341
H	2.467173	0.831397	1.872905
C	1.695691	-1.494863	2.572814
C	-0.544992	-0.697675	1.777540
C	0.764956	1.858808	-1.559899
H	2.678835	1.443636	-0.703792
C	-0.226949	2.972864	-1.817324
C	0.636991	0.642459	-2.283153
H	0.248598	3.682622	-2.506597
H	-1.126991	2.611703	-2.328107
H	-0.502369	3.548744	-0.928991
H	1.411972	-2.453845	2.129462
H	2.749566	-1.304108	2.357155

H 1.595033 -1.594395 3.661334
H -0.177914 0.555885 -2.995587
H 1.515183 0.052705 -2.526042
H -0.844093 -1.736689 1.875525
H -1.347844 0.015450 1.915274
Ru 0.352951 0.120549 -0.115431
N 1.889221 -1.250261 -0.495680
N 1.566597 -2.468140 -0.991788
C 3.227424 -1.241573 -0.418204
C 2.662808 -3.223153 -1.227539
C 3.760526 -2.462552 -0.865339
H 3.747859 -0.374970 -0.039606
H 2.580885 -4.224204 -1.625142
H 4.800460 -2.747599 -0.914334
H 0.587622 -2.663957 -1.150417
O -3.624484 -0.311659 0.328764
C -4.749261 -0.331688 -0.165485
C -5.763703 -1.322117 0.177871
H -5.051269 0.425359 -0.916382
H -0.673812 -0.971124 -0.757969
C -6.972041 -1.284184 -0.403234
H -5.492733 -2.072917 0.914920
H -7.746939 -2.005971 -0.166997
H -7.223231 -0.522489 -1.138011
H -2.294896 0.705097 0.162712
O -1.514764 1.321358 0.193401
H -1.674496 1.986511 -0.487211

t-OH-I_{3O}
E(gas): -979.51618
E(H_2O): -979.80573; G(H_2O): -979.45472

C -2.295531 -2.328520 1.207231
C -2.126797 -2.412368 -0.334215
H -3.303441 -2.007467 1.485315
H -2.690560 -1.622651 -0.832417
H -2.155285 -3.320608 1.650487
H -2.497794 -3.366541 -0.737896
C -1.201819 -1.394811 1.740190
C -0.631572 -2.282525 -0.566838
C 0.207417 -1.752891 -1.591452
H -0.100938 -3.042320 0.008878
C 1.553441 -2.406843 -1.823908
C -0.045912 -0.511962 -2.195575
C -1.354579 -0.020809 2.017878
H -0.318793 -1.890490 2.137334
C -2.706725 0.643252 2.122774
C -0.171993 0.791438 2.078411
H -3.009177 0.584643 3.177196
H -2.668574 1.700515 1.852939
H -3.486949 0.159451 1.533789
H 2.342388 -1.677318 -2.025285
H 1.861220 -3.033967 -0.984663
H 1.461982 -3.052887 -2.706999
H -0.313825 1.861395 2.206651
H 0.715878 0.420418 2.590539
H 0.733143 -0.077046 -2.813972
H -1.051381 -0.178731 -2.417256
Ru -0.107813 -0.138534 0.091979
N -1.653701 1.170817 -0.614227
N -1.307908 2.473692 -0.755778
C -2.924433 1.101637 -1.037418
C -2.317681 3.216932 -1.258625
C -3.388063 2.361533 -1.450115
H -3.460372 0.165908 -1.021125
H -2.200615 4.275631 -1.438832
H -4.367272 2.6091 -1.830987
H -0.349096 2.722006 -0.553365
H 5.644778 0.323769 -1.320149
C 4.870601 0.475860 -0.547504
C 5.135429 1.549131 0.425200
O 3.873441 -0.240267 -0.564558
H 6.127003 1.993070 0.397395
H 2.516993 -0.719737 0.330327
O 1.737222 -1.116676 0.797018
H 1.902433 -0.988831 1.740541
C 4.197780 1.993938 1.272882
H 4.397310 2.799083 1.972383
H 0.866293 1.094389 -0.338985
H 3.197017 1.570734 1.267932

t-OH-I_{3N}
E(gas): -979.51964
E(H_2O): -979.80860; G(H_2O): -979.45706

C -3.797641 0.323841 0.041933
C -3.207278 0.186445 1.469676
H -4.570853 -0.427246 -0.151126

H	-3.030279	-0.861136	1.722350
H	-4.290667	1.297142	-0.058821
H	-3.890491	0.590213	2.231559
C	-2.634831	0.266438	-0.963438
C	-1.918039	0.994064	1.427880
C	-0.623163	0.890599	1.993702
H	-2.124175	2.011252	1.088457
C	0.180896	2.163201	2.162787
C	0.053725	-0.345633	2.157805
C	-2.168776	-0.918522	-1.591182
H	-2.372366	1.204916	-1.440625
C	-2.959241	-2.209673	-1.552995
C	-0.859064	-0.931426	-2.138661
H	-3.638991	-2.204835	-2.414937
H	-2.318939	-3.090367	-1.679539
H	-3.596843	-2.325783	-0.670691
H	1.248888	1.998833	1.998143
H	-0.161273	2.971122	1.511267
H	0.057575	2.500425	3.200254
H	-0.471429	-1.873315	-2.514758
H	-0.447818	-0.048816	-2.617727
H	1.109808	-0.307507	2.405608
H	-0.476483	-1.216027	2.529347
Ru	-0.642139	-0.355113	0.026436
N	0.430964	1.260298	-0.732769
N	1.783677	1.247543	-0.692514
C	0.095672	2.414209	-1.332098
C	2.301914	2.367987	-1.237579
C	1.242664	3.147383	-1.671151
H	-0.939869	2.674811	-1.487218
H	3.370118	2.525257	-1.273254
H	1.288369	4.108682	-2.159881
H	2.283534	0.493116	-0.212714
H	4.812482	-1.144333	2.200943
C	4.437321	-1.020678	1.168248
C	5.200967	-1.728659	0.125389
O	3.444205	-0.326873	0.975347
H	6.090893	-2.258667	0.454576
H	-1.967765	-2.864324	0.315423
O	-1.405710	-2.337704	0.901145
H	-0.565630	-2.816105	0.962663
C	4.822559	-1.739134	-1.1608
H	5.389658	-2.269070	-1.918129
H	0.724055	-1.227167	-0.139045
H	3.926040	-1.217038	-1.482119

t-OH-I_{4O}

E(gas): -979.51267

E(H_2O): -979.81976; G(H_2O): -979.46124

C	-2.001075	-2.663472	0.146930
C	-1.326683	-2.496535	-1.245506
H	-3.044171	-2.338388	0.119098
H	-1.832921	-1.733136	-1.841074
H	-2.008143	-3.717116	0.446750
H	-1.365581	-3.426817	-1.829252
C	-1.163984	-1.871285	1.144891
C	0.112520	-2.126995	-0.966396
C	1.027532	-1.266452	-1.663362
H	0.638593	-2.902425	-0.410484
C	2.481131	-1.646239	-1.737711
C	0.577873	-0.008847	-2.055978
C	-1.552780	-0.675537	1.818905
H	-0.353391	-2.432153	1.608858
C	-2.954092	-0.129026	1.827732
C	-0.486113	0.055368	2.388985
H	-3.435554	-0.519517	2.734919
H	-2.970128	0.961344	1.894826
H	-3.558425	-0.441416	0.976326
H	3.127250	-0.781379	-1.898106
H	2.808169	-2.168580	-0.837854
H	2.599163	-2.323290	-2.594704
H	-0.683154	1.065798	2.742834
H	0.328622	-0.448565	2.899417
H	1.308413	0.743613	-2.347480
H	-0.438462	0.166740	-2.380202
Ru	0.072240	-0.251585	0.243080
N	-1.580340	1.072604	-0.515649
N	-1.488855	2.400921	-0.253533
C	-2.699996	0.944804	-1.240842
C	-2.511382	3.101135	-0.797774
C	-3.322448	2.187697	-1.444776
H	-3.021161	-0.028657	-1.579835
H	-2.580787	4.173491	-0.684905
H	-4.234468	2.387783	-1.986512
H	-0.686341	2.756162	0.245666
H	5.100619	1.644715	-0.455086
C	4.146529	1.398164	0.005699

C	3.188516	2.340766	0.129639
O	4.107288	0.120121	0.399866
H	3.385350	3.316719	-0.299815
H	3.207288	-0.199885	0.681206
O	1.771361	-1.076144	1.003178
H	1.753042	-1.213069	1.958894
C	1.916145	2.134026	0.876004
H	1.444824	3.084029	1.150880
H	1.1491	1.572385	0.249568
H	2.048705	1.539435	1.781839

t-OH-I_{4N}
E(gas): -979.50908
E(H_2O): -979.81684; G(H_2O): -979.45861

C	-3.391991	0.723660	0.638364
C	-2.555318	0.515060	1.929249
H	-4.168463	-0.040332	0.545089
H	-2.494443	-0.549392	2.170349
H	-3.904094	1.691388	0.664798
H	-3.004739	1.021777	2.794255
C	-2.410377	0.722821	-0.530211
C	-1.187380	1.093041	1.627949
C	0.111535	0.678611	2.073087
H	-1.225460	2.149086	1.358378
C	1.212223	1.683557	2.281595
C	0.374015	-0.691068	2.098937
C	-2.223786	-0.334587	-1.476800
H	-2.104233	1.707447	-0.871767
C	-3.126859	-1.540078	-1.552663
C	-1.056961	-0.248202	-2.251422
H	-3.956068	-1.289240	-2.227114
H	-2.621823	-2.403786	-1.999754
H	-3.579459	-1.815434	-0.596368
H	2.195848	1.244004	2.103531
H	1.092541	2.572842	1.659078
H	1.168584	1.999895	3.332808
H	-0.749305	-1.104052	-2.847624
H	-0.637497	0.707076	-2.545502
H	1.401797	-1.030389	2.188569
H	-0.404728	-1.399681	2.357037
Ru	-0.443687	-0.207398	-0.031239
N	0.669855	1.359222	-0.678736
N	1.980080	1.059175	-0.795262
C	0.447121	2.636666	-1.078164
C	2.590941	2.160466	-1.267055
C	1.664691	3.190824	-1.465654
H	-0.537199	3.083937	-1.064746
H	3.660496	2.154677	-1.430599
H	1.843641	4.190931	-1.832598
H	2.853923	-0.193936	0.078843
H	4.113633	-2.504040	1.284284
C	3.427275	-2.027206	0.588542
C	2.698746	-2.759015	-0.279053
O	3.405740	-0.694103	0.746951
H	2.822416	-3.836491	-0.254874
H	-1.814088	-2.823053	-0.089204
O	-1.276743	-2.346906	0.559094
H	-0.521112	-2.921945	0.753744
C	1.770715	-2.163950	-1.282148
H	1.325054	-2.917013	-1.937102
H	0.897789	-1.636109	-0.782898
H	2.220143	-1.376949	-1.893789

t-OH-TS_1
E(gas): -979.50554;
Frecuencia imaginaria: -51.6 cm^{-1}
E(H_2O): -979.80731; G(H_2O): -979.44989

C	-2.868578	-1.951782	0.221715
C	-2.363556	-1.517367	1.628990
H	-2.760390	-3.031732	0.090551
H	-1.574109	-2.190549	1.969038
H	-3.933930	-1.724498	0.108438
H	-3.172579	-1.542869	2.371926
C	-2.083483	-1.155146	-0.813550
C	-1.836159	-0.102703	1.469460
C	-0.778128	0.568996	2.202019
H	-2.620109	0.590504	1.160684
C	-0.939088	2.033836	2.539835
C	0.427343	-0.063575	2.427205
C	-1.003986	-1.640097	-1.619547
H	-2.590568	-0.271790	-1.197520
C	-0.630409	-3.088102	-1.785848
C	-0.214467	-0.611711	-2.181246
H	-1.121257	-3.442621	-2.701996
H	0.446039	-3.215942	-1.931919
H	-0.978993	-3.735524	-0.976294

H	0.024513	2.547630	2.599970
H	-1.583466	2.564445	1.836084
H	-1.4108	2.101144	3.529256
H	0.772246	-0.862594	-2.566904
H	-0.669259	0.298127	-2.557172
H	1.271605	0.526013	2.778310
H	0.550342	-1.138824	2.419538
Ru	-0.220076	-0.335368	0.035968
N	-0.678102	1.713242	-0.598157
N	0.350867	2.551336	-0.870731
C	-1.783276	2.413709	-0.889415
C	-0.077490	3.753365	-1.320301
C	-1.459456	3.703255	-1.344661
H	-2.761750	1.974272	-0.758858
H	0.619288	4.536937	-1.580856
H	-2.138747	4.485878	-1.646860
H	1.299919	2.222913	-0.756264
O	2.807926	-1.402017	-0.989975
C	3.177305	-0.142715	-0.471933
C	4.189150	-0.206819	0.638337
H	3.559538	0.461088	-1.303186
H	2.262032	0.388814	-0.086737
C	5.323825	0.492577	0.655526
H	3.946590	-0.881279	1.459543
H	6.028242	0.420136	1.478200
H	5.598640	1.156386	-0.161325
H	2.232584	-1.825236	-0.316764
O	0.669680	-2.043999	0.628703
H	0.379443	-2.852898	0.191389

t-OH-TS$_2$
E(gas): -979.50086;
Frecuencia imaginaria: -801.3 cm^{-1}
E(H$_2$O): -979.80134; G(H$_2$O): -979.444648

C	3.371329	-0.9283	-0.160614
C	2.908707	-0.6908	1.300971
H	4.173815	-0.241156	-0.444097
H	2.913413	0.374206	1.539582
H	3.778250	-1.939782	-0.267958
H	3.559232	-1.201181	2.025304
C	2.135903	-0.803205	-1.059453
C	1.504389	-1.267007	1.345874
C	0.327639	-0.942602	2.091431
H	1.504327	-2.313277	1.033709
C	-0.629937	-2.050564	2.466415
C	-0.061165	0.388429	2.273635
C	1.764324	0.364707	-1.787127
H	1.715185	-1.739093	-1.418075
C	2.682430	1.547467	-1.978091
C	0.424310	0.430407	-2.232504
H	3.230483	1.383563	-2.915454
H	2.130055	2.484450	-2.100320
H	3.437764	1.658770	-1.195508
H	-1.672122	-1.719305	2.448724
H	-0.525990	-2.936270	1.836015
H	-0.400434	-2.352058	3.496807
H	0.067244	1.364824	-2.659176
H	-0.092526	-0.460581	-2.573503
H	-1.062097	0.585597	2.648214
H	0.656158	1.188285	2.396890
Ru	0.344817	0.142275	0.0445
N	-1.011110	-1.398079	-0.525899
N	-2.338320	-1.121740	-0.540635
C	-0.909673	-2.675886	-0.918622
C	-3.067328	-2.191919	-0.929270
C	-2.177281	-3.220447	-1.182501
H	0.056957	-3.152477	-0.987911
H	-4.144643	-2.141716	-0.994146
H	-2.408511	-4.222755	-1.509696
H	-2.661605	-0.190039	-0.295853
O	-0.669032	3.233689	0.776286
C	-1.469102	2.567043	0.008796
C	-2.856533	2.296650	0.499253
H	-1.427940	2.746045	-1.082425
H	-1.011143	1.262988	-0.073593
C	-3.906678	2.153695	-0.318861
H	-2.968929	2.268162	1.581246
H	-4.911707	2.003915	0.062987
H	-3.801814	2.232960	-1.399300
H	0.480410	2.693846	0.694743
O	1.346476	1.957564	0.608358
H	1.992669	2.344697	0.005832

t-OH-TS$_{3O}$
E(gas): -979.49773;
Frecuencia imaginaria: -519.8 cm^{-1}
E(H$_2$O): -979.79993; G(H$_2$O): -979.44415

C	-2.120380	-2.634702	0.154668
C	-1.592092	-2.317477	-1.272402
H	-3.177241	-2.372902	0.256917
H	-2.090780	-1.446960	-1.699070
H	-2.050290	-3.710677	0.348691
H	-1.769314	-3.152009	-1.966549
C	-1.225304	-1.8966	1.155489
C	-0.104248	-2.089138	-1.099480
C	0.881746	-1.268287	-1.724364
H	0.358975	-2.962428	-0.638449
C	2.286137	-1.812672	-1.845943
C	0.644020	0.090812	-1.985828
C	-1.542720	-0.686071	1.820140
H	-0.408240	-2.484073	1.569155
C	-2.932264	-0.102677	1.868642
C	-0.455792	0.065269	2.357087
H	-3.383135	-0.447701	2.809038
H	-2.920718	0.989160	1.894034
H	-3.583888	-0.430133	1.058477
H	3.051581	-1.050928	-1.684132
H	2.472089	-2.643037	-1.162212
H	2.398857	-2.191021	-2.870932
H	-0.674767	1.054633	2.751814
H	0.358219	-0.438724	2.874215
H	1.497083	0.716419	-2.239046
H	-0.315363	0.441598	-2.344373
Ru	0.062295	-0.218607	0.225890
N	-1.476745	1.137252	-0.462180
N	-1.194419	2.460879	-0.369430
C	-2.675118	1.084278	-1.063163
C	-2.172951	3.230595	-0.895305
C	-3.155602	2.371759	-1.352330
H	-3.153447	0.137506	-1.254233
H	-2.098380	4.308426	-0.901117
H	-4.089903	2.633877	-1.825161
H	-0.298005	2.730755	0.007774
H	5.079590	1.453919	-0.495346
C	4.136837	1.189365	0.008909
C	3.207723	2.239309	0.252455
O	3.958199	-0.015606	0.309712
H	3.344050	3.183064	-0.266139
H	2.672071	-0.722039	0.751439
O	1.824763	-1.253398	0.982077
H	1.8540	-1.417529	1.933520
C	2.126327	2.036158	1.104863
H	1.525285	2.894844	1.400598
H	1.029175	1.221285	0.453499
H	2.228055	1.288976	1.884743

t-OH-TS$_{3N}$

E(gas): -979.50105;

Frecuencia imaginaria: -741.7 cm^{-1}

E(H_2O): -979.80942; G(H_2O): -979.45449

C	-3.340304	0.950131	0.645285
C	-2.563055	0.541418	1.924733
H	-4.207362	0.303629	0.484485
H	-2.598239	-0.542104	2.062049
H	-3.727336	1.969789	0.745918
H	-2.992026	0.998792	2.827277
C	-2.347123	0.919415	-0.518453
C	-1.144178	1.029977	1.703166
C	0.120784	0.500338	2.108966
H	-1.103659	2.103815	1.513754
C	1.278477	1.423451	2.387786
C	0.327791	-0.882418	2.025877
C	-2.240688	-0.113405	-1.499430
H	-1.948726	1.885997	-0.808336
C	-3.264844	-1.215219	-1.634789
C	-1.051165	-0.150381	-2.251941
H	-4.045860	-0.854878	-2.317023
H	-2.845173	-2.112673	-2.103629
H	-3.771893	-1.472937	-0.700556
H	2.234566	0.951555	2.148328
H	1.195048	2.376320	1.859508
H	1.270638	1.638511	3.464974
H	-0.855096	-1.014738	-2.881806
H	-0.527095	0.756447	-2.530864
H	1.338923	-1.270353	2.101852
H	-0.4772	-1.569974	2.259841
Ru	-0.459690	-0.232939	-0.042183
N	0.826702	1.285941	-0.611221
N	2.151768	1.012515	-0.662863
C	0.658441	2.555790	-1.040446
C	2.812242	2.097133	-1.104413
C	1.896724	3.111902	-1.366832
H	-0.319374	3.010240	-1.100401

H	3.889766	2.076718	-1.191837
H	2.093324	4.106817	-1.737300
H	2.653561	0.060921	-0.138188
H	4.061307	-2.564842	1.153563
C	3.355865	-2.051447	0.489489
C	2.548656	-2.809097	-0.332259
O	3.337292	-0.761658	0.585913
H	2.563099	-3.889626	-0.238147
H	-2.138501	-2.596512	-0.201710
O	-1.536601	-2.233064	0.462664
H	-0.846243	-2.900694	0.591987
C	1.637568	-2.167969	-1.270369
H	1.081318	-2.857561	-1.908683
H	0.803216	-1.540154	-0.692276
H	2.079419	-1.372330	-1.874992

Tautomería ceto-enol
(1-propen-1-ol → propanal)

Enol·$(H_2O)_4$
E(gas): -498.88342;
E(H_2O): -499.087043; G(H_2O): -498.93903

C 1.932467 0.295938 -0.25741500
C 1.371647 0.324496 0.96665500
H 1.472886 0.876914 -1.05635100
H 1.817912 -0.209141 1.80584800
O 0.239346 0.968144 1.33377800
H -0.150399 1.462113 0.54902700
C 3.239285 -0.395435 -0.546530
H 3.158326 -1.102276 -1.38383500
H 4.020310 0.325529 -0.82389500
H 3.601359 -0.952174 0.32589800
H -1.535229 1.302974 -1.00163100
O -0.864227 2.019883 -0.80034300
H -1.367319 2.836298 -0.69560500
H -1.906081 -0.728003 -1.40638500
O -2.503600 -0.032275 -1.08392600
H -2.574696 -0.272406 -0.12977600
H 0.403694 -1.311118 -0.52754700
O -0.349992 -1.910708 -0.69886500
H 0.036766 -2.746201 -0.98748900
H -1.439136 -1.577655 0.96699800
O -1.959648 -0.920950 1.46147100
H -1.293810 -0.247598 1.69157300

ceto·$(H_2O)_4$
E(gas): -498.89106;
E(H_2O): -499.094061; G(H_2O): -498.94858

C 1.953026 0.070488 -0.417910
C 1.196034 -0.363993 0.80133900
H 1.758804 1.130268 -0.60916900
H 1.421236 -1.384693 1.16764500
O 0.359949 0.307562 1.39101900
H -0.224556 1.810829 0.494180
C 3.454208 -0.245978 -0.33006500
H 3.947908 -0.006548 -1.27654200
H 3.942703 0.335721 0.45944700
H 3.627206 -1.308761 -0.12399300
H -1.794813 1.254796 -0.92618500
O -0.563905 2.426489 -0.18606700
H -0.986014 3.145602 0.29950700
H -1.282594 -0.849645 -1.27621700
O -2.353126 0.472164 -1.11588200
H -2.610671 0.142617 -0.23023400
H 1.492893 -0.505685 -1.23429800
O -0.744285 -1.660016 -1.05825300
H -1.048604 -2.338973 -1.67260800
H -1.777171 -1.571159 0.58930400
O -2.265565 -1.048354 1.25517500
H -1.550478 -0.600244 1.73104300

TS-tautomerización
E(gas): -498.85594;
Frecuencia imaginaria: -1023.0 cm^{-1}
E(H_2O): -499.06008; G(H_2O): -498.91755

C 1.806701 -0.158069 0.31504700
C 0.989694 -1.123108 -0.28700800
H 1.594944 0.039558 1.36990200
H 1.321352 -1.490225 -1.27836200
O -0.143032 -1.539111 0.12502400
H -0.766890 -0.750291 1.44992100
C 3.249416 0.014837 -0.12835100
H 3.586295 1.055488 -0.03712900
H 3.946098 -0.597861 0.46074600
H 3.374140 -0.271463 -1.18050600
H -1.763817 0.894361 0.863130
O -1.236619 -0.104500 2.05461400
H -1.929675 -0.611205 2.49529600
H -0.726477 1.675417 -0.354660
O -1.875765 1.347365 -0.02868700
H -2.144054 0.595470 -0.63385100
H 1.028429 1.002879 -0.27721700
O 0.399076 1.903354 -0.64047100
H 0.695429 2.690306 -0.16231400
H -2.034312 -0.909602 -2.30956300
O -2.263235 -0.905380 -1.37230300
H -1.499730 -1.338616 -0.90893500

Ciclo con El complejo 1.2k
(*ruta cis-hidroxo-k*)

[Ru]H_2Obenzimidazolato
E(gas): -940.01206;
E(H_2O): -940,32096; G(H_2O): -940,00120

C -2.244724 2.486921 -0.415904
C -2.369257 2.059007 1.065087
H -3.226385 2.572511 -0.892242
H -3.236938 1.403386 1.200312
H -1.770334 3.470528 -0.489829
H -2.526418 2.916322 1.733292
C -1.349070 1.465050 -1.108446
C -1.070131 1.347709 1.412534
C -0.887838 0.223470 2.281433
H -0.192807 1.987605 1.329155
C 0.385627 0.054284 3.063547
C -1.817841 -0.819143 2.156737
C -1.805053 0.351038 -1.883926
H -0.338050 1.792885 -1.325853
C -3.269534 0.046620 -2.086170
C -0.801623 -0.567013 -2.213737
H -3.671122 0.719256 -2.855637
H -3.424430 -0.981251 -2.422043
H -3.869114 0.216767 -1.182789
H 0.636520 -0.997472 3.222777
H 1.230876 0.549670 2.581095
H 0.237762 0.517309 4.048335
H -1.074019 -1.523395 -2.651992
H 0.233747 -0.259303 -2.319052
H -1.615105 -1.769274 2.646836
H -2.872246 -0.628760 1.945703
Ru -1.101214 -0.428707 0.077469
N 0.917328 -0.642242 0.118390
C 1.986567 0.191231 -0.215404
C 3.130404 -0.654482 -0.230886
H -1.768196 -3.253719 0.442762
O -1.508029 -2.687126 -0.296843
C 4.405793 -0.137782 -0.494389
C 2.122260 1.572074 -0.440452
H 1.287419 2.262223 -0.384833
C 3.396095 2.065496 -0.708919
H 3.521734 3.129633 -0.886481
C 4.525383 1.223114 -0.742952
H 5.267334 -0.798259 -0.488732
H 5.500939 1.651037 -0.952044
C 1.476999 -1.899161 0.259534
H 0.883196 -2.753475 0.559665
N 2.772217 -1.956420 0.079186
H -0.7926 -3.152096 -0.755997

c-OH-k-I_0
E(gas): -940.039614;
E(H_2O): -940,32391; G(H_2O): -940,00100

C -1.834538 2.637536 0.381717
C -2.111684 1.730075 1.593946
H -2.741377 3.136773 0.022286
H -3.054791 1.190316 1.456262
H -1.135399 3.432644 0.662501
H -2.212366 2.295109 2.531725
C -1.180415 1.772259 -0.693196
C -0.931617 0.769065 1.661405
C -0.935171 -0.578303 2.173470
H 0.018164 1.284031 1.799216
C 0.287975 -1.140052 2.856335
C -1.991076 -1.395764 1.809720
C -1.882461 0.963922 -1.622469
H -0.164172 2.027416 -0.975981
C -3.388941 0.921492 -1.719003
C -1.077661 0.021384 -2.323338
H -3.706313 1.664865 -2.463754
H -3.745633 -0.054930 -2.058711
H -3.887556 1.173438 -0.779244
H 0.368867 -2.222537 2.720046
H 1.207802 -0.663460 2.505646
H 0.211037 -0.946475 3.933695
H -1.568395 -0.689698 -2.983738
H -0.054379 0.273390 -2.590253
H -1.946283 -2.470798 1.946283
H -2.971043 -0.998786 1.550064
Ru -1.090978 -0.495523 -0.192324
N 0.981878 -0.615521 -0.323611
C 2.101514 0.223283 -0.188048
C 3.257490 -0.558128 -0.418851
H -1.439099 -2.552182 -1.637766
O -1.571357 -2.375894 -0.696252

H 3.360547 -2.655080 -0.877652
C 4.552328 -0.038886 -0.359888
C 2.247543 1.583406 0.128635
H 1.395657 2.217568 0.332546
C 3.534115 2.105711 0.187982
H 3.665741 3.155342 0.430984
C 4.671981 1.310519 -0.054935
H 5.422909 -0.661094 -0.541620
H 5.658152 1.759678 0.001989
C 1.450372 -1.827630 -0.610300
H 0.820468 -2.692267 -0.756919
N 2.797095 -1.840541 -0.678448

c-OH-k-I_1
E(gas): -1133.177709;
E(H_2O): -1133,51330; G(H_2O): -1133,11379

C 0.444166 2.989053 -1.817991
C 0.644361 3.466242 -0.366269
H -0.365163 3.530196 -2.319630
H -0.323161 3.675713 0.103859
H 1.3522 3.173821 -2.401664
H 1.224780 4.397405 -0.301721
C 0.190206 1.481647 -1.771974
C 1.373288 2.325193 0.331206
C 1.283691 1.907599 1.696356
H 2.337798 2.112293 -0.126305
C 2.471320 1.285854 2.387568
C 0.013157 1.861376 2.276752
C -1.098915 0.887197 -1.645637
H 0.959472 0.846980 -2.203288
C -2.362230 1.705914 -1.514200
C -1.111524 -0.490522 -1.362144
H -2.669655 2.031845 -2.517833
H -3.169522 1.112735 -1.076975
H -2.217866 2.620909 -0.925672
H 2.170486 0.542908 3.132142
H 3.163125 0.822434 1.679421
H 3.019523 2.077814 2.913585
H -2.048123 -0.960865 -1.075707
H -0.307715 -1.128587 -1.717414
H -0.117098 1.391762 3.247823
H -0.771341 2.566838 1.996995
Ru -0.161126 0.666043 0.354124
N 1.199691 -0.881659 0.332940
C 2.421463 -1.138442 -0.310439
C 2.836654 -2.437542 0.061933
H 1.823042 -3.823861 1.354354
H -3.060045 -0.712142 0.789269
O -3.834271 -0.656613 0.184323
C -4.815477 -1.628962 0.543114
C -6.097448 -1.325128 -0.174405
H -4.481630 -2.648567 0.294713
H -4.993453 -1.599776 1.630996
C -6.763371 -2.197120 -0.929965
H -6.484014 -0.317048 -0.027845
H -7.704883 -1.940223 -1.405627
H -6.395484 -3.207483 -1.094058
H -1.616557 -0.100221 2.351577
O -1.452839 -0.520284 1.498289
H -0.018637 -2.054485 1.605949
N 1.848417 -2.917027 0.909948
C 0.898450 -1.969293 1.038361
C 4.023730 -3.014086 -0.393375
C 3.224686 -0.382767 -1.177602
C 4.405652 -0.954044 -1.638109
C 4.802401 -2.250171 -1.253575
H 4.321768 -4.013388 -0.092193
H 5.732534 -2.658201 -1.635538
H 5.038853 -0.385751 -2.312060
H 2.944890 0.615065 -1.487368

c-OH-k-I_2
E(gas): -1133.168802;
E(H_2O): -1133,50406; G(H_2O): -1133,09856

C -1.023311 2.824852 -0.851682
C -1.330245 2.600108 0.647159
H -1.918748 3.099564 -1.416526
H -2.293470 2.092911 0.765949
H -0.315814 3.653142 -0.968752
H -1.390209 3.541217 1.211996
C -0.367048 1.539587 -1.366612
C -0.166811 1.744905 1.127115
C -0.064465 0.765568 2.163979
H 0.782656 2.241905 0.936860

C 1.239783 0.564918 2.896363
C -1.108299 -0.143770 2.329707
C -1.064448 0.485557 -2.026616
H 0.699544 1.589157 -1.565085
C -2.495976 0.589853 -2.479048
C -0.376457 -0.742014 -2.103734
H -2.475279 0.940246 -3.520335
H -2.988384 -0.384476 -2.462281
H -3.085160 1.307832 -1.905578
H 1.412011 -0.486654 3.144209
H 2.097793 0.945597 2.338753
H 1.185610 1.120696 3.841451
H -0.920753 -1.634146 -2.397950
H 0.698378 -0.767832 -2.247565
H -0.962880 -1.005670 2.976706
H -2.139049 0.151344 2.171606
Ru -0.510281 -0.232852 0.088360
N 1.551865 -0.721894 0.029726
C 2.768481 -0.043101 -0.166493
C 3.808221 -1.002021 -0.160707
H 3.628420 -3.130936 0.069246
H -2.442562 -2.4060 -0.487176
O -3.331672 -2.005467 -0.721927
C -3.486966 -0.976211 0.176632
C -4.727104 -0.176104 -0.063733
H -3.4308 -1.299139 1.226801
H -2.573512 -0.238922 0.082898
C -5.457396 0.352483 0.921173
H -5.023687 -0.053085 -1.101839
H -6.354829 0.927135 0.716397
H -5.201108 0.211829 1.968935
H -1.109962 -2.540221 1.143005
O -0.912546 -2.314738 0.224533
H 1.095847 -2.777222 0.229538
N 3.183042 -2.225337 0.028098
C 1.854919 -2.012586 0.127473
C 3.094992 1.310212 -0.349525
C 5.154399 -0.670197 -0.322099
C 5.452260 0.674756 -0.500535
C 4.433911 1.647694 -0.515053
H 2.339659 2.084262 -0.365107
H 5.931132 -1.428367 -0.310760
H 6.485031 0.980777 -0.632019
H 4.700458 2.689959 -0.659436

c-OH-k-I_3
E(gas): -1133.204615;
E(H_2O): -1133,52362; G(H_2O): -1133,12914

C -2.071689 -3.152997 0.488009
C -1.204662 -2.874160 1.737747
H -1.982710 -4.196421 0.169156
H -0.307353 -3.497745 1.711568
H -3.131682 -2.987704 0.712518
H -1.735477 -3.115439 2.670023
C -1.641743 -2.167364 -0.595814
C -0.838723 -1.398048 1.699556
C 0.416041 -0.793905 2.025080
H -1.696069 -0.739384 1.830123
C 0.516856 0.590409 2.618842
C 1.548461 -1.520528 1.616198
C -0.752698 -2.439270 -1.679669
H -2.333997 -1.346317 -0.769052
C -0.216075 -3.812172 -2.002469
C -0.319210 -1.281181 -2.369409
H -0.920716 -4.301664 -2.688086
H 0.752117 -3.755101 -2.507320
H -0.111787 -4.447334 -1.120325
H 1.4258 1.104010 2.290130
H -0.352024 1.205449 2.371413
H 0.565706 0.506660 3.712514
H 0.469961 -1.378595 -3.112376
H -0.993807 -0.443552 -2.515443
H 2.517014 -1.027340 1.629219
H 1.583749 -2.599898 1.686500
Ru 0.238819 -1.048056 -0.203159
H 5.527741 1.344051 2.020241
C 5.027457 1.351578 1.036247
C 5.738773 2.060209 -0.038993
O 3.942788 0.782974 0.923758
H 6.713875 2.465893 0.216597
H 2.789881 0.347169 -0.284403
O 2.121250 0.108662 -0.970887
H 2.559239 -0.530827 -1.547331
C 5.222989 2.218866 -1.266364
H 5.761328 2.749497 -2.044778
H 1.081329 -2.366994 -0.338489

H 4.242803 1.824823 -1.520106
C -2.159472 1.579247 -0.087925
C -0.193004 2.052898 -0.859110
C -2.178114 2.946889 -0.448608
C -3.325790 0.995953 0.433256
H 0.832462 1.972510 -1.188533
C -3.304286 3.759267 -0.303955
C -4.452428 1.797522 0.579628
H -3.362604 -0.049875 0.712680
H -0.566769 4.087020 -1.292914
C -4.444020 3.159697 0.219028
H -3.293664 4.807160 -0.587537
H -5.363092 1.363212 0.980460
H -5.345002 3.750727 0.349625
N -0.905921 3.207085 -0.933970
N -0.888161 1.050045 -0.357127

c-OH-k-I_4
E(gas): -1133.204615;
E(H_2O): -1133,52205; G(H_2O): -1133,11959

C -2.071689 -3.152997 0.488009
C -1.204662 -2.874160 1.737747
H -1.982710 -4.196421 0.169156
H -0.307353 -3.497745 1.711568
H -3.131682 -2.987704 0.712518
H -1.735477 -3.115439 2.670023
C -1.641743 -2.167364 -0.595814
C -0.838723 -1.398048 1.699556
C 0.416041 -0.793905 2.025080
H -1.696069 -0.739384 1.830123
C 0.516856 0.590409 2.618842
C 1.548461 -1.520528 1.616198
C -0.752698 -2.439270 -1.679669
H -2.333997 -1.346317 -0.769052
C -0.216075 -3.812172 -2.002469
C -0.319210 -1.281181 -2.369409
H -0.920716 -4.301664 -2.688086
H 0.752117 -3.755101 -2.507320
H -0.111787 -4.447334 -1.120325
H 1.4258 1.104010 2.290130
H -0.352024 1.205449 2.371413
H 0.565706 0.506660 3.712514
H 0.469961 -1.378595 -3.112376
H -0.993807 -0.443552 -2.515443
H 2.517014 -1.027340 1.629219
H 1.583749 -2.599898 1.686500
Ru 0.238819 -1.048056 -0.203159
H 5.527741 1.344051 2.020241
C 5.027457 1.351578 1.036247
C 5.738773 2.060209 -0.038993
O 3.942788 0.782974 0.923758
H 6.713875 2.465893 0.216597
H 2.789881 0.347169 -0.284403
O 2.121250 0.108662 -0.970887
H 2.559239 -0.530827 -1.547331
C 5.222989 2.218866 -1.266364
H 5.761328 2.749497 -2.044778
H 1.081329 -2.366994 -0.338489
H 4.242803 1.824823 -1.520106
C -2.159472 1.579247 -0.087925
C -0.193004 2.052898 -0.859110
C -2.178114 2.946889 -0.448608
C -3.325790 0.995953 0.433256
H 0.832462 1.972510 -1.188533
C -3.304286 3.759267 -0.303955
C -4.452428 1.797522 0.579628
H -3.362604 -0.049875 0.712680
H -0.566769 4.087020 -1.292914
C -4.444020 3.159697 0.219028
H -3.293664 4.807160 -0.587537
H -5.363092 1.363212 0.980460
H -5.345002 3.750727 0.349625
N -0.905921 3.207085 -0.933970
N -0.888161 1.050045 -0.357127

c-OH-k-I_5
E(gas): -1133.184934;
E(H_2O): -1133,52321; G(H_2O): -1133,11822

C -0.683553 3.177269 0.866500
C -1.131216 2.176408 1.956341
H -1.506671 3.819721 0.540792
H -2.155482 1.838269 1.767969
H 0.091902 3.844251 1.259182
H -1.120673 2.615859 2.963720

C	-0.086933	2.347169	-0.274624
C	-0.139022	1.029109	1.852362
C	-0.307935	-0.370452	2.099647
H	0.885408	1.365538	2.010553
C	0.842846	-1.191306	2.627006
C	-1.462855	-0.996965	1.634197
C	-0.764468	2.008053	-1.483548
H	0.995362	2.351847	-0.344642
C	-2.092897	2.594489	-1.885283
C	-0.170812	0.976384	-2.235699
H	-1.878173	3.508109	-2.456762
H	-2.654787	1.926351	-2.541740
H	-2.722169	2.880675	-1.041321
H	0.829892	-2.211407	2.232890
H	1.814444	-0.735782	2.422472
H	0.733796	-1.260117	3.717195
H	-0.715280	0.571022	-3.085591
H	0.908071	0.868260	-2.278326
H	-1.505962	-2.080776	1.589504
H	-2.431945	-0.506380	1.607495
Ru	-0.579382	0.125369	-0.172321
H	-4.974694	-2.703715	0.989698
C	-4.295531	-2.099213	0.390316
C	-4.511315	-0.763268	0.269755
O	-3.318026	-2.823953	-0.139518
H	-5.337022	-0.345516	0.836009
H	-2.585296	-2.289006	-0.599798
O	-1.276870	-1.631462	-1.144604
H	-1.305957	-1.484033	-2.097679
C	-3.750409	0.133202	-0.629322
H	-4.276808	1.072937	-0.806366
H	-2.731609	0.4497	-0.207324
H	-3.498095	-0.330904	-1.585444
C	2.695123	-0.188313	-0.173420
C	1.481162	-1.894288	-0.8203
C	3.579070	-1.234034	-0.528359
C	3.227384	1.018721	0.306609
H	0.613210	-2.491828	-1.067781
C	4.967734	-1.120568	-0.443573
C	4.610077	1.139088	0.392005
H	2.595826	1.839095	0.619879
H	3.071375	-3.196608	-1.241452
C	5.471195	0.088405	0.019630
H	5.622635	-1.939708	-0.723512
H	5.036565	2.067038	0.759712
H	6.544740	0.223823	0.101733
N	1.381261	-0.644951	-0.378155
N	2.767813	-2.286335	-0.926011

c-OH-k-TS$_{1'}$

E(gas): -1133.167911;

Frecuencia imaginaria: -45.983 cm^{-1}

E(H_2O): -1133,50737; G(H_2O): -1133,10164

C	-1.117603	2.816655	-0.825724
C	-1.370191	2.623978	0.688486
H	-2.040396	3.048806	-1.364723
H	-2.337980	2.141156	0.851291
H	-0.439336	3.660930	-0.992409
H	-1.379725	3.576064	1.237887
C	-0.443074	1.536167	-1.326191
C	-0.217105	1.742688	1.138692
C	-0.123796	0.755011	2.169593
H	0.741455	2.217796	0.936506
C	1.176418	0.526432	2.900493
C	-1.197626	-0.116871	2.342363
C	-1.109080	0.479021	-2.018673
H	0.626165	1.604818	-1.507738
C	-2.516361	0.570482	-2.542133
C	-0.387245	-0.727105	-2.092423
H	-2.452559	0.943921	-3.573279
H	-2.989146	-0.413071	-2.574150
H	-3.146638	1.261618	-1.980648
H	1.326637	-0.528265	3.149681
H	2.041636	0.886618	2.340836
H	1.135254	1.084799	3.844884
H	-0.898595	-1.629339	-2.416032
H	0.691278	-0.723618	-2.202899
H	-1.070124	-0.9898	2.979530
H	-2.217058	0.224753	2.215501
Ru	-0.570568	-0.221108	0.104326
H	-2.107874	-2.414974	-0.258914
O	-3.151485	-2.077715	-0.633666
C	-3.433166	-1.079504	0.159343
C	-4.617893	-0.248013	-0.156579
H	-3.302595	-1.247888	1.237704
H	-2.343472	-0.165683	0.070581

C	-5.306105	0.397043	0.792345
H	-4.939657	-0.235155	-1.193001
H	-6.201553	0.963694	0.559059
H	-5.013827	0.362462	1.839535
H	-1.047111	-2.649757	1.163648
O	-0.941346	-2.380516	0.241600
C	2.809668	-0.028526	-0.155410
C	1.909577	-1.992038	0.127912
C	3.856917	-0.978905	-0.180257
C	3.119313	1.329625	-0.332048
H	1.172901	-2.776257	0.229070
C	5.196763	-0.633705	-0.365847
C	4.451352	1.681270	-0.521441
H	2.353455	2.094624	-0.327276
H	3.687847	-3.110950	0.024987
C	5.477755	0.716268	-0.536855
H	5.981444	-1.383655	-0.379454
H	4.707063	2.726834	-0.661970
H	6.504897	1.032806	-0.687009
N	1.596741	-0.706269	0.051160
N	3.239565	-2.206375	0.004713

c-OH-k-TS$_1$

E(gas): -1133.163327;

Frecuencia imaginaria: -947.295 cm^{-1}

E(H_2O): -1133,49634; G(H_2O): -1133,09606

C	-0.847474	2.921351	-0.818878
C	-1.181670	2.671302	0.668172
H	-1.723098	3.247135	-1.388344
H	-2.150587	2.166976	0.759647
H	-0.104501	3.721718	-0.904218
H	-1.252344	3.600680	1.250694
C	-0.239971	1.624403	-1.361810
C	-0.035452	1.798815	1.160889
C	0.015591	0.797037	2.177945
H	0.926099	2.283435	1.0472
C	1.297567	0.546272	2.933694
C	-1.051449	-0.098553	2.287559
C	-0.993074	0.590940	-1.994023
H	0.820289	1.644885	-1.597503
C	-2.453584	0.714615	-2.341130
C	-0.336940	-0.648459	-2.116492
H	-2.505945	1.059413	-3.383564
H	-2.958416	-0.253153	-2.280903
H	-2.989808	1.445165	-1.731619
H	1.431028	-0.512807	3.173129
H	2.177756	0.9043	2.395028
H	1.245388	1.094139	3.883353
H	-0.908475	-1.528330	-2.395309
H	0.733408	-0.694858	-2.287777
H	-0.945440	-0.972578	2.925386
H	-2.074692	0.209189	2.092734
Ru	-0.429812	-0.152516	0.088062
H	-2.594163	-2.263662	-0.545339
O	-3.504667	-1.946918	-0.766612
C	-3.788965	-0.961963	0.184227
C	-5.094165	-0.286135	-0.107949
H	-3.786666	-1.350844	1.216629
H	-2.971937	-0.176797	0.165163
C	-5.991884	0.032694	0.825223
H	-5.282677	-0.057943	-1.155273
H	-6.920191	0.535504	0.573733
H	-5.841221	-0.211706	1.874383
H	-1.237066	-2.401982	1.091275
O	-0.993318	-2.179933	0.183445
C	2.805956	-0.125438	-0.170878
C	1.802507	-2.058617	0.106264
C	3.799358	-1.131843	-0.171612
C	3.191451	1.213518	-0.340576
H	1.009327	-2.787892	0.204126
C	5.159441	-0.859525	-0.328463
C	4.544532	1.490855	-0.501300
H	2.469346	2.018704	-0.350313
H	3.524171	-3.252543	0.041978
C	5.517623	0.472160	-0.494514
H	5.901149	-1.652010	-0.323032
H	4.858833	2.521014	-0.635992
H	6.563309	0.732259	-0.622418
N	1.561571	-0.752691	0.017388
N	3.119336	-2.327664	0.006381

c-OH-k-TS$_2$

E(gas): -1133.180190;

Frecuencia imaginaria: -409.0099cm^{-1}

E(H_2O): -1133,51994; G(H_2O): -1133,11845

C	-0.904864	3.130118	0.808131
C	-1.204013	2.160659	1.977916
H	-1.812174	3.640391	0.473553
H	-2.228438	1.784809	1.906995
H	-0.205571	3.913315	1.121887
H	-1.103821	2.645371	2.959097
C	-0.253940	2.295026	-0.294147
C	-0.197238	1.032501	1.831393
C	-0.351799	-0.365464	2.102068
H	0.830380	1.377469	1.947758
C	0.804181	-1.181388	2.624438
C	-1.532472	-0.980938	1.686690
C	-0.864457	1.915299	-1.531080
H	0.830831	2.342015	-0.322547
C	-2.154638	2.484735	-2.055790
C	-0.178814	0.893769	-2.216262
H	-1.889935	3.329420	-2.706015
H	-2.705151	1.768519	-2.671286
H	-2.812991	2.871942	-1.277006
H	0.789925	-2.204908	2.238909
H	1.772692	-0.727103	2.405195
H	0.704623	-1.241054	3.716283
H	-0.652891	0.436993	-3.084163
H	0.904426	0.841273	-2.200195
H	-1.576553	-2.066747	1.654747
H	-2.496251	-0.485815	1.715795
Ru	-0.638041	0.096758	-0.148644
H	-5.064490	-2.667770	0.862234
C	-4.314927	-2.088105	0.300424
C	-4.434483	-0.672388	0.333332
O	-3.421614	-2.732085	-0.303656
H	-5.112273	-0.232247	1.058222
H	-2.143001	-2.168670	-0.851668
O	-1.225735	-1.825366	-1.177955
H	-1.289003	-1.730366	-2.136286
C	-3.705984	0.146433	-0.545271
H	-4.017517	1.184659	-0.612910
H	-2.389138	0.382676	-0.150983
H	-3.433012	-0.289379	-1.503662
C	2.798932	-0.159431	-0.156710
C	1.660796	-1.928425	-0.702092
C	3.732291	-1.176314	-0.465540
C	3.268623	1.099621	0.249091
H	0.841635	-2.599517	-0.915202
C	5.113958	-0.987447	-0.399199
C	4.643342	1.295990	0.316936
H	2.591231	1.902088	0.513596
H	3.305649	-3.190748	-1.079048
C	5.5546	0.270046	-0.004367
H	5.811245	-1.783294	-0.641564
H	5.025545	2.263343	0.627619
H	6.620238	0.464883	0.061420
N	1.503389	-0.671482	-0.321197
N	2.965446	-2.280675	-0.804132

c-OH-k-TS$_2$'

E(gas): -1133.180390;

E(H_2O): -1133,52152; G(H_2O): -1133,11955

C	-0.829028	3.142684	0.831445
C	-1.181074	2.158989	1.972829
H	-1.706598	3.706010	0.502656
H	-2.206233	1.793770	1.860447
H	-0.096066	3.882044	1.173171
H	-1.112445	2.625961	2.965265
C	-0.2039	2.308207	-0.288589
C	-0.176669	1.026866	1.839791
C	-0.332227	-0.371495	2.105327
H	0.849454	1.371623	1.967188
C	0.825880	-1.185175	2.626797
C	-1.502089	-0.995886	1.674914
C	-0.843958	1.949352	-1.515671
H	0.879963	2.339831	-0.337627
C	-2.147767	2.530673	-1.991047
C	-0.196912	0.921305	-2.227034
H	-1.899988	3.403322	-2.610779
H	-2.704577	1.835649	-2.624249
H	-2.793863	2.879444	-1.184533
H	0.812601	-2.208316	2.240456
H	1.793720	-0.728440	2.408738
H	0.727143	-1.246214	3.718536
H	-0.702020	0.481438	-3.085269
H	0.885121	0.845559	-2.236230
H	-1.542852	-2.080995	1.639897
H	-2.472358	-0.508377	1.675959

Ru	-0.621968	0.101204	-0.154531
H	-4.934183	-2.727489	0.887017
C	-4.217339	-2.114770	0.325349
C	-4.417401	-0.736531	0.309207
O	-3.262428	-2.755839	-0.237382
H	-5.183742	-0.323367	0.956601
H	-2.227037	-2.175149	-0.761829
O	-1.260284	-1.758566	-1.163426
H	-1.362666	-1.641051	-2.115665
C	-3.668316	0.143003	-0.556986
H	-4.097051	1.140336	-0.646958
H	-2.536124	0.386495	-0.163728
H	-3.444880	-0.272940	-1.540787
C	2.736306	-0.157370	-0.166065
C	1.573568	-1.904325	-0.760869
C	3.653178	-1.182307	-0.497083
C	3.228579	1.081528	0.274069
H	0.738669	-2.549519	-0.993923
C	5.037716	-1.020307	-0.422326
C	4.606565	1.250861	0.349778
H	2.568615	1.889946	0.560982
H	3.200490	-3.175459	-1.160250
C	5.500731	0.218130	0.004573
H	5.719987	-1.823414	-0.682681
H	5.004103	2.203042	0.686791
H	6.569433	0.391969	0.077805
N	1.434679	-0.651846	-0.349779
N	2.871983	-2.267304	-0.864740

Ciclo con el complejo 1.2k
(*ruta trans-hidroxo-k*)

t-OH-k-I_0
E(gas): -940,04483;
E(H_2O): -940,32552; G(H_2O): -940,00152

C 1.8041310 -1.5351760 1.9943750
C 1.9528550 -0.0286660 2.3251150
H 2.7708440 -2.0464990 2.0313970
H 2.9058660 0.3536610 1.9474380
H 1.1626730 -2.0236550 2.7358040
H 1.9417550 0.1525230 3.4093650
C 1.1416040 -1.6426850 0.6236950
C 0.7806310 0.6639490 1.6514280
C 0.7277560 2.0294140 1.1595550
H -0.1793070 0.3202280 2.0317330
C -0.5747070 2.7910860 1.2530230
C 1.7995340 2.5535710 0.4794970
C 1.8409490 -1.8311090 -0.6132790
H 0.10650 -1.9738190 0.6220510
C 3.3086920 -2.1674960 -0.6984200
C 1.0471440 -1.5589070 -1.7505170
H 3.4187600 -3.2414450 -0.4985300
H 3.7124620 -1.9954170 -1.7006960
H 3.9211870 -1.6304900 0.0297280
H -0.6554260 3.5579610 0.4769290
H -1.4469480 2.1356450 1.2016010
H -0.6074830 3.3006450 2.2246420
H 1.5185200 -1.4966730 -2.7291340
H -0.0120190 -1.79400 -1.7565570
H 1.6953130 3.4872320 -0.0670820
H 2.8005030 2.1484910 0.5380030
Ru 1.1569940 0.2652120 -0.4628990
N -1.0491050 0.2241880 -0.6621250
C -2.2015630 -0.2799960 -0.0348110
C -3.32980 0.0899120 -0.8033010
H 3.3243300 0.0666340 -1.7213410
O 2.8586950 0.7674960 -1.2451880
H -3.3527290 1.2219260 -2.6302630
C -4.6371510 -0.2567070 -0.4561560
C -2.3898860 -1.0301050 1.1381280
H -1.5599570 -1.3345600 1.7634180
C -3.6885640 -1.3799010 1.4889960
H -3.8537120 -1.9605090 2.3910720
C -4.7974810 -1.08970 0.7056110
H -5.4863170 0.0395990 -1.0637850
H -5.7944980 -1.2956890 1.0166020
C -1.4779290 0.8534540 -1.7457260
H -0.8370720 1.3468680 -2.4634640
N -2.8234430 0.8091840 -1.8754670

t-OH-k-I_1
E(gas): -1133,19396;
E(H_2O): -1133,51719; G(H_2O): -1133,11057

C 1.1107410 -3.4234630 0.0694000
C 1.3769990 -2.7983960 1.4648910
H 2.0224750 -3.8598690 -0.3481350
H 2.3941810 -2.4077650 1.5180780
H 0.3826950 -4.2389150 0.1442220
H 1.2469850 -3.5294820 2.2747080
C 0.5245920 -2.3212950 -0.8138810
C 0.3587700 -1.6796390 1.5835190
C 0.4173430 -0.4276270 2.2958540
H -0.6598120 -2.0614280 1.5292940
C -0.8390230 0.1142380 2.9370970
C 1.5551820 0.3577540 2.2216670
C 1.2256110 -1.6105200 -1.8396460
H -0.5554820 -2.3409840 -0.9300320
C 2.5775790 -1.9906910 -2.3839730
C 0.5901780 -0.4244110 -2.2488190
H 2.4044380 -2.5476040 -3.3143230
H 3.1782870 -1.1139660 -2.6421940
H 3.1515920 -2.6517240 -1.7295360
H -0.8635730 1.2078950 2.9309430
H -1.7493210 -0.2661380 2.4694520
H -0.8483460 -0.2090790 3.9862700
H 1.1452830 0.2984460 -2.8419500
H -0.4898030 -0.3680740 -2.3189850
H 1.5014170 1.3835870 2.5785160
H 2.5391820 -0.0469680 2.0215110
Ru 0.9098250 -0.2698630 -0.0234420
O 2.1243080 1.6722040 -0.6442160
C 2.5666970 2.9278240 -0.0777750
C 1.4271670 3.7843890 0.3856310
H 3.2383060 2.7182530 0.7658190

H 3.1430330 3.4592170 -0.8441810
C 1.0990270 4.9501800 -0.1759190
H 0.8806210 3.4350950 1.2616730
H 0.30860 5.5718920 0.2176330
H 1.6382950 5.3378210 -1.0367650
H 2.8262710 0.9702170 -0.4597720
O 2.97680 -0.5185980 0.1291380
H 3.3673090 -1.1673280 -0.4643880
C -2.4622400 -0.0516380 -0.1905540
C -1.3122180 1.7756880 -0.4568980
C -3.3824280 0.9851890 -0.4694840
C -2.9467740 -1.3533110 0.0181950
H -0.5006540 2.4829340 -0.5527000
C -4.7617610 0.7825700 -0.5455590
C -4.3189260 -1.5641230 -0.0585710
H -2.2845970 -2.1814840 0.2357350
H -2.9394940 3.0528520 -0.8485840
C -5.2161040 -0.5133900 -0.3351560
H -5.4466150 1.5969710 -0.7599760
H -4.7095010 -2.5645120 0.0994950
H -6.2802110 -0.7206410 -0.3851220
N -1.1645540 0.4884830 -0.1832010
N -2.6092570 2.1243680 -0.6289090

t-OH-k-I_2
E(gas): -1133,17585;
E(H_2O): -1133,50976; G(H_2O): -1133,10643

C 0.9216830 -3.4499670 -0.1225830
C 1.1570820 -2.9316880 1.3243060
H 1.8408340 -3.8757200 -0.5342660
H 2.1855090 -2.5861350 1.4304180
H 0.1741060 -4.2509770 -0.1302300
H 0.9714560 -3.7149330 2.0721110
C 0.3924340 -2.2795800 -0.9470660
C 0.1823570 -1.7840880 1.5091840
C 0.2916100 -0.5763510 2.2874050
H -0.8533680 -2.1087640 1.4100860
C -0.9473500 -0.0150930 2.9451240
C 1.4667900 0.1609290 2.2675350
C 1.1273850 -1.5181930 -1.9099800
H -0.6861940 -2.2506240 -1.0703770
C 2.4684990 -1.9091230 -2.4726630
C 0.5365790 -0.2797700 -2.2340640
H 2.2809770 -2.4047880 -3.4343540
H 3.0988670 -1.0392090 -2.6803920
H 3.0177990 -2.6247950 -1.8559330
H -0.9246310 1.0770540 2.9996190
H -1.8689140 -0.3318220 2.4524860
H -0.9779360 -0.3939850 3.9751950
H 1.1181530 0.4453210 -2.8009690
H -0.5399610 -0.1771570 -2.3114090
H 1.4597790 1.1724050 2.6668340
H 2.4358810 -0.2822130 2.0836720
Ru 0.8341450 -0.3098390 -0.0077430
O 3.5252980 1.8574560 0.3702270
C 2.4424240 2.3214100 -0.3453460
C 1.9759150 3.6553240 0.1570080
H 2.5970550 2.3448530 -1.4377350
H 1.5468300 1.5987820 -0.2148550
C 1.5368080 4.6414970 -0.6293060
H 2.0274530 3.7824170 1.2373430
H 1.2135870 5.5939520 -0.2208880
H 1.5206810 4.5456890 -1.7128200
H 3.5224050 0.8663550 0.2771970
O 2.8556060 -0.6707950 0.1724100
H 3.2588770 -1.1815760 -0.5366980
C -2.5224010 0.1157020 -0.2025730
C -1.2887920 1.9053550 -0.1268600
C -3.3906600 1.2270950 -0.3021800
C -3.0677020 -1.1785050 -0.2163650
H -0.4526600 2.5910150 -0.0804930
C -4.7761320 1.1053980 -0.4254360
C -4.4461720 -1.3086390 -0.3410560
H -2.4475580 -2.0611790 -0.1249140
H -2.8508940 3.3067070 -0.2913400
C -5.2904040 -0.1849850 -0.4464130
H -5.4206680 1.9754930 -0.5006700
H -4.8844610 -2.3015750 -0.3550250
H -6.3615100 -0.3308500 -0.5421450
N -1.2016800 0.5832260 -0.0934520
N -2.5655790 2.3389950 -0.2468140

t-OH-k-I_{3a}
E(gas): -1133,19262;
E(H_2O): -1133,51678; G(H_2O): -1133,12015

C 0.3627780 3.3550450 -0.1050970
C -0.1767030 2.9326100 1.2883380
H -0.2928020 4.0907420 -0.5841610
H -1.2542340 2.7657030 1.2674190
H 1.3307970 3.8548370 0.0177900
H 0.0104960 3.7134090 2.0408850
C 0.5800920 2.0924380 -0.9602030
C 0.5919880 1.66720 1.6407340
C 0.3216010 0.4278340 2.2675780
H 1.6627280 1.8745510 1.6206950
C 1.4858680 -0.3134750 2.8954810
C -0.89990 -0.2854910 2.1213380
C -0.3818610 1.5377440 -1.8443550
H 1.6094310 1.7935400 -1.1244770
C -1.6208190 2.2873630 -2.2840770
C -0.2489940 0.1737270 -2.2133800
H -1.3830040 2.7725660 -3.2397530
H -2.4655080 1.6180070 -2.4735090
H -1.9256680 3.0963020 -1.6109650
H 1.4183690 -1.3931650 2.7344180
H 2.4573940 0.0368310 2.5395260
H 1.4484810 -0.14180 3.9791130
H -1.0521350 -0.2805940 -2.7857880
H 0.7321160 -0.2585880 -2.3813750
H -0.9155840 -1.3043560 2.4978730
H -1.8542960 0.2260890 2.1530030
Ru -0.2996360 0.2140470 0.0365180
O -4.2360640 -0.6275180 -0.5816650
C -5.1714020 -1.0409540 0.1013200
C -6.2412900 -1.8833060 -0.4212580
H -5.2426300 -0.7802070 1.1756970
H -1.1345150 -1.1509450 -0.2208460
C -7.2355910 -2.2904130 0.3817980
H -6.1911600 -2.1527580 -1.4725840
H -8.0471020 -2.9142780 0.0219180
H -7.2670050 -2.0072770 1.4315880
H -3.0125270 0.3565290 -0.0152660
O -2.3611820 1.0664990 0.2417200
H -2.5722560 1.8145760 -0.3304070
C 2.8383930 -0.7673340 -0.2231170
C 1.3032510 -2.3062830 -0.3413510
C 3.4929500 -1.9963400 -0.4675360
C 3.6096450 0.3970630 -0.0797590
H 0.3507520 -2.8115240 -0.3548440
C 4.8789240 -2.1126620 -0.5915670
C 4.9902060 0.2901860 -0.2035590
H 3.1546170 1.3542370 0.1372200
H 2.5923480 -3.9331270 -0.6931430
C 5.6190550 -0.9447560 -0.4592790
H 5.3551740 -3.0697280 -0.7802830
H 5.6007120 1.1813460 -0.0960540
H 6.6999220 -0.9845710 -0.5488520
N 1.4540500 -1.0027710 -0.1537500
N 2.4830770 -2.9425770 -0.5325880

t-OH-k-I_{3b}
E(gas): -1133,17534;
E(H_2O): -1133,50551; G(H_2O): -1133,11010

C 0.6910150 3.2833250 1.1049960
C 0.7638250 3.0789040 -0.4306140
H 1.6902220 3.3451730 1.5461960
H 1.6315180 2.4730120 -0.6873790
H 0.1888650 4.2289240 1.3377490
H 0.8676970 4.0297660 -0.9755920
C -0.1376860 2.1319220 1.6674500
C -0.5244670 2.3812570 -0.8282400
C -0.8458690 1.4624620 -1.8775880
H -1.3963060 2.9556540 -0.5135450
C -2.2140200 1.5151730 -2.5193720
C 0.0046470 0.3890610 -2.1419310
C 0.3409470 0.9224930 2.1833010
H -1.1937580 2.3505200 1.8067180
C 1.79020 0.7206760 2.5590070
C -0.5870750 -0.1891480 2.2500530
H 1.9160500 1.0745720 3.5912090
H 2.0748800 -0.3326410 2.5395960
H 2.4884710 1.2787820 1.9328190
H -2.5931470 0.5192270 -2.7647160
H -2.9467860 2.0236390 -1.8892380
H -2.1315730 2.0833580 -3.4551240
H -0.1892330 -1.1350710 2.6108480
H -1.6016180 -0.0049690 2.6095300
H -0.3371310 -0.4052500 -2.7981200
H 1.0772790 0.4676600 -2.0211280
Ru -0.5275380 0.3123740 0.1422320
H -5.8554730 -1.7700430 -1.7105050

C -5.1307930 -1.5865400 -0.8974090
C -5.2086950 -2.5048020 0.2524410
O -4.3359800 -0.6589670 -1.0152500
H -6.0658300 -3.1724940 0.2808850
H -3.2355130 0.2588710 -0.1044800
O -2.6594940 0.9014740 0.3837880
H -2.9321620 0.8405680 1.3089600
C -4.2568940 -2.5545680 1.1943240
H -4.3162720 -3.2483110 2.0266820
H -1.1749960 -1.0908960 -0.3177040
H -3.3820270 -1.9122860 1.1379770
C 2.6509870 -0.7993760 -0.2998300
C 1.1139060 -2.2382570 0.2384450
C 3.2605650 -2.0744870 -0.2763700
C 3.4347080 0.3188420 -0.6180680
H 0.1710320 -2.6903800 0.4985610
C 4.6118200 -2.2824370 -0.5592220
C 4.7807580 0.1225470 -0.9050930
H 3.0164280 1.3155600 -0.6346330
H 2.3287720 -3.9563920 0.1746410
C 5.3646210 -1.1592050 -0.8775590
H 5.0530280 -3.2738450 -0.5309090
H 5.3982220 0.9798410 -1.1544130
H 6.4196740 -1.2704620 -1.1063330
N 1.2911580 -0.9411330 0.0319250
N 2.2502960 -2.95510 0.0741630

t-OH-k-I_4

E(gas): -1133,17966;
E(H_2O): -1133,52464; G(H_2O): -1133,12214

C 0.4643840 3.3114740 0.1943650
C 0.1222900 2.8735140 -1.2590290
H 1.5458560 3.3137550 0.3520370
H 0.9673950 2.3579430 -1.7202520
H 0.1139170 4.3316340 0.3872870
H -0.0997080 3.7387520 -1.8989770
C -0.2580950 2.3563900 1.1291790
C -1.0989260 1.9826600 -1.2009570
C -1.3603040 0.7649780 -1.9102860
H -2.0058630 2.4972890 -0.8899660
C -2.7535970 0.4184380 -2.3603220
C -0.3124540 -0.1500610 -1.9776040
C 0.3349780 1.4212640 2.0265060
H -1.2866450 2.6402460 1.3501630
C 1.8069210 1.3789090 2.3341050
C -0.5546470 0.4337080 2.5180220
H 1.9793870 2.0812880 3.1613980
H 2.1227450 0.3908090 2.6747290
H 2.4437090 1.6862030 1.5037140
H -2.8899070 -0.6616350 -2.4583370
H -3.5128950 0.8124340 -1.6844560
H -2.9080530 0.8694690 -3.3496210
H -0.1346250 -0.4189130 3.0485890
H -1.5654370 0.6903050 2.8207950
H -0.5107510 -1.1703660 -2.2977410
H 0.7223750 0.1629400 -2.0202670
Ru -0.6834990 0.3535590 0.2927380
H -5.3291490 -2.5551410 -1.0132670
C -4.4867580 -2.1413570 -0.4633690
C -3.3926220 -2.8888140 -0.2246560
O -4.72180 -0.8736960 -0.0822690
H -3.3687850 -3.8870050 -0.6486820
H -3.9035540 -0.4066190 0.2217060
O -2.6586580 0.7476250 0.5872000
H -2.8660200 0.9620010 1.5056600
C -2.2512320 -2.4627920 0.6476130
H -1.7057010 -3.3307750 1.0328870
H -1.4975750 -1.8428590 0.0946650
H -2.5864740 -1.8610890 1.4964580
C 2.5868820 -0.6067470 -0.2643370
C 1.3118910 -1.97710 0.8348710
C 3.3479550 -1.7687100 -0.0104640
C 3.1748040 0.4664910 -0.9486020
H 0.4741960 -2.4303740 1.3433780
C 4.6733370 -1.9138370 -0.4260120
C 4.4931450 0.3303270 -1.3678930
H 2.6271260 1.3820150 -1.1352980
H 2.7136040 -3.5370520 1.0344970
C 5.2318990 -0.8434880 -1.1140610
H 5.2413020 -2.8157290 -0.2210030
H 4.9679190 1.1481510 -1.9007680
H 6.2588800 -0.9100520 -1.4584180
N 1.3045210 -0.7745150 0.2793620
N 2.4999440 -2.6107950 0.6930310

t-OH-k-TS_1,

E(gas): -1133,17348;
Frecuencia imaginaria: -53.98 cm^{-1}
E(H_2O): -1133,50633; G(H_2O): -1133,10359

C 0.2358790 -3.5800580 0.1149950
C 0.6446890 -2.9861620 1.4903260
H 1.0113010 -4.2509820 -0.2653830
H 1.7292420 -2.8640140 1.5394210
H -0.6778390 -4.1763200 0.2126770
H 0.3461710 -3.6432580 2.3192630
C -0.0379500 -2.4098720 -0.8233880
C -0.0577340 -1.6450630 1.5950970
C 0.3808660 -0.4580470 2.2980650
H -1.1422520 -1.7382680 1.5689700
C -0.6477330 0.4390560 2.9462950
C 1.7030480 -0.0764550 2.2260960
C 0.8561260 -1.9176630 -1.8271030
H -1.0857770 -2.1780800 -0.9904610
C 2.0971160 -2.6448280 -2.2736820
C 0.5258360 -0.6266560 -2.2919000
H 1.7907360 -3.3933330 -3.0162740
H 2.8037520 -1.9785080 -2.7790470
H 2.6080240 -3.1771460 -1.4678330
H -0.3215100 1.4828620 2.9723370
H -1.6251060 0.3782070 2.4631920
H -0.7752230 0.1108860 3.9861090
H 1.2446600 -0.0855450 -2.9044880
H -0.5081840 -0.3195340 -2.4024180
H 2.0079620 0.9185770 2.5360890
H 2.5027690 -0.7653750 1.9915470
Ru 0.8233870 -0.5286870 -0.0713390
O 3.5482560 1.8125180 0.5287020
C 2.8105840 2.4763360 -0.4711510
C 2.2166920 3.7453890 0.0792930
H 3.4162090 2.6991910 -1.3647470
H 1.9819030 1.8201310 -0.8256010
C 2.0159780 4.8619720 -0.6231750
H 1.9369220 3.7001720 1.1320450
H 1.5658970 5.7434140 -0.1769650
H 2.3216040 4.9472380 -1.6636010
H 3.5458720 0.8600570 0.3048380
O 2.8062340 -0.7883380 -0.1003980
H 3.1619690 -1.1988960 -0.8971310
C -2.4930550 0.3032470 -0.1914990
C -0.9999990 1.8793350 -0.3492230
C -3.1856620 1.5228830 -0.3745290
C -3.2328600 -0.8831030 -0.0496210
H -0.0703140 2.4309100 -0.3928640
C -4.5778030 1.6111140 -0.4344780
C -4.6195150 -0.8035980 -0.1091300
H -2.7570610 -1.8424600 0.1094200
H -2.3354850 3.4841830 -0.5996880
C -5.2854160 0.4233560 -0.3010340
H -5.0828770 2.5611010 -0.5778580
H -5.2052220 -1.7112190 -0.0025750
H -6.3697070 0.4404030 -0.3419350
N -1.1114010 0.5686850 -0.1827710
N -2.1997320 2.4923590 -0.4652400

t-OH-k-TS_1
E(gas): -1133,02090;
Frecuencia imaginaria: -683.77 cm^{-1}
E(H_2O): -1133,49751; G(H_2O): -1133,09895

C 0.9654300 -3.4109790 -0.1347390
C 1.2586140 -2.8933020 1.3001720
H 1.8551130 -3.8654130 -0.5808290
H 2.2751340 -2.5040590 1.3694840
H 0.2019950 -4.1965980 -0.1057410
H 1.1511530 -3.6894390 2.0503450
C 0.4210920 -2.2353800 -0.9539900
C 0.2269870 -1.8036770 1.5345690
C 0.2380890 -0.5760740 2.2677750
H -0.7845260 -2.1983810 1.4346940
C -1.0484240 -0.0956860 2.8993090
C 1.3384050 0.2883720 2.2109540
C 1.1661490 -1.4531970 -1.8857560
H -0.6547570 -2.2147590 -1.0907850
C 2.5324940 -1.8351540 -2.40400
C 0.6089980 -0.2028030 -2.2282530
H 2.3826790 -2.3570940 -3.3543550
H 3.1545940 -0.9608320 -2.6153900
H 3.0758210 -2.5313240 -1.7550760
H -1.1348690 0.9942720 2.8804660
H -1.9364840 -0.5330510 2.4384180
H -1.0355390 -0.4058840 3.9525030
H 1.2122430 0.4918420 -2.8085920

H -0.4637990 -0.0781980 -2.3260350
H 1.2144700 1.2967240 2.5973830
H 2.3569640 -0.0708090 2.1502470
Ru 0.8084290 -0.2223900 0.0223560
O 3.5279140 1.7581430 0.2112760
C 2.4996510 2.2848700 -0.3661690
C 1.9265270 3.5351650 0.2257040
H 2.4479270 2.2757990 -1.4724370
H 1.4131110 1.4358660 -0.1942620
C 1.3164270 4.4790440 -0.5012090
H 2.0799430 3.6525380 1.2967850
H 0.9523040 5.3984830 -0.0531640
H 1.2098990 4.3865700 -1.5806420
H 3.3636430 0.4704290 0.1933550
O 2.9417500 -0.5658400 0.2144910
H 3.3887480 -1.0668420 -0.4776430
C -2.4885970 0.0648810 -0.2223610
C -1.27940 1.8858020 -0.1356190
C -3.3715670 1.1631400 -0.3320860
C -3.0155700 -1.2369680 -0.2343350
H -0.4109010 2.5454090 -0.0708520
C -4.7542450 1.01930 -0.4678220
C -4.3902770 -1.3886200 -0.3710490
H -2.3840590 -2.1097560 -0.1279770
H -2.8746150 3.2441500 -0.3174280
C -5.2502220 -0.2777830 -0.4895110
H -5.4105240 1.8799970 -0.5508640
H -4.8137380 -2.3880300 -0.3834440
H -6.3181460 -0.4398620 -0.5944620
N -1.1847130 0.5607740 -0.1013310
N -2.5646210 2.2848350 -0.2682030

t-OH-k-TS$_2$
E(gas): -1133,15895;
Frecuencia imaginaria: -462.89 cm^{-1}
E(H_2O): -1133,50112; G(H_2O): -1133,10084

C -0.2024510 3.4519770 -0.2194390
C -0.4468560 2.7176150 1.1220500
H -1.1399130 3.7915980 -0.6702510
H -1.3364350 2.0995260 1.0334700
H 0.4118830 4.3436750 -0.0559460
H -0.6094640 3.4148170 1.9577260
C 0.5671960 2.4813640 -1.1126670
C 0.8268370 1.9128320 1.3322920
C 1.2441090 0.7033760 1.9662950
H 1.6827110 2.5824190 1.2328220
C 2.6453830 0.6718290 2.5388260
C 0.5449950 -0.5116390 1.8341050
C -0.0233330 1.5704230 -2.0109070
H 1.6319690 2.6742210 -1.2183470
C -1.4897950 1.6539510 -2.3680200
C 0.7951440 0.49460 -2.4835770
H -1.6161310 2.4901320 -3.0680480
H -1.8377420 0.7517710 -2.8744970
H -2.1377100 1.8415340 -1.5089010
H 3.1389220 -0.2915200 2.3964200
H 3.2852360 1.4529790 2.1235470
H 2.5607010 0.8475800 3.6196360
H 0.3367160 -0.2330970 -3.1485410
H 1.8407110 0.6809510 -2.7262280
H 1.0668360 -1.4225660 2.1196200
H -0.5315830 -0.57140 1.8840520
Ru 0.7691480 0.2777240 -0.2904960
H 4.5705710 -3.1629650 1.2840400
C 3.9417410 -2.5308890 0.6362800
C 2.7816150 -3.1330400 0.0631490
O 4.2893940 -1.3390620 0.4738880
H 2.4233060 -4.0664240 0.4863540
H 3.4433730 -0.16580 -0.0811210
O 2.9168210 0.6554240 -0.3867360
H 3.2466310 0.8652710 -1.2703680
C 2.1122430 -2.5230790 -0.9865260
H 1.3197170 -3.0707740 -1.4898350
H 1.2044790 -1.3646270 -0.5040060
H 2.6648320 -1.8352280 -1.6178900
C -2.5109930 -0.5469420 0.3373380
C -1.4908030 -1.4884480 -1.3336360
C -3.4297880 -1.4323090 -0.2735950
C -2.9172420 0.1452790 1.4918760
H -0.7496350 -1.7884060 -2.0555250
C -4.7351390 -1.6258210 0.1817480
C -4.2144920 -0.0439540 1.9550860
H -2.2490350 0.7957530 2.0385210
H -3.0872380 -2.7069360 -1.9667180
C -5.1175950 -0.9088920 1.3075980

H -5.4153600 -2.3091300 -0.3169340
H -4.5358280 0.4854270 2.8465400
H -6.1220940 -1.0257840 1.7012980
N -1.2939480 -0.5940120 -0.3772990
N -2.7399570 -2.0064380 -1.3278380

Mecanismo con el complejo 1.2j (*ruta cis-hidroxo-j*)

c-OH-j-I_0

E(gas): -786,40217

E(H_2O): -786,652094; G(H_2O): -786,3715086

C	1.9339790	0.2182470	2.1865500
C	1.6671990	1.6092720	1.5625430
H	3.0038480	-0.0079880	2.2087190
H	2.3870780	1.8104700	0.7641520
H	1.5850700	0.1970400	3.2245810
H	1.7741730	2.4151550	2.3021780
C	1.1399150	-0.8093600	1.3840350
C	0.2485070	1.5582940	1.0244070
C	-0.2900730	2.2068400	-0.1412920
H	-0.4892230	1.3958170	1.8103370
C	-1.7343140	2.6425080	-0.1773390
C	0.4922990	2.2406400	-1.2874070
C	1.6726760	-1.6307500	0.3343460
H	0.2624130	-1.2127530	1.8853360
C	3.1300790	-1.6774360	-0.0335910
C	0.6825990	-2.26800	-0.4365430
H	3.5982620	-2.4746030	0.5600810
H	3.2623410	-1.9083880	-1.0905290
H	3.6532030	-0.74410	0.1838640
H	-2.1584040	2.5672470	-1.1833480
H	-2.3595470	2.0800770	0.5196510
H	-1.7790630	3.6983590	0.1190980
H	0.9597620	-2.7283430	-1.3801910
H	-0.2447890	-2.6047740	0.0147890
H	0.0441620	2.5291950	-2.2354020
H	1.5745850	2.2824410	-1.2373780
Ru	0.3823460	-0.0098490	-0.5338670
N	-1.6322180	-0.5126330	0.0922240
C	-2.29720	-0.6372930	1.3010370
C	-3.5887530	-1.0275070	1.0698440
H	1.7375110	0.5580930	-2.5903080
O	1.6895790	-0.1865230	-1.9774770
C	-2.5114450	-0.8278840	-0.8526140
H	-2.3136450	-0.8474600	-1.9140310
N	-3.7033730	-1.1410310	-0.2975370
H	-4.4102100	-1.2285560	1.7398010
H	-1.8196640	-0.4415400	2.2478440
H	-4.5313770	-1.4196450	-0.8059440

c-OH-j-I_1

E(gas): -979,5255528;

E(H_2O): -979,828138; G(H_2O): -979,4674172

C	0.7276270	2.3615850	1.8601400
C	0.8734760	2.7041120	0.3603090
H	1.6907870	2.3687130	2.3781490
H	1.7842760	2.2517760	-0.0461270
H	0.0998400	3.1085850	2.3578510
H	0.9412470	3.7857530	0.1763840
C	0.0268490	1.0022630	1.9298670
C	-0.3797350	2.1157310	-0.2699950
C	-0.62540	1.6066570	-1.5863140
H	-1.2791520	2.5224450	0.1947050
C	-1.9878740	1.7435360	-2.2205070
C	0.3434480	0.7972430	-2.1741480
C	0.6981640	-0.2452680	2.0688610
H	-1.0160100	1.0152740	2.2366560
C	2.1720940	-0.3662540	2.3514710
C	-0.0707700	-1.3909540	1.7696590
H	2.2895890	-0.3745490	3.4439590
H	2.5687290	-1.3069970	1.9653890
H	2.7643330	0.4661350	1.9659530
H	-2.2459600	0.8719930	-2.8295440
H	-2.7789490	1.9103870	-1.4864280
H	-1.9662620	2.6162390	-2.8858230
H	0.4316740	-2.3468640	1.6590370
H	-1.1236360	-1.4344090	2.0270030
H	0.1017700	0.2508800	-3.0826380
H	1.3991720	0.9682710	-1.9976750
Ru	-0.1011860	-0.1200990	-0.0766290
H	1.5500640	-2.4964200	-0.5769050
O	2.4962190	-2.3035880	-0.3157830
C	2.7216660	-1.0330330	-0.7915790
C	4.0771330	-0.5113030	-0.4360170
H	2.5364160	-0.9289550	-1.8709040
H	1.9342570	-0.2965540	-0.3172790
C	4.8018390	0.2556710	-1.2538700
H	4.4636940	-0.80500	0.5361810
H	5.7849920	0.6165630	-0.9697990

H 4.4523720 0.5326150 -2.2460690
H 0.0849390 -1.8902740 -1.9759350
O -0.0119300 -2.0084420 -1.0220090
C -3.1714170 0.3387380 0.6783780
C -2.7225490 -1.5222350 -0.3749980
C -4.3535520 -0.3380100 0.5527440
H -2.9928610 1.2962020 1.1397600
H -2.1644550 -2.3145610 -0.8522030
H -5.3557550 -0.0945180 0.8689870
H -4.6964640 -2.2382310 -0.3606430
N -2.1628610 -0.4072940 0.0899950
N -4.0466790 -1.5048140 -0.1131450

c-OH-j-I_2
E(gas): -979,5661511;
E(H_2O): -979,854369; G(H_2O): -979,5039739

C -2.4169430 -2.5886460 -1.1246970
C -2.9384070 -2.2630850 0.2948000
H -2.0293780 -3.6101270 -1.1801980
H -2.3832680 -2.8424450 1.0370800
H -3.2260490 -2.5211220 -1.8606610
H -4.0018300 -2.5135020 0.4174060
C -1.3573560 -1.5411600 -1.4573210
C -2.7090940 -0.7731810 0.4947260
C -2.2889050 -0.0956840 1.6864020
H -3.3192050 -0.1579540 -0.1691020
C -2.7803600 1.2898220 2.0272050
C -1.2826470 -0.7245410 2.4324530
C 0.0593650 -1.7420710 -1.4458280
H -1.7025430 -0.7399300 -2.1096750
C 0.7273120 -3.0801640 -1.2430930
C 0.8036470 -0.5470030 -1.5351850
H 0.8839920 -3.5370010 -2.2295660
H 1.7061210 -2.9649880 -0.7698750
H 0.1303210 -3.7704560 -0.6440580
H -2.0123690 1.8847480 2.5321440
H -3.1243430 1.8334080 1.1444920
H -3.6303600 1.1978060 2.7159420
H 1.8758390 -0.5725660 -1.3613680
H 0.4383220 0.2850760 -2.1289680
H -0.7887270 -0.1469940 3.2139530
H -1.2497810 -1.7970840 2.5700760
Ru -0.5411380 -0.4122690 0.2757110
H 2.0728320 0.4686250 0.9046630
O 3.5931140 0.0760860 0.1964970
C 4.7517460 0.3082430 0.5371560
C 5.9192750 -0.1153280 -0.2264480
H 4.9614670 0.8668290 1.4702760
H -0.0329130 -1.7884560 0.8411190
C 7.1546650 0.17060 0.2117970
H 5.7385420 -0.6632720 -1.1470930
H 8.0425610 -0.1322430 -0.3333890
H 7.3142100 0.7199380 1.1369630
H 1.27910 0.2140570 2.2106260
O 1.2030300 0.6382280 1.3460850
C -1.9502270 2.1288730 -1.5127650
C -0.3858080 2.7977510 -0.1780550
C -1.8442130 3.4821460 -1.6967000
H -2.6214970 1.4391370 -2.0023670
H 0.4031720 2.8216670 0.5581540
H -2.3712750 4.1693340 -2.3401180
H -0.5101700 4.8350670 -0.7226240
N -1.0371050 1.7115750 -0.5622720
N -0.8449180 3.8896170 -0.8395060

c-OH-j-I_3
E(gas): -979,5420638;
E(H_2O): -979,845124; G(H_2O): -979,4843842

C -0.0422420 3.1198300 1.1700510
C -0.4866700 2.0245040 2.1630920
H -0.8562520 3.8108570 0.9366110
H -1.5246300 1.7354530 1.9722130
H 0.7612830 3.7251410 1.6039830
H -0.4320760 2.3531080 3.2109880
C 0.4947560 2.3915460 -0.0660080
C 0.4703670 0.8697440 1.9101410
C 0.2767040 -0.5413990 2.0584030
H 1.5078450 1.1722730 2.0575730
C 1.4226950 -1.4289120 2.4829180
C -0.9123120 -1.0971720 1.6029850
C -0.2442170 2.1556340 -1.2624740
H 1.5735960 2.3755770 -0.1673380
C -1.5819790 2.7896520 -1.5479540
C 0.3011230 1.1799190 -2.1311050

H -1.3752690 3.7654070 -2.0096500
H -2.1684610 2.2116750 -2.2654680
H -2.1860010 2.9690130 -0.6560300
H 1.3644580 -2.4198720 2.0241400
H 2.3979390 -0.9854960 2.2671000
H 1.3600940 -1.5693210 3.5693150
H -0.2938660 0.8620830 -2.9841910
H 1.3755010 1.0933100 -2.2621760
H -0.9970510 -2.1707170 1.4676640
H -1.8536690 -0.5582420 1.6136930
Ru -0.0136340 0.1585790 -0.1714810
N 1.9801570 -0.4401290 -0.4115450
C 3.1919460 0.1915710 -0.1701350
C 4.2001630 -0.6671590 -0.5017660
H 3.2617530 1.1911550 0.2286300
H 4.0449470 -2.6533290 -1.2970590
H 5.2712920 -0.5602980 -0.4585320
H 1.4939760 -2.3713930 -1.1811910
H -4.2705770 -2.9279110 0.6409830
C -3.5757760 -2.2565280 0.1408600
C -3.8413860 -0.9153140 0.0754520
O -2.5151920 -2.9163160 -0.3306340
H -4.7179400 -0.5583640 0.6092920
H -1.7614700 -2.3179360 -0.7288540
O -0.5419200 -1.6176330 -1.1903520
H -0.6034810 -1.4269520 -2.1439310
C -3.0624580 0.0544950 -0.7020110
H -3.6002650 1.060 -0.8257860
H -2.0664530 0.3888780 -0.1975830
H -2.7589390 -0.3282840 -1.6750820
C 2.2514030 -1.6526220 -0.8926730
N 3.5823860 -1.8197330 -0.9620130

c-OH-j-I_4

E(gas): -979,5420637;
E(H_2O): -979,847282; G(H_2O): -979,4865403

-0.04430 3.1425440 1.1361560
C -0.4873050 2.0604680 2.1251450
H -0.7905920 3.8557290 0.8840820
H -1.5203450 1.7741210 1.9014890
H 0.8130350 3.7238430 1.5831170
H -0.4682390 2.3997510 3.1705380
C 0.5404760 2.3968340 -0.0865070
C 0.4723550 0.9011520 1.9075250
C 0.2775550 -0.5105660 2.0700610
H 1.5079260 1.2057900 2.0695700
C 1.4188960 -1.3866090 2.5254380
C -0.8976230 -1.0759470 1.5896060
C -0.1984440 2.1476380 -1.2759880
H 1.6218690 2.3792410 -0.1898080
C -1.5408990 2.7763360 -1.5511310
C 0.3354230 1.1637090 -2.1412570
H -1.3474750 3.7579180 -2.0054960
H -2.1236540 2.1954980 -2.2687770
H -2.1417700 2.9460260 -0.6557360
H 1.3635640 -2.3883070 2.0896770
H 2.3965360 -0.9496810 2.3062380
H 1.3471010 -1.4986630 3.6149770
H -0.2667600 0.8432800 -2.9886530
H 1.4085040 1.0649760 -2.2736880
H -0.9737270 -2.1519860 1.4713730
H -1.8468030 -0.5482520 1.5850440
Ru 0.0089750 0.1593330 -0.1706900
N 1.9791450 -0.4765650 -0.4141290
C 3.2001540 0.1369930 -0.1864530
C 4.2018520 -0.7381040 -0.5064480
H 3.2856790 1.1419680 0.1929250
H 4.0256080 -2.7351120 -1.2431010
H 5.2757390 -0.6424610 -0.4690940
H 1.4720730 -2.4156890 -1.1358420
H -4.3166940 -2.8814190 0.7260090
C -3.63730 -2.2271440 0.1819040
C -3.8976870 -0.8967220 0.1090030
O -2.6122200 -2.8946160 -0.3365390
H -4.7613060 -0.5346130 0.6568120
H -1.8850850 -2.3161770 -0.7462100
O -0.5704600 -1.5867880 -1.2032070
H -0.5443890 -1.4183740 -2.1532550
C -3.1338230 0.0674040 -0.7156620
H -3.6887150 0.9939650 -0.8742400
H -2.14940 0.4032320 -0.2332170
H -2.8228430 -0.3433120 -1.6787900
C 2.2364940 -1.7027380 -0.8649780
N 3.5720870 -1.8880400 -0.9296000

c-OH-j-TS_1

E(gas): -979,5197331;
Frecuencia imaginaria: -963.059 cm^{-1}
E(H_2O): -979,817569; G(H_2O): -979,4621019

C 0.8228310 2.3871360 1.7834700
C 0.9013720 2.7457810 0.2813950
H 1.8118810 2.37350 2.2496680
H 1.8150640 2.3348670 -0.1576100
H 0.2325380 3.1351520 2.3241100
H 0.9125030 3.8309370 0.1062210
C 0.1090420 1.0365530 1.8706700
C -0.3397040 2.1055810 -0.3179580
C -0.5732740 1.5649550 -1.6249680
H -1.2484980 2.4950370 0.1435100
C -1.9306440 1.6562500 -2.2771850
C 0.4348500 0.7885680 -2.1907000
C 0.7580720 -0.2197710 2.0590600
H -0.9331280 1.0749360 2.1797200
C 2.2182560 -0.3633890 2.3931440
C -0.0403520 -1.3500710 1.7904450
H 2.3079400 -0.3131930 3.4869010
H 2.5986520 -1.3360550 2.0754650
H 2.8429420 0.4272260 1.9739300
H -2.1606050 0.7646800 -2.8686500
H -2.7339610 1.8194360 -1.5562640
H -1.9214210 2.5134910 -2.9627360
H 0.4357990 -2.3230780 1.7106060
H -1.0957250 -1.3568100 2.0389750
H 0.2180250 0.2081540 -3.0851610
H 1.4787560 1.0229830 -2.0251620
Ru -0.0481300 -0.1049650 -0.08500
H 1.1725940 -2.4146660 -0.7393780
O 2.2844720 -2.3475020 -0.4075860
C 2.6420550 -1.1632770 -0.8230270
C 3.9578180 -0.6371900 -0.3907030
H 2.3975560 -0.9038080 -1.8629230
H 1.7144730 -0.2305950 -0.2672800
C 4.6588200 0.2226490 -1.1383190
H 4.3574170 -1.0313470 0.5383020
H 5.6442160 0.5640140 -0.8386260
H 4.2849800 0.5969750 -2.0887880
H -0.0609660 -2.0225610 -1.9842180
O -0.0165330 -2.0831940 -1.0208570
C -3.1987880 0.4155070 0.6886400
C -2.7843030 -1.4886360 -0.2769240
C -4.3895500 -0.2564540 0.6268170
H -3.0045700 1.3929600 1.1013930
H -2.2587310 -2.3182450 -0.7249080
H -5.3828250 0.0070130 0.9552990
H -4.7637870 -2.1972050 -0.1825190
N -2.2045400 -0.3599870 0.1167410
N -4.1048760 -1.4564300 0.0124790

c-OH-j-TS_2
E(gas): -979,5420633;
Frecuencia imaginaria: -510.219 cm^{-1}
E(H_2O): -979,847274; G(H_2O): -979,4848817

C 0.0050470 3.1435010 1.1350510
C -0.4847360 2.0624430 2.1236860
H -0.7829520 3.8591870 0.8833010
H -1.5179980 1.7778340 1.8988150
H 0.8203350 3.7221050 1.5822070
H -0.4662400 2.4017520 3.1690780
C 0.5436990 2.3966030 -0.0878800
C 0.4732790 0.9016220 1.9068370
C 0.2768210 -0.5097830 2.0703550
H 1.5092480 1.2050540 2.0685930
C 1.4172990 -1.3869570 2.5258450
C -0.8991560 -1.0740570 1.5907280
C -0.1971540 2.1474210 -1.2760490
H 1.6249350 2.3774950 -0.1925450
C -1.5393280 2.7775190 -1.5494260
C 0.3344340 1.1623710 -2.1416300
H -1.3455100 3.7592890 -2.0032230
H -2.1232630 2.1977390 -2.2669530
H -2.1392080 2.9470390 -0.6533120
H 1.3604720 -2.3888590 2.0907450
H 2.3953720 -0.9514190 2.3058330
H 1.3459390 -1.4981930 3.6154940
H -0.2693460 0.8425200 -2.9881140
H 1.4072310 1.0626050 -2.2757850
H -0.9766270 -2.1500700 1.4731250
H -1.8476400 -0.5451160 1.5858840
Ru 0.0089440 0.1593630 -0.1709370
N 1.9787880 -0.4779180 -0.4143120

C 3.2002910 0.1344650 -0.1860220
C 4.2013090 -0.7413530 -0.5061350
H 3.2865980 1.1391470 0.1939540
H 4.0235130 -2.7378540 -1.2437910
H 5.2752690 -0.6466990 -0.4683970
H 1.4701860 -2.4162730 -1.1369120
H -4.3192060 -2.8788580 0.7268240
C -3.6391190 -2.2253200 0.1826970
C -3.8992020 -0.8949360 0.1081410
O -2.6136810 -2.8935510 -0.3340890
H -4.7632800 -0.5320960 0.6547430
H -1.8861480 -2.31570 -0.7439670
O -0.5713300 -1.5873740 -1.2020460
H -0.5477730 -1.4185700 -2.1520950
C -3.1341250 0.0683920 -0.7163840
H -3.6877840 0.9957340 -0.8746200
H -2.1492540 0.4022440 -0.2336210
H -2.8237410 -0.3423700 -1.6797030
C 2.2352060 -1.7041020 -0.8656670
N 3.5706460 -1.8905410 -0.9299950

Mecanismo con el complejo 1.2j (*ruta trans-hidroxo-j*)

t-OH-j-I_0
E(gas): -786,4010207;
E(H_2O): -786,650957;
G(H_2O): -786,3713863

C 1.9315850 0.1815950 2.1744560
C 1.6420710 1.5760490 1.5667880
H 3.0047210 -0.0314630 2.1866200
H 2.3586100 1.8036320 0.7722600
H 1.5910710 0.1432820 3.2145520
H 1.7290560 2.3749970 2.3167090
C 1.1440950 -0.8430940 1.3615410
C 0.2274320 1.5014180 1.02050
C -0.3270070 2.2449480 -0.0957250
H -0.5054910 1.2972780 1.8007440
C -1.7771570 2.6698790 -0.0574290
C 0.4213310 2.4071940 -1.2373470
C 1.6859330 -1.6275040 0.2902790
H 0.2779830 -1.2736410 1.8602600
C 3.1571510 -1.6767310 -0.0377820
C 0.7005470 -2.2490440 -0.5083730
H 3.6411120 -2.3496300 0.6822370
H 3.3424980 -2.0972190 -1.0305690
H 3.6491300 -0.7039730 0.0334300
H -2.2032960 2.7545850 -1.0615090
H -2.3960030 1.9950250 0.5383600
H -1.8335670 3.6615650 0.4094180
H 0.9912330 -2.7168460 -1.4466490
H -0.2194510 -2.6201020 -0.0688520
H -0.0463450 2.7624790 -2.1516850
H 1.4985270 2.3145130 -1.2624450
Ru 0.3964250 -0.0289820 -0.5367600
N -1.6358550 -0.5503800 0.0730260
C -2.3043740 -0.7130500 1.2753010
C -3.5975050 -1.0889730 1.0296410
H 2.2724170 -0.6057450 -2.1100640
O 1.6999670 0.1592440 -1.9621230
H -4.5394040 -1.4099540 -0.8600580
C -2.5151100 -0.8300470 -0.8827340
H -2.3173690 -0.8127530 -1.9443700
N -3.7102160 -1.1555760 -0.3410390
H -4.4211370 -1.3085260 1.6910870
H -1.8281870 -0.5503880 2.2292950

t-OH-j-I_1
E(gas): -979,53253;
E(H_2O): -979,836754; G(H_2O): -979,476866

C -3.4540720 0.5315910 -0.0926030
C -2.9336710 0.3974210 1.3645440
H -4.1410110 -0.2823250 -0.3384760
H -2.8624870 -0.6557080 1.6403470
H -4.0135490 1.4649150 -0.2189620
H -3.5962320 0.8997280 2.0829330
C -2.2313760 0.5653770 -1.0062000
C -1.5639220 1.0506760 1.3579320
C -0.3913090 0.7736850 2.1511330
H -1.6194370 2.1011830 1.0665710
C 0.4995530 1.9177660 2.5768410
C 0.0132510 -0.5355530 2.3529910
C -1.7508900 -0.5190570 -1.8052060
H -1.9278250 1.5566720 -1.3355040
C -2.52330 -1.7838400 -2.0728320
C -0.4220660 -0.3664360 -2.2553440
H -3.0634910 -1.6381820 -3.0178060
H -1.8644620 -2.6459960 -2.2155150
H -3.2739310 -2.0139730 -1.3131260
H 1.5498560 1.6180890 2.6370960
H 0.4120390 2.7898750 1.9252950
H 0.1888430 2.2273870 3.5832210
H 0.0814860 -1.22490 -2.6962810
H -0.0420660 0.6023800 -2.5601230
H 1.0078410 -0.7284010 2.7474450
H -0.6702190 -1.3733180 2.3315220
Ru -0.3911570 -0.2109600 -0.0193970
O 1.2319200 -3.1269740 0.8564920
C 1.8645480 -2.3059540 -0.0527090
C 3.2777160 -2.0097100 0.3525180
H 1.8207850 -2.6655570 -1.0946730
H 1.3299710 -1.2784090 -0.0998740
C 4.2978170 -1.9099780 -0.5036740
H 3.4321830 -1.8845680 1.4231810
H 5.3067700 -1.6971900 -0.1644020
H 4.1676640 -2.0746840 -1.5710660
H 0.2554240 -2.9630540 0.7586520

O -1.1513320 -2.0493490 0.5228450
H -1.7350080 -2.4713060 -0.1161290
C 0.4872950 2.8411430 -0.8209210
C 2.1574810 1.4804550 -0.5481320
C 1.6219780 3.5661510 -1.0661490
H -0.5371270 3.1776640 -0.8525330
H 2.7650520 0.6046690 -0.3636900
H 1.7715570 4.5983030 -1.3423150
H 3.6487300 2.8990920 -0.9942110
N 0.8308660 1.5393240 -0.4950750
N 2.6663710 2.6875340 -0.8872020

t-OH-j-I_2
E(gas): -979,5500358;
E(H_2O): -979,841802; G(H_2O): -979,4863462

C 1.6183760 3.0246750 0.2859230
C 1.0411120 2.4877250 1.6237690
H 1.1188990 3.9473400 -0.0284190
H -0.0483690 2.5550590 1.6443020
H 2.6733590 3.2872430 0.4248080
H 1.4130830 3.0670780 2.4822570
C 1.5356350 1.9038540 -0.7661530
C 1.5298080 1.0482570 1.7027840
C 1.0281860 -0.1942160 2.1652230
H 2.6191610 1.0284870 1.6241310
C 2.0308190 -1.2473870 2.5941030
C -0.3182340 -0.6087790 1.9988750
C 0.4462150 1.7117730 -1.6551100
H 2.4753360 1.4345560 -1.0407480
C -0.6169950 2.7665940 -1.8750830
C 0.2699080 0.4321070 -2.2478000
H -0.2951870 3.3788090 -2.7277450
H -1.5821370 2.3306480 -2.1506100
H -0.7433100 3.4653300 -1.0409000
H 1.7273250 -2.2522580 2.2861380
H 3.0399430 -1.0529730 2.2227530
H 2.0769220 -1.2409690 3.6908240
H -0.6337920 0.2585310 -2.8240710
H 1.1282010 -0.1528570 -2.5630530
H -0.5406320 -1.6495870 2.2154710
H -1.1401990 0.0782430 2.1585490
Ru 0.3095630 0.0996440 -0.0311560
O -3.7194720 0.0061510 -0.4771790
C -4.5953810 -0.5435170 0.1876920
C -5.7902920 -1.1456960 -0.3933320
H -4.5110850 -0.6047890 1.2906190
H -0.7408480 -1.0647270 -0.4488600
C -6.7078680 -1.7253820 0.3947800
H -5.8942120 -1.0968990 -1.4737030
H -7.6076720 -2.1792880 -0.0072050
H -6.5843950 -1.7613920 1.4749070
H -2.3345290 0.7093400 0.1302790
O -1.5551360 1.2573520 0.4244840
H -1.6524270 2.0994130 -0.0367940
C 3.2142350 -1.1110800 -0.5652300
C 1.5966660 -2.5320500 -0.8582810
C 3.7953520 -2.2847150 -0.9606960
H 3.6928250 -0.1786760 -0.3143360
H 0.6198510 -2.9828540 -0.9247870
H 4.8262080 -2.5582370 -1.1223250
H 2.8364440 -4.1321670 -1.4378890
N 1.8399640 -1.2751120 -0.5022010
N 2.7560470 -3.1702760 -1.1406470

t-OH-j-I_3
E(gas): -979,555311123;
E(H_2O): -979,848789; G(H_2O): -979,499153

C 1.3958340 3.1490330 0.7896210
C 0.8593640 2.3850290 2.0222950
H 0.8108300 4.0533130 0.59690
H -0.2197020 2.5350060 2.1111570
H 2.4279550 3.4764320 0.9575610
H 1.3129690 2.7368320 2.9600430
C 1.3748300 2.1731250 -0.3846100
C 1.1833210 0.9185180 1.7883670
C 0.3812380 -0.2257240 2.1064320
H 2.2557560 0.7178130 1.7696670
C 0.9935170 -1.5447490 2.5097970
C -0.9946740 -0.0924840 1.8720620
C 0.3949690 2.1270440 -1.4225810
H 2.3451630 1.7546170 -0.6463690
C -0.6908420 3.1591410 -1.6030160
C 0.45980 0.9636120 -2.2263450
H -0.3014320 3.9553010 -2.2516870
H -1.5686970 2.7313390 -2.0949580

H -1.0063760 3.6160440 -0.6631900
H 0.4297330 -2.3937700 2.1102440
H 2.0349970 -1.6294670 2.1913830
H 0.9715130 -1.6212020 3.6046890
H -0.3348240 0.7891990 -2.9502380
H 1.4175910 0.5152020 -2.4715370
H -1.6169700 -0.9844750 1.8743330
H -1.5199030 0.8332170 2.0660590
Ru 0.1619260 0.3169820 -0.0883490
N 1.9707390 -1.1155630 -0.4805650
C 3.3376480 -0.9163310 -0.4161450
C 3.9923400 -2.0714320 -0.7527160
H 3.7659040 0.0338100 -0.1337300
H 3.1360030 -3.9473440 -1.3072750
H 5.0409320 -2.3157840 -0.8215640
H 0.8473720 -2.8589170 -0.9927540
H -5.2709360 -2.4602130 0.9960660
C -4.6372570 -1.7722950 0.4085800
C -5.3395450 -0.6581570 -0.2493800
O -3.4286660 -1.9848320 0.3565440
H -6.4245820 -0.6682700 -0.1895030
H -1.9597570 -1.5538030 -0.4238410
O -1.0926330 -1.4324810 -0.8806390
H -1.3001840 -1.2752160 -1.8098670
C -4.6877500 0.3392010 -0.8631740
H -5.2179610 1.1628150 -1.3301580
H -1.1475970 1.1977210 0.0074620
H -3.6018170 0.3606420 -0.8975860
C 1.8019040 -2.3753690 -0.8519080
N 2.9994690 -2.9870800 -1.0258440

t-OH-j-I$_4$

E(gas): -979,5365776;
E(H_2O): -979,845773; G(H_2O): -979,4866964

C -1.8836240 -2.7508860 0.1228980
C -1.2321810 -2.5297270 -1.2719240
H -2.9420290 -2.4786770 0.1093330
H -1.7829260 -1.7840360 -1.8502340
H -1.8334920 -3.8074840 0.4077800
H -1.2291980 -3.4512750 -1.8707940
C -1.0769280 -1.9308140 1.1226830
C 0.1890880 -2.0906200 -1.0012210
C 1.0427760 -1.1707270 -1.6991110
H 0.7638440 -2.8454370 -0.4659490
C 2.5151970 -1.4610590 -1.8038450
C 0.5095830 0.06040 -2.0683260
C -1.5150030 -0.7603460 1.8070820
H -0.2350980 -2.4562050 1.5718310
C -2.9422180 -0.2844600 1.8214910
C -0.4800520 0.0123770 2.3847140
H -3.4231070 -0.7587670 2.6880700
H -3.0111210 0.7962880 1.9629910
H -3.5137060 -0.5642240 0.9361480
H 3.0995070 -0.5581040 -1.9909220
H 2.8949070 -1.9513010 -0.9067070
H 2.6570840 -2.1396800 -2.6558700
H -0.7213120 1.0116830 2.7427990
H 0.3527430 -0.4583240 2.8979790
H 1.1850760 0.8608040 -2.3637760
H -0.5215820 0.1757400 -2.3722900
Ru 0.0771480 -0.2396460 0.2407560
H 5.1234730 1.6713540 -0.4307210
C 4.1670720 1.4216320 0.0239240
C 3.1938950 2.3513770 0.1162500
O 4.1409170 0.1521920 0.4500860
H 3.3821400 3.3206080 -0.3325620
H 3.2337620 -0.1736620 0.6986150
O 1.7955290 -1.0585660 0.9805650
H 1.7804090 -1.1918580 1.9368160
C 1.9170470 2.1470750 0.8587140
H 1.4487330 3.0973050 1.1336410
H 1.1436230 1.6034900 0.2308430
H 2.0511100 1.5498180 1.7626340
C -2.7084710 0.8994010 -1.2437390
C -1.6113040 2.3991550 -0.1310220
C -3.3895060 2.0748140 -1.4059990
H -2.9541940 -0.0726860 -1.6402780
H -0.8815240 2.9139450 0.4740330
H -4.2904970 2.3170010 -1.9478690
H -2.9033090 3.9946840 -0.6083040
N -1.5965100 1.1085990 -0.4442460
N -2.6794400 3.0126690 -0.6916300

t-OH-j-TS$_1$

E(gas): -979,521726;
Frecuencia imaginaria: -813.040 cm^{-1}
E(H_2O): -979,824327; G(H_2O): -979,469425

	H 2.8440710 0.3478980 -0.3143090
C -3.3775390 0.8380250 -0.1576120	H 2.1977040 4.3826690 -1.4204450
C -2.9155720 0.5981070 1.3040610	H 3.9260460 2.5469030 -1.0039540
H -4.1589820 0.1311210 -0.4517050	N 1.0032920 1.43790 -0.5001540
H -2.8979880 -0.4685210 1.5328220	N 2.9288920 2.4188380 -0.9028110
H -3.8140340 1.8381180 -0.2563650	
H -3.5809100 1.0873220 2.0296800	**t-OH-j-TS$_2$**
C -2.1353250 0.7589920 -1.0527640	E(gas): -979,5196559;
C -1.5240100 1.2043440 1.3620810	Frecuencia imaginaria: -483.929 cm^{-1}
C -0.3419120 0.8974060 2.1065830	E(H$_2$O): -979,823841; G(H$_2$O): -979,4679061
H -1.5488590 2.2560500 1.0695540	
C 0.5824030 2.0259680 2.5043480	
C 0.0860710 -0.4245610 2.2687110	C -1.8726800 -2.8446960 0.2455540
C -1.7265310 -0.3868300 -1.7949840	C -1.4176210 -2.4749100 -1.1906130
H -1.7416680 1.7111220 -1.3978530	H -2.9542430 -2.7365820 0.3668690
C -2.6094440 -1.5912080 -2.0159820	H -2.0120320 -1.6487820 -1.5797430
C -0.3815660 -0.4099780 -2.2306360	H -1.6399540 -3.8951580 0.4509380
H -3.1336740 -1.4364380 -2.9683710	H -1.5395210 -3.3135860 -1.8920980
H -2.0315470 -2.5143350 -2.1246930	C -1.0732690 -1.9681450 1.2123500
H -3.3853580 -1.7241570 -1.2570830	C 0.0488670 -2.1134270 -1.0438340
H 1.6320320 1.7182630 2.5035130	C 0.9663200 -1.2371220 -1.6979100
H 0.46830 2.9125730 1.8763930	H 0.58420 -2.9322280 -0.5609410
H 0.3281550 2.3166770 3.5320230	C 2.4089070 -1.6769780 -1.8035140
H 0.0030630 -1.3281310 -2.6687180	C 0.6256370 0.0905080 -2.0010990
H 0.1118250 0.4986400 -2.5592320	C -1.5156660 -0.7495940 1.7701200
H 1.0927610 -0.5966450 2.6400310	H -0.2070490 -2.4415540 1.6684640
H -0.6061210 -1.2478800 2.3801240	C -2.9583560 -0.3098460 1.6985890
Ru -0.3252910 -0.1514030 0.0029650	C -0.5205870 0.1288240 2.3079990
O 0.6965100 -3.2584260 0.7347730	H -3.4844820 -0.7835420 2.5381690
C 1.5043630 -2.5859470 -0.0175560	H -3.0627940 0.7703740 1.8181130
C 2.8984720 -2.3751900 0.4704930	H -3.4666880 -0.6110980 0.7812590
H 1.4451500 -2.7207580 -1.1137080	H 3.1102420 -0.8445120 -1.7255610
H 1.0583250 -1.2456410 -0.0574780	H 2.6729480 -2.4253380 -1.0538390
C 3.9518100 -2.2860890 -0.3489970	H 2.5391590 -2.1343340 -2.7935240
H 3.0143110 -2.3607230 1.5522120	H -0.8497720 1.1057500 2.6544340
H 4.9646760 -2.1936570 0.0302460	H 0.3035340 -0.2758770 2.8935190
H 3.8387030 -2.3462650 -1.4295610	H 1.4271800 0.7730820 -2.2738160
H -0.4514290 -2.7186070 0.6549380	H -0.3550890 0.3596980 -2.3700530
O -1.3175250 -1.9841470 0.5866780	Ru 0.0815700 -0.1903310 0.2175630
H -1.9674410 -2.3616050 -0.0174220	H 5.0923640 1.6124940 -0.4942310
C 0.7684330 2.7533810 -0.8656530	C 4.1431440 1.3377130 -0.0064360
C 2.3210630 1.2675850 -0.5352010	C 3.1462200 2.3518060 0.1003050
C 1.9614400 3.3744010 -1.1180780	O 4.0182430 0.1586330 0.3972640
H -0.2244290 3.1707280 -0.9148480	H 3.2473590 3.2417390 -0.5131220

H 2.7203750 -0.5683720 0.8089680
O 1.8883340 -1.1178230 1.0406640
H 1.8931320 -1.2124700 2.0020320
C 2.0599580 2.1881520 0.9482360
H 1.4051580 3.0374160 1.1261290
H 0.9745080 1.2772820 0.3437900
H 2.1674670 1.5160840 1.7928590
C -2.5620990 0.9890370 -1.3569880
C -1.5688830 2.3861270 -0.0325920
C -3.2427270 2.1706270 -1.4612100
H -2.7641350 0.0653060 -1.8725410
H -0.8919720 2.8419400 0.6701090
H -4.1025940 2.4555650 -2.0470790
H -2.8415290 4.0105770 -0.4551840
N -1.5156300 1.1287070 -0.4583940
N -2.6001500 3.0421140 -0.6121600

Mecanismo con el complejo 1.2l (*ruta cis-hidroxo-l*)

c-OH-l-I_0

E(gas): -825,5708507; E(H_2O): -825,965548; G(H_2O): -825,6596313

C 2.3616580 0.1465110 2.0551520
C 2.2368880 1.5121460 1.3382700
H 3.3889440 -0.2277030 2.0208750
H 2.9139550 1.5524360 0.4800920
H 2.0986970 0.2501570 3.1134140
H 2.5083020 2.34670 2.00070
C 1.3714820 -0.8126420 1.3990680
C 0.7868650 1.6214670 0.9011940
C 0.2564790 2.2492010 -0.2789840
H 0.0950180 1.6262870 1.7435690
C -1.1129590 2.8824960 -0.2594270
C 0.9484110 2.0827750 -1.4712240
C 1.6989650 -1.7773960 0.3876400
H 0.4902510 -1.0468860 1.9927360
C 3.1001600 -2.0613450 -0.0803330
C 0.5703140 -2.3235270 -0.2509910
H 3.4931700 -2.8899350 0.5246400
H 3.1105060 -2.3612990 -1.1282710
H 3.7713580 -1.2086220 0.0422890
H -1.6154530 2.7990320 -1.2280180
H -1.7559430 2.4613010 0.5165980
H -0.9911120 3.9517270 -0.0434940
H 0.7014710 -2.8892480 -1.1685560
H -0.3544680 -2.4839390 0.2929620
H 0.4743440 2.3588250 -2.4102670
H 2.0268740 1.9726070 -1.4948550
Ru 0.5793720 -0.0612110 -0.5237550
N -1.4183740 -0.2204940 0.2806590
C -2.0029050 -0.1535780 1.5268350
C -3.3492110 -0.3684950 1.4246950
H 1.7852900 0.13170 -2.7383100
O 1.6879700 -0.5491340 -2.0607910
C -2.4101880 -0.4790640 -0.5701930
H -2.3020130 -0.6113710 -1.6368580
N -3.5871320 -0.5722790 0.0823430
H -4.1459360 -0.3968730 2.1701890
H -1.4335880 0.0429220 2.4205780
C -4.8861680 -0.8490940 -0.5258780
H -4.7593770 -0.9727700 -1.6023960
H -5.3055970 -1.7686810 -0.1097650
H -5.5710120 -0.0173250 -0.3415600

c-OH-l-I_1

E(gas): -1018,876493; E(H_2O): -1019,16777; G(H_2O): -1018,792084

C 1.2964190 2.5084880 1.6014830
C 1.4358990 2.6777560 0.0716310
H 2.2693080 2.4371290 2.0961030
H 2.2781220 2.08430 -0.2996470
H 0.7888920 3.3776770 2.0335710
H 1.6218620 3.7196910 -0.2253770
C 0.4269250 1.2689930 1.8224810
C 0.1061330 2.1785240 -0.4753940
C -0.2233130 1.5805160 -1.7365870
H -0.7272630 2.7391160 -0.0494470
C -1.5670870 1.8264400 -2.3769970
C 0.6318870 0.6075140 -2.2433550
C 0.9274800 -0.0370150 2.0828560
H -0.5972620 1.4544690 2.1361440
C 2.3792960 -0.3276640 2.3594200
C 0.0061270 -1.0950010 1.9147930
H 2.5247020 -0.2346460 3.4445920
H 2.6338700 -1.3501460 2.0748150
H 3.0684870 0.3684990 1.8768690
H -1.9298070 0.9475500 -2.9183200
H -2.3257110 2.1379420 -1.6558110
H -1.4523430 2.6389940 -3.1060390
H 0.3789270 -2.1146700 1.8990190
H -1.0363380 -0.9739360 2.1894650
H 0.3159320 0.0055540 -3.0920140
H 1.7022700 0.6606790 -2.0801520
Ru 0.0990510 -0.0320330 -0.0543470
H 1.3721750 -2.6558390 -0.3209450
O 2.3418320 -2.5776760 -0.0859270
C 2.7356260 -1.4074810 -0.6924250
C 4.1630710 -1.0589830 -0.4140540
H 2.5355710 -1.3854160 -1.7735920
H 2.0788420 -0.5196530 -0.2824690

C 4.9666410 -0.4993310 -1.3213830
H 4.5320140 -1.3026020 0.5786190
H 6.03540 -0.2603980 -1.0935740
H 4.6301340 -0.2797200 -2.3322430
H -0.0154630 -1.9838640 -1.7729770
O -0.1055900 -1.9930580 -0.8112360
C -2.8566870 0.9174250 0.6927190
C -2.7038250 -1.0744860 -0.1806120
C -4.1223130 0.3982950 0.6472260
H -2.5396900 1.8804930 1.0588750
H -2.2753710 -1.9795570 -0.5859620
H -5.0727950 0.8084450 0.9529500
C -5.1017780 -1.8017490 -0.1466170
N -1.9771700 -0.0107360 0.1654180
N -4.0079430 -0.8596900 0.0931510
H -5.8247370 -1.3669430 -0.8413360
H -5.5987660 -2.0434880 0.7961080
H -4.6913220 -2.7148140 -0.5797210

c-OH-l-I_2
E(gas): -1018,837028;
E(H_2O): -1019,14159; G(H_2O): -1018,755861

C -2.3779540 -2.7506670 -1.2564100
C -2.8776830 -2.5341780 0.1911870
H -1.9910070 -3.7644720 -1.3958330
H -2.3025360 -3.1581910 0.8802710
H -3.1989900 -2.6285460 -1.9718430
H -3.9356260 -2.8073390 0.3134950
C -1.3251700 -1.6782190 -1.5255810
C -2.6633440 -1.0591790 0.4929370
C -2.2311960 -0.4631200 1.7230380
H -3.2910780 -0.4072660 -0.1170250
C -2.73320 0.8846270 2.1797350
C -1.2067380 -1.1391400 2.4018310
C 0.0918490 -1.8704650 -1.5327420
H -1.6771840 -0.8352750 -2.1186860
C 0.7655960 -3.2159730 -1.4173680
C 0.8305130 -0.6677680 -1.5493120
H 0.9119580 -3.6130580 -2.4309380
H 1.7493890 -3.1263350 -0.9489580
H 0.1769250 -3.9425510 -0.8539310
H -1.9594990 1.4534320 2.7058090
H -3.1114460 1.4868410 1.3506720
H -3.5612400 0.7282030 2.8835140
H 1.9035630 -0.7001510 -1.3821780
H 0.4602220 0.1971030 -2.0908980
H -0.7038020 -0.6201740 3.2182030
H -1.1673740 -2.2186170 2.4605140
Ru -0.5079250 -0.6502470 0.2714430
H 2.0842740 0.2585450 0.9368790
O 3.6130760 -0.0641910 0.2066170
C 4.7668510 0.1787360 0.5553290
C 5.9417730 -0.1833930 -0.2287120
H 4.9667540 0.6999880 1.5120260
H 0.0608520 -2.0390480 0.7453120
C 7.1714740 0.1122790 0.2187450
H 5.7707890 -0.6946070 -1.1720590
H 8.0644870 -0.1451240 -0.3412340
H 7.3210430 0.6241580 1.1667780
H 1.2999330 -0.0634370 2.2331490
O 1.2127260 0.3931130 1.3862980
C -2.0221110 1.9332940 -1.3546160
C -0.4341340 2.5782100 -0.0439610
C -1.9432250 3.2959900 -1.4775270
H -2.6976410 1.2559580 -1.8560980
H 0.3762440 2.5882820 0.6696650
H -2.5034920 4.01940 -2.0739300
C -0.4651110 5.0641440 -0.4243770
N -1.0739520 1.4919110 -0.4536990
N -0.9262890 3.6955260 -0.6355280
H -1.2810910 5.6840520 -0.0432790
H -0.0946340 5.4882790 -1.3616140
H 0.3450640 5.0555350 0.3067960

c-OH-l-I_3
E(gas): -1018,85369;
E(H_2O): -1019,160862; G(H_2O): -1018,774799

C 0.5937480 3.6111390 0.4079720
C 0.1751020 2.9322270 1.7315950
H -0.1359130 4.3651580 0.0974490
H -0.9149870 2.8837030 1.7939530
H 1.5492600 4.1336790 0.5284890
H 0.5257350 3.4862570 2.6142120
C 0.7694230 2.4995650 -0.6241070

C 0.7764510 1.5363880 1.6992520
C 0.1947610 0.3142610 2.1671170
H 1.8675820 1.5421160 1.7067090
C 1.0285200 -0.8015910 2.7479110
C -1.1758820 0.1588790 1.9101610
C -0.1742480 2.1268080 -1.6278190
H 1.8044790 2.2455130 -0.8458950
C -1.4365660 2.8987700 -1.9240660
C 0.1231360 0.8999650 -2.2714650
H -1.2013990 3.6632780 -2.6767570
H -2.2116860 2.2500490 -2.3412160
H -1.8425260 3.4055140 -1.0463890
H 0.6376760 -1.7860050 2.4710020
H 2.0743360 -0.7360130 2.4388500
H 0.9978640 -0.7312930 3.84300
H -0.6166490 0.4836850 -2.9540340
H 1.1522360 0.6218590 -2.4787590
H -1.6242700 -0.8250630 2.0254790
H -1.8675610 0.9877110 1.9853080
Ru -0.0604760 0.5040650 -0.0709620
N 2.0090750 -0.5564050 -0.2742870
C 3.3009920 -0.0695070 -0.2597530
C 4.1852250 -1.1003110 -0.4429770
H 3.5198780 0.9783370 -0.1172620
H 5.2633260 -1.1254580 -0.4930030
H 1.2940510 -2.5562540 -0.5216350
H -4.8616920 -3.00880 1.5078980
C -4.3702610 -2.4252860 0.7030810
C -5.2671430 -1.8512990 -0.3141830
O -3.1475550 -2.3112560 0.7237190
H -6.3154440 -2.1293670 -0.2465050
H -1.7801120 -1.7720980 -0.1727960
O -0.9091390 -1.5591330 -0.5867830
H -1.0413500 -1.6025700 -1.5416570
C -4.8330060 -1.0038220 -1.2568860
H -5.5050020 -0.5738880 -1.9921970
H -1.5231290 1.0894230 -0.1038470
H -3.7882700 -0.7093280 -1.3024660
C 2.1210360 -1.8642150 -0.4659190
N 3.4195540 -2.2400740 -0.5722940
C 3.9146690 -3.5958390 -0.7934170
H 3.0687620 -4.2853690 -0.7967460
H 4.4315620 -3.6597990 -1.7548870
H 4.6016290 -3.8808840 0.0076270

c-OH-l-I_4
E(gas): -1018,869921;
E(H_2O): -1019,161062; G(H_2O): -1018,786511

C 1.0997210 -3.2005140 0.8389630
C 1.3748890 -2.1112710 1.8989380
H 2.0204360 -3.6700100 0.4802380
H 2.2762760 -1.5455820 1.6400990
H 0.4900100 -4.0010610 1.2711760
H 1.5333400 -2.5253380 2.9048220
C 0.3022870 -2.5227800 -0.2778980
C 0.1342340 -1.2330160 1.8534620
C -0.0318260 0.1606340 2.1522390
H -0.7714490 -1.8133310 2.0376810
C -1.3253830 0.6589900 2.7493110
C 0.9163480 1.0573880 1.6774150
C 0.8708080 -1.9752710 -1.4596050
H -0.7501190 -2.7838600 -0.3362330
C 2.3143620 -2.1829920 -1.8431960
C 0.0379010 -1.1005560 -2.1995160
H 2.3679730 -3.1358650 -2.3878740
H 2.6729790 -1.40260 -2.5170870
H 2.9922170 -2.2583130 -0.9905350
H -1.5665160 1.6703360 2.4096770
H -2.1674840 -0.0042450 2.5353840
H -1.2060430 0.6976280 3.8397160
H 0.4790310 -0.5527110 -3.0294020
H -1.0280460 -1.2902090 -2.2857910
H 0.7047450 2.1217600 1.6682930
H 1.9651710 0.8005830 1.5628030
Ru 0.2199150 -0.2248930 -0.1590110
N -1.8572660 -0.1503310 -0.2241590
C -2.8432670 -1.0894680 0.0162380
C -4.0648810 -0.4941610 -0.1482820
H -2.6266860 -2.1071660 0.2976240
H -5.0666300 -0.8843850 -0.0513480
H -1.9609720 1.9067730 -0.7690100
H 3.6180730 3.8334190 0.8176340
C 3.1067690 3.0605450 0.2459960
C 3.7244370 1.8751930 0.0143010
O 1.8927600 3.4470710 -0.1362530
H 4.7006690 1.7345020 0.4662990

H 1.3270700 2.7238960 -0.5670180
O 0.2276330 1.6928880 -1.0296230
H 0.1654320 1.6058660 -1.9887620
C 3.1937290 0.8014740 -0.8596700
H 3.9706580 0.0873270 -1.1394990
H 2.3846100 0.1689150 -0.3598350
H 2.7085240 1.1837800 -1.7607620
C -2.4788060 0.9901470 -0.5289300
N -3.8168530 0.8184990 -0.49100
C -4.8221980 1.8433730 -0.7759690
H -4.3154350 2.7896320 -0.9699190
H -5.4067590 1.5607150 -1.6550950
H -5.4863840 1.9617110 0.0835340

c-OH-l-TS$_1$
E(gas): -1018,830968;
Frecuencia imaginaria: -985.476 cm^{-1}
E(H_2O): -1019,131595; G(H_2O): -1018,750766

C 1.4112010 2.4123860 1.6341360
C 1.4913690 2.6800540 0.1129500
H 2.4032590 2.2782910 2.0741760
H 2.3306540 2.1300400 -0.3225970
H 0.9527270 3.2640210 2.1486730
H 1.6405310 3.7436540 -0.1213800
C 0.5151460 1.1854590 1.8124190
C 0.1590520 2.1816360 -0.4239920
C -0.1772720 1.6121140 -1.6965820
H -0.6762410 2.7172570 0.0296450
C -1.5226140 1.8605990 -2.3323860
C 0.7040950 0.6787250 -2.2345830
C 0.9813680 -0.1397550 2.0611190
H -0.5027390 1.3920250 2.1361430
C 2.4116860 -0.4767890 2.3854320
C 0.0243420 -1.1570980 1.8680540
H 2.5289440 -0.3810950 3.4735860
H 2.6384720 -1.5108270 2.1190600
H 3.1377750 0.1884230 1.9151420
H -1.8825830 0.9876980 -2.8856130
H -2.2822320 2.1576360 -1.6068100
H -1.4112410 2.6829040 -3.0511050
H 0.3576160 -2.1905860 1.8348000
H -1.0160540 -1.0010400 2.1299540
H 0.3927190 0.0849330 -3.0917410
H 1.7731190 0.7759360 -2.0947220
Ru 0.1510540 -0.0266090 -0.0730900
H 1.0149540 -2.5066670 -0.6361020
O 2.1385630 -2.5887230 -0.3174850
C 2.6575930 -1.4873380 -0.7863270
C 4.0402050 -1.1403370 -0.3788040
H 2.4488590 -1.2429750 -1.8383130
H 1.8776940 -0.4099820 -0.2789000
C 4.8508430 -0.4132160 -1.1555110
H 4.3876250 -1.5604760 0.5597630
H 5.8777300 -0.2085170 -0.87100
H 4.5256500 -0.0165170 -2.1146880
H -0.1619790 -1.9973930 -1.8795960
O -0.1113080 -2.0303210 -0.9153930
C -2.8717360 0.9653160 0.7225150
C -2.7599860 -1.01300 -0.1627110
C -4.1468690 0.4664140 0.6996250
H -2.5347120 1.9211860 1.0922900
H -2.3698710 -1.9289250 -0.5803830
H -5.0863130 0.8853810 1.0269970
C -5.1692220 -1.7140110 -0.0923130
N -2.0103970 0.0337610 0.1744060
N -4.0598410 -0.7888090 0.1352210
H -5.89560 -1.2687620 -0.7770450
H -5.6585360 -1.9516380 0.8555710
H -4.7782020 -2.6324640 -0.5324350

c-OH-l-TS$_2$
E(gas): -1018,847463;
Frecuencia imaginaria: -514.556 cm^{-1}
E(H_2O): -1019,15224; G(H_2O): -1018,769679

C 1.24010 -3.1153340 0.7993710
C 1.3824170 -2.0874190 1.9459850
H 2.2144930 -3.4703470 0.4524260
H 2.2923800 -1.4959910 1.8144010
H 0.6903040 -3.9990940 1.1413540
H 1.4435890 -2.5651310 2.9340810
C 0.4321200 -2.4246770 -0.2992510
C 0.1425900 -1.2174150 1.8412290
C -0.0261300 0.1751570 2.1322380
H -0.7737880 -1.7948310 1.9755630

C -1.3226120 0.6983100 2.6996200
C 0.9735900 1.0441620 1.6988200
C 0.9689440 -1.8812570 -1.5042020
H -0.6158610 -2.7118600 -0.3472440
C 2.3801640 -2.1186820 -1.9709380
C 0.0901680 -1.0254180 -2.2064300
H 2.3732420 -3.0436660 -2.5634350
H 2.7351050 -1.3205790 -2.6271880
H 3.0926870 -2.2606190 -1.1563540
H -1.5521210 1.7038160 2.3345810
H -2.1674390 0.03790 2.4906280
H -1.2140020 0.7627520 3.7901880
H 0.4887840 -0.4584740 -3.0465390
H -0.9729140 -1.2382790 -2.2565120
H 0.7691560 2.1111390 1.6750650
H 2.0232710 0.7763270 1.6917500
Ru 0.2757080 -0.1866060 -0.1324680
N -1.9585700 -0.1806710 -0.2101170
C -2.9060140 -1.1659200 -0.0122130
C -4.1573970 -0.6288900 -0.1632070
H -2.6423510 -2.1846690 0.2282650
H -5.1409190 -1.0679280 -0.0897080
H -2.1865370 1.8922220 -0.6780380
H 3.7145090 3.8023350 0.7196450
C 3.1318480 3.0361910 0.1833530
C 3.6864480 1.7275230 0.1226650
O 2.0330320 3.3873370 -0.3109480
H 4.5273010 1.4982840 0.7700970
H 0.9307400 2.4639360 -0.7841500
O 0.1367110 1.8637030 -1.0440960
H 0.1158290 1.8344950 -2.0087160
C 3.1765660 0.7553760 -0.7465750
H 3.7790920 -0.1347400 -0.8984820
H 2.0169090 0.0779130 -0.2537530
H 2.6767420 1.1102910 -1.6446390
C -2.6357370 0.9313370 -0.4772400
N -3.9700710 0.7050140 -0.4576800
C -5.0188400 1.6920610 -0.7099200
H -4.5553960 2.6660960 -0.8741770
H -5.5931460 1.4139890 -1.5974680
H -5.6876190 1.7560510 0.1520620

Mecanismo con el complejo 1.2l (*ruta trans-hidroxo-l*)

t-OH-l-I_0

E(gas): -825,5695707;

E(H_2O): -825,264772; G(H_2O): -825,964597

C	2.3375430	0.0913080	2.0653920
C	2.2033420	1.4684980	1.3729650
H	3.3694470	-0.2717740	2.0338170
H	2.8884090	1.5355410	0.5227340
H	2.0641400	0.1705990	3.1228630
H	2.4545050	2.2955340	2.0521020
C	1.3629810	-0.8613790	1.3774720
C	0.7571430	1.5627860	0.9181900
C	0.2429190	2.2945380	-0.2230070
H	0.0569070	1.5257790	1.7526260
C	-1.1285460	2.9249110	-0.1483210
C	0.9365140	2.2554350	-1.4096950
C	1.7130290	-1.7752230	0.3295450
H	0.4864410	-1.1366200	1.9602130
C	3.1351920	-2.0422870	-0.0960740
C	0.5933700	-2.3074300	-0.3485580
H	3.5796640	-2.7370940	0.6287100
H	3.1867470	-2.5320680	-1.0725830
H	3.7558490	-1.1436990	-0.1191800
H	-1.5996520	2.9900480	-1.1335920
H	-1.7957310	2.3922490	0.5332370
H	-1.0187840	3.9480320	0.2335490
H	0.7427390	-2.8716550	-1.2667240
H	-0.3287890	-2.51960	0.1822080
H	0.4707060	2.5982580	-2.3294940
H	1.9881430	2.0114540	-1.4763150
Ru	0.5872990	-0.0788530	-0.5263660
N	-1.4247840	-0.2631630	0.2728910
C	-2.0144550	-0.2346260	1.5182020
C	-3.3621680	-0.4334950	1.4042790
H	2.1186070	-1.0813100	-2.2486170
O	1.7102430	-0.2165290	-2.1057320
C	-2.4158290	-0.4830920	-0.5895820
H	-2.3062690	-0.5751990	-1.6604700
N	-3.5966700	-0.5876220	0.0546950
H	-4.1622830	-0.4799880	2.1450290
H	-1.4474970	-0.0730140	2.4206100
C	-4.8960420	-0.8293760	-0.5673640
H	-5.5757680	-0.0019690	-0.3479320
H	-4.7678790	-0.9062160	-1.6480500
H	-5.3225500	-1.7634230	-0.1925620

t-OH-l-I_1,

E(gas): -1018.85721270;

E(H_2O): -1019.158732; G(H_2O): -1018,77348

C	3.514760	-0.924755	-0.428106
C	3.199754	-0.723326	1.076496
H	4.259826	-0.205128	-0.778633
H	3.271790	0.333601	1.340049
H	3.935905	-1.920735	-0.604312
H	3.886404	-1.286658	1.723468
C	2.186862	-0.813036	-1.178346
C	1.774461	-1.221748	1.232502
C	0.753191	-0.844681	2.180505
H	1.684699	-2.269444	0.938803
C	-0.178137	-1.905248	2.720719
C	0.511239	0.491227	2.444124
C	1.746135	0.325987	-1.923697
H	1.734167	-1.759053	-1.467654
C	2.617923	1.500821	-2.281872
C	0.369689	0.327381	-2.220406
H	3.017038	1.314008	-3.287726
H	2.046893	2.432356	-2.332917
H	3.479814	1.631354	-1.622658
H	-1.159088	-1.496498	2.980602
H	-0.311143	-2.742193	2.031804
H	0.265446	-2.306606	3.641335
H	-0.095322	1.243774	-2.574784
H	-0.149474	-0.592538	-2.464413
H	-0.390225	0.756610	2.991654
H	1.256621	1.264847	2.308942
Ru	0.565648	0.176116	0.018431
N	-0.892029	-1.413704	-0.317206
C	-2.201053	-1.184955	-0.320385
C	-0.740235	-2.750087	-0.635423
N	-2.893560	-2.308822	-0.619254
C	-1.973852	-3.314894	-0.823052
H	0.227652	-3.222059	-0.704561
H	-2.270847	-4.321313	-1.076526

H -2.668277 -0.230880 -0.131087
O -0.801251 2.045006 -0.053987
C -1.861502 2.566615 0.776108
C -2.215664 3.969823 0.379066
H -2.726977 1.909192 0.648391
H -1.554864 2.524290 1.830273
C -3.417205 4.336114 -0.065831
H -1.423974 4.710332 0.490056
H -3.641891 5.366525 -0.322194
H -4.228237 3.626 -0.179021
H 0.089049 2.453471 0.190167
O 1.616689 1.934997 0.469213
H 2.258327 2.215913 -0.190513
C -4.347222 -2.432286 -0.719768
H -4.712385 -3.166164 0.003049
H -4.801088 -1.463549 -0.505459
H -4.627599 -2.742592 -1.729490000

t-OH-l-I_1

E(gas): -1018,860512;
E(H_2O): -1019,155085; G(H_2O): -1018,778275

C 3.2336740 -1.6698640 -0.2154850
C 2.9017240 -1.2952510 1.2544490
H 4.1434090 -1.1650900 -0.5510530
H 3.2204420 -0.2721050 1.4610100
H 3.4177530 -2.7458530 -0.3075430
H 3.4005560 -1.9643410 1.9693000
C 2.0135100 -1.3066870 -1.0578800
C 1.3938910 -1.4252850 1.3654940
C 0.4544920 -0.7150460 2.1975810
H 1.0555240 -2.4380620 1.1394890
C -0.7507590 -1.4436600 2.7447760
C 0.5574470 0.6600660 2.3307920
C 1.8881860 -0.1581300 -1.9008060
H 1.3546130 -2.1371420 -1.3015180
C 3.0351110 0.7375940 -2.2891060
C 0.5618530 0.1515460 -2.2689680
H 3.4276700 0.3646460 -3.2445200
H 2.7115900 1.7687590 -2.4615990
H 3.8664490 0.7255100 -1.5802190
H -1.6197420 -0.7854360 2.8347480
H -1.0247410 -2.3190400 2.1519490
H -0.4995320 -1.7949690 3.7540930
H 0.3618810 1.1139170 -2.7365920
H -0.1569840 -0.6311260 -2.4844550
H -0.2727360 1.2156600 2.7598360
H 1.4918680 1.1939490 2.2224600
Ru 0.6420500 0.1124810 -0.0267360
O 0.1838920 3.4492010 0.7512840
C -0.7578610 2.8629580 -0.0691110
C -2.1531030 3.1050650 0.4244900
H -0.6647600 3.1388660 -1.1331410
H -0.6210350 1.7136210 -0.0721750
C -3.1981420 3.3480620 -0.3707290
H -2.2689130 3.0798150 1.5070080
H -4.1910190 3.5228690 0.0319840
H -3.0911160 3.4197460 -1.4509210
H 1.0343490 2.9542250 0.6063540
O 2.0217420 1.5995910 0.3418440
H 2.6658050 1.7601630 -0.3552870
C -1.2962480 -2.4740700 -0.5635800
C -2.3629340 -0.6026600 -0.3304840
C -2.6288020 -2.7553890 -0.7085680
H -0.4625470 -3.1576660 -0.6100510
H -2.6108460 0.4406540 -0.1872600
H -3.1492410 -3.6815390 -0.9003070
C -4.7405580 -1.3541640 -0.6296560
N -1.1368230 -1.1218550 -0.3236690
N -3.2937150 -1.5580070 -0.5575650
H -5.2402640 -1.9351970 0.1495220
H -4.9556890 -0.2950970 -0.4801690
H -5.1131430 -1.6606950 -1.6102030

t-OH-l-I_2

E(gas): -1018,843855;
E(H_2O): -1019,149479; G(H_2O): -1018,764455

C -1.2879660 -3.3742110 -0.2124760
C -0.7464340 -3.0521580 1.2057490
H -0.7464120 -4.2080360 -0.6719200
H 0.3442100 -3.0679450 1.2253110
H -2.3325810 -3.6979120 -0.1397630
H -1.0948490 -3.7862120 1.9476760
C -1.2397440 -2.0856890 -1.0520160
C -1.2990440 -1.6697140 1.5217260
C -0.8552650 -0.5113280 2.2086620

H -2.3867970 -1.6766970 1.4220280
C -1.9026210 0.4129190 2.7970640
C 0.4773190 -0.0324240 2.1502820
C -0.1506060 -1.7004240 -1.8762150
H -2.1941940 -1.6106220 -1.2570630
C 0.9562260 -2.6594850 -2.2572390
C -0.0195270 -0.3310680 -2.2333090
H 0.6722410 -3.1195270 -3.2128250
H 1.9083380 -2.1477870 -2.4304160
H 1.0974450 -3.4904930 -1.5583800
H -1.6348350 1.4664110 2.6736410
H -2.8995190 0.2503520 2.3805310
H -1.9593870 0.2127990 3.8748980
H 0.8809610 -0.0284570 -2.7594750
H -0.8973680 0.2665820 -2.4568890
H 0.6609920 0.9590390 2.5539510
H 1.3184270 -0.7127160 2.2021130
Ru -0.0962220 -0.3860850 0.0069840
O 3.9881570 -0.0918430 -0.0488730
C 4.2125790 1.0959770 0.1720680
C 5.5211280 1.7137820 -0.0207050
H 3.4053330 1.7604420 0.5360650
H 0.9010810 0.8877920 -0.1771990
C 5.7027750 3.0151330 0.2469140
H 6.32200 1.0737150 -0.3803060
H 6.6640570 3.5012180 0.1168700
H 4.8870040 3.6366730 0.6094870
H 2.5610720 -0.9084990 0.1972180
O 1.7957910 -1.5401030 0.2957600
H 1.9722910 -2.2482090 -0.3357340
C -3.0562210 0.7481280 -0.3463890
C -1.5263060 2.2824240 -0.4074380
C -3.6963450 1.9392400 -0.5584770
H -3.4863020 -0.2348670 -0.2431370
H -0.5760370 2.7916770 -0.3974420
H -4.7416380 2.1788880 -0.6809340
C -2.9147440 4.3365280 -0.8073570
N -1.6947440 0.9714720 -0.2511810
N -2.7132980 2.9048070 -0.5951820
H -3.5566350 4.7459210 -0.0231210
H -1.9469080 4.8392350 -0.7745500
H -3.3747220 4.5108250 -1.7835320

t-OH-l-I_3

E(gas): -1018,846841;
E(H_2O): -1019,141998; G(H_2O): -1018,764889

C -1.4730930 -3.1231460 0.9328540
C -1.3786810 -2.9425270 -0.6056430
H -2.5110580 -3.1039860 1.2784280
H -2.1394150 -2.2460250 -0.9586820
H -1.0710420 -4.1019540 1.2168920
H -1.5430880 -3.8886650 -1.1437030
C -0.6082750 -2.0328400 1.5752880
C 0.0305510 -2.4287430 -0.8481190
C 0.6692080 -1.5789450 -1.7989180
H 0.7526940 -3.1130350 -0.4002100
C 2.1152940 -1.8619530 -2.1497140
C 0.1070110 -0.3606860 -2.2087070
C -1.0695840 -0.7822430 2.0281490
H 0.3852440 -2.3475150 1.8863640
C -2.5395850 -0.4891750 2.2170700
C -0.1060330 0.2732130 2.1969380
H -2.8098190 -0.8207840 3.2287170
H -2.7547430 0.5792420 2.1552350
H -3.1886140 -1.0161200 1.5157550
H 2.6997400 -0.9474190 -2.2811100
H 2.6088630 -2.4889940 -1.4040780
H 2.1282140 -2.4062380 -3.1032420
H -0.4894210 1.2519930 2.4740750
H 0.8567150 0.0542730 2.6608400
H 0.7309360 0.3255360 -2.7729820
H -0.9576080 -0.2454660 -2.3638430
Ru 0.0854700 -0.3295750 0.1056650
H 5.6455680 1.5146170 -1.1943140
C 4.8174060 1.4092210 -0.4709680
C 4.7569590 2.4302130 0.5888690
O 4.0312230 0.4766850 -0.6076630
H 5.6157980 3.0911070 0.6723000
H 2.7963850 -0.3739190 0.2067040
O 2.1391470 -0.9695760 0.6477730
H 2.3034500 -0.8731140 1.5951680
C 3.6862350 2.5771470 1.3812950
H 3.6468010 3.3473760 2.1447820
H 0.7420210 1.1258470 -0.1653370
H 2.8124710 1.9414430 1.2641970
C -2.9528690 0.3652540 -0.8941060

C -1.7824980 2.0616140 -0.2347020
C -3.7333390 1.4756600 -1.0670460
H -3.2035910 -0.6597570 -1.1103820
H -0.9808440 2.6821470 0.1311840
H -4.7375660 1.5929990 -1.4450710
C -3.3837420 3.9507910 -0.6498730
N -1.7290170 0.7379340 -0.3676500
N -2.9781230 2.5469780 -0.6416170
H -3.5996410 4.2735060 -1.6716520
H -2.5698240 4.5569870 -0.2491730
H -4.2720560 4.0888290 -0.0281480

t-OH-l-I_4
E(gas): -1018,848006;
E(H_2O): -1019,158938; G(H_2O): -1018,774505

C -0.7071370 -3.3497780 0.0305310
C -0.2073120 -2.8686180 -1.3608460
H -1.7957790 -3.4457240 0.0460340
H -0.9869910 -2.3139360 -1.8884260
H -0.2999080 -4.3397130 0.2633750
H 0.0719530 -3.7118390 -2.0081380
C -0.1876920 -2.3486900 1.0556190
C 1.0047920 -2.0062130 -1.0887940
C 1.4937060 -0.8302360 -1.7512780
H 1.8062630 -2.5555970 -0.5962910
C 2.9769560 -0.6162270 -1.8845180
C 0.5773570 0.1718130 -2.0554500
C -0.9685580 -1.4146480 1.7964960
H 0.7890030 -2.5896500 1.4736520
C -2.4721530 -1.4358970 1.8424070
C -0.2303390 -0.3696060 2.3996930
H -2.7526950 -2.0948550 2.6756330
H -2.8875650 -0.4483230 2.0542450
H -2.9383160 -1.8310640 0.9394950
H 3.2259990 0.4352200 -2.0393820
H 3.5180570 -0.9855990 -1.0127150
H 3.3140180 -1.1785790 -2.7657850
H -0.7763840 0.4799140 2.8057560
H 0.7228920 -0.5613340 2.8825110
H 0.9453640 1.1613890 -2.3191220
H -0.4428490 -0.0447520 -2.3396080
Ru 0.3291530 -0.3425830 0.2390440
H 4.4762460 3.1201550 -0.3943800
C 3.6598020 2.5592940 0.0559600
C 2.4406940 3.1216500 0.1877280
O 4.0528150 1.3363430 0.4350660
H 2.3001510 4.1146080 -0.2254580
H 3.3032360 0.7248280 0.6722380
O 2.2381680 -0.5817540 0.9246810
H 2.2902990 -0.7544820 1.8731820
C 1.3085830 2.4934040 0.9285840
H 0.5676100 3.2346060 1.2440410
H 0.7356970 1.7567620 0.2845150
H 1.6427500 1.9391630 1.8076880
C -2.7052260 -0.1112990 -1.1753080
C -2.1442470 1.5984230 0.0215630
C -3.7343910 0.7872130 -1.2622840
H -2.6308880 -1.0844410 -1.6348420
H -1.6109200 2.2902320 0.6553420
H -4.6760890 0.7503980 -1.7888780
C -4.1407310 3.0941510 -0.2924940
N -1.7082320 0.4024310 -0.3662020
N -3.3649780 1.8702930 -0.4954670
H -4.3112280 3.5919370 -1.2502720
H -3.5821160 3.7639280 0.3630810
H -5.1005710 2.8562100 0.1726100

t-OH-l-TS_1'
E(gas): -1018.83658151;
Frecuencia imaginaria: -52.934 cm^{-1}
E(H_2O): -1019.145980; G(H_2O): -1018,76262

C 2.2547440 -2.8197750 -0.0063000
C 1.9505850 -2.3538450 1.4481320
H 3.3059780 -2.6476040 -0.2523020
H 2.6282070 -1.5461940 1.7300590
H 2.0770650 -3.8953700 -0.1130310
H 2.0789490 -3.1729390 2.1689610
C 1.3078060 -2.0704360 -0.9343440
C 0.5121250 -1.8671090 1.4496520
C -0.0967300 -0.8339570 2.2671580
H -0.1911060 -2.6678990 1.2150740
C -1.5061530 -1.0437720 2.7712620
C 0.5245980 0.3873350 2.4312850
C 1.6407970 -0.9786440 -1.7991290

H 0.4025600 -2.6135170 -1.2003950
C 3.0353340 -0.5393270 -2.1537970
C 0.5135380 -0.2408100 -2.2242130
H 3.2716970 -0.9797230 -3.1315630
H 3.1018260 0.5465790 -2.2652270
H 3.8039640 -0.8927040 -1.4607640
H -2.0294150 -0.0958840 2.9262950
H -2.1012770 -1.6784270 2.1108740
H -1.4456990 -1.5491350 3.7440850
H 0.6670210 0.7528710 -2.6407340
H -0.4170540 -0.7376820 -2.4741810
H -0.0416030 1.2104690 2.8618460
H 1.5872970 0.5406910 2.2913890
Ru 0.5239870 -0.2312170 0.0129520
N -1.6041570 -0.6731720 -0.3556490
C -2.5248380 0.2850490 -0.4123620
C -2.2729770 -1.8556450 -0.6100820
N -3.7473780 -0.2269050 -0.6840690
C -3.6015330 -1.5909710 -0.8138830
H -1.7730540 -2.8120510 -0.6281480
H -4.4363240 -2.2390110 -1.0343250
H -2.3429200 1.3411660 -0.2769940
O 1.4726690 2.7300700 -1.1106300
C 0.3366050 3.1619200 -0.3860220
C 0.6420890 4.20450 0.6579840
H -0.3930070 3.5478170 -1.1070370
H -0.1492680 2.2844150 0.1148370
C 0.0103140 5.3694750 0.7594800
H 1.4389940 3.9445900 1.3566230
H 0.2596660 6.0901390 1.5320930
H -0.7746800 5.6564220 0.0630840
H 1.9824670 2.1456520 -0.5056500
O 2.3174900 0.6475780 0.4310430
H 3.0805220 0.3183690 -0.0571070
C -4.9928130 0.5288480 -0.8212720
H -5.7176040 0.1946000 -0.0748230
H -4.7832110 1.5883180 -0.6665990
H -5.4068680 0.3886560 -1.8227880

t-OH-l-TS$_1$
E(gas): -1018,833014;
Frecuencia imaginaria: -772.934 cm^{-1}
E(H_2O): -1019,137266; G(H_2O): -1018,756798

C 3.0604200 -1.9267400 -0.3004760
C 2.8322780 -1.4867450 1.1692630
H 4.0133920 -1.5541620 -0.6876520
H 3.1909690 -0.4684390 1.3248030
H 3.1081420 -3.0195300 -0.3641030
H 3.3539480 -2.1427470 1.8806240
C 1.8552770 -1.4439870 -1.1161190
C 1.3278390 -1.5778920 1.3570950
C 0.3851130 -0.8572570 2.1550510
H 0.9691100 -2.5826010 1.1238730
C -0.8388050 -1.5799510 2.6705700
C 0.4510730 0.5361100 2.2682740
C 1.8136820 -0.2487770 -1.8914030
H 1.1304300 -2.2072330 -1.3863820
C 3.0409940 0.5641580 -2.2270040
C 0.5313260 0.2337540 -2.2406900
H 3.4132090 0.2039930 -3.1952730
H 2.8106890 1.6263050 -2.3566150
H 3.8649080 0.4453520 -1.5179540
H -1.7147460 -0.9260460 2.7085400
H -1.0841070 -2.4725680 2.0904430
H -0.6262540 -1.9028810 3.6980910
H 0.4577760 1.2180330 -2.6973000
H -0.2734930 -0.4506860 -2.4866730
H -0.4038060 1.0576940 2.6901590
H 1.3906800 1.0710760 2.2929860
Ru 0.5631630 0.0698720 0.0034570
O 0.7118880 3.3588810 0.6260210
C -0.3313840 2.9787620 -0.0355280
C -1.6732050 3.2691780 0.5503750
H -0.3176170 3.0562400 -1.1390500
H -0.3707290 1.5692990 -0.0323150
C -2.7530240 3.5284760 -0.19500
H -1.7047400 3.3190520 1.6367550
H -3.7048430 3.7978600 0.2521030
H -2.7082330 3.5229280 -1.2822030
H 1.6050150 2.4523020 0.5054320
O 2.1641960 1.4709330 0.4225260
H 2.8539240 1.5886170 -0.2408920
C -1.5074950 -2.3139850 -0.6202810
C -2.4399080 -0.3788120 -0.3168590
C -2.8561010 -2.4924860 -0.7757480
H -0.7240980 -3.0518470 -0.6880800

H -2.6038210 0.6733230 -0.1300730
H -3.4405100 -3.3716590 -1.09990
C -4.8626880 -0.9486290 -0.6472650
N -1.2547420 -0.9857820 -0.3306760
N -3.4345030 -1.2570380 -0.5802010
H -5.4073920 -1.5319210 0.0993520
H -5.0042960 0.1137730 -0.4438530
H -5.2489680 -1.1777160 -1.6435940

t-OH-l-TS$_2$
E(gas): -1018,830934;
Frecuencia imaginaria: -475. 610 cm^{-1}
E(H_2O): -1019,136845; G(H_2O): -1018,755598

C -0.5384110 -3.4567980 0.2006580
C -0.2768920 -2.9205670 -1.2319250
H -1.5836140 -3.7491430 0.3369280
H -1.1385490 -2.3600950 -1.5927720
H 0.0622450 -4.3556570 0.3770010
H -0.1016700 -3.7341450 -1.9514950
C -0.0928670 -2.3694860 1.1814130
C 0.9650700 -2.0592010 -1.0922730
C 1.5046230 -0.8981870 -1.7222730
H 1.7642270 -2.6445160 -0.6349990
C 3.0090700 -0.7964630 -1.8402230
C 0.7188980 0.2377470 -1.9818050
C -0.9388970 -1.4042430 1.7682170
H 0.8906320 -2.5082830 1.6245230
C -2.4438780 -1.5160320 1.7083360
C -0.3224840 -0.2356800 2.3198920
H -2.7532130 -2.2003960 2.5094750
H -2.9301800 -0.5563320 1.8938320
H -2.8191910 -1.9202450 0.7666900
H 3.3773260 0.2202990 -1.6913620
H 3.5277930 -1.4583080 -1.1439800
H 3.2782890 -1.1050510 -2.8592820
H -0.9792040 0.5485760 2.6893720
H 0.6004550 -0.3232580 2.8916120
H 1.2325180 1.1638930 -2.2298970
H -0.2952490 0.1625110 -2.3505610
Ru 0.3274480 -0.2801130 0.2180740
H 4.3146150 3.2471690 -0.4906220
C 3.5399570 2.6362270 0.07420
C 2.2424300 3.2130980 0.1365060
O 3.8613900 1.4875850 0.3818240
H 2.08220 4.0859740 -0.4620720
H 2.9266840 0.3151850 0.7860850
O 2.36030 -0.5048050 1.0092290
H 2.4109550 -0.60840 1.9682360
C 1.3044860 2.6498480 0.9887860
H 0.3825600 3.1919540 1.1824610
H 0.6219200 1.40540 0.3713360
H 1.6609240 2.0507610 1.8197990
C -2.5625720 -0.0850040 -1.3497600
C -2.1700550 1.4988320 0.0677450
C -3.6338400 0.7651710 -1.3989090
H -2.4070510 -0.9829060 -1.9243720
H -1.7135160 2.1311780 0.8112590
H -4.5380700 0.7432420 -1.9880500
C -4.2266070 2.9177110 -0.20080
N -1.6452760 0.3782350 -0.4232300
N -3.3725900 1.7667290 -0.4905630
H -4.3424370 3.5349480 -1.09452400

MATERIAL SUPLEMENTARIO

CAPÍTULO 4

Tabla S4.1. Datos cristalográficos para el compuesto **4.1c**.

	4.1c
Chem formula	$RuC_{20}H_{27}ClO_2$
fw	435.94
T (K)	293(2)
wavelength (Å)	1.54184
space group	$P2_1/n$
a, Å	8.7941(3)
b, Å	17.6238(6)
c, Å	12.5849(4)
α, deg	90
β, deg	102.288(3)
γ, deg	90
Z	4
V, Å^3	1905.79(11)
ρ_{calcd}, gcm^{-3}	1.519
μ, mm^{-1}	8.010
goodness of fit on F^2	1.182
weight function (*a*,*b*)	0.1602,0.4375
R1[a] ($I > 2\sigma(I)$)	0.0719
wR2[a] ($I > 2\sigma(I)$)	0.2041
R1[a] (all data)	0.0834
wR2[a] (all data)	0.2416
F(0)	896

[a] $R1 = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|$; $wR2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/ \Sigma[w(F_o^2)^2]\}^{1/2}$.

Figura S4.1. Espectros del complejo **4.1c**.

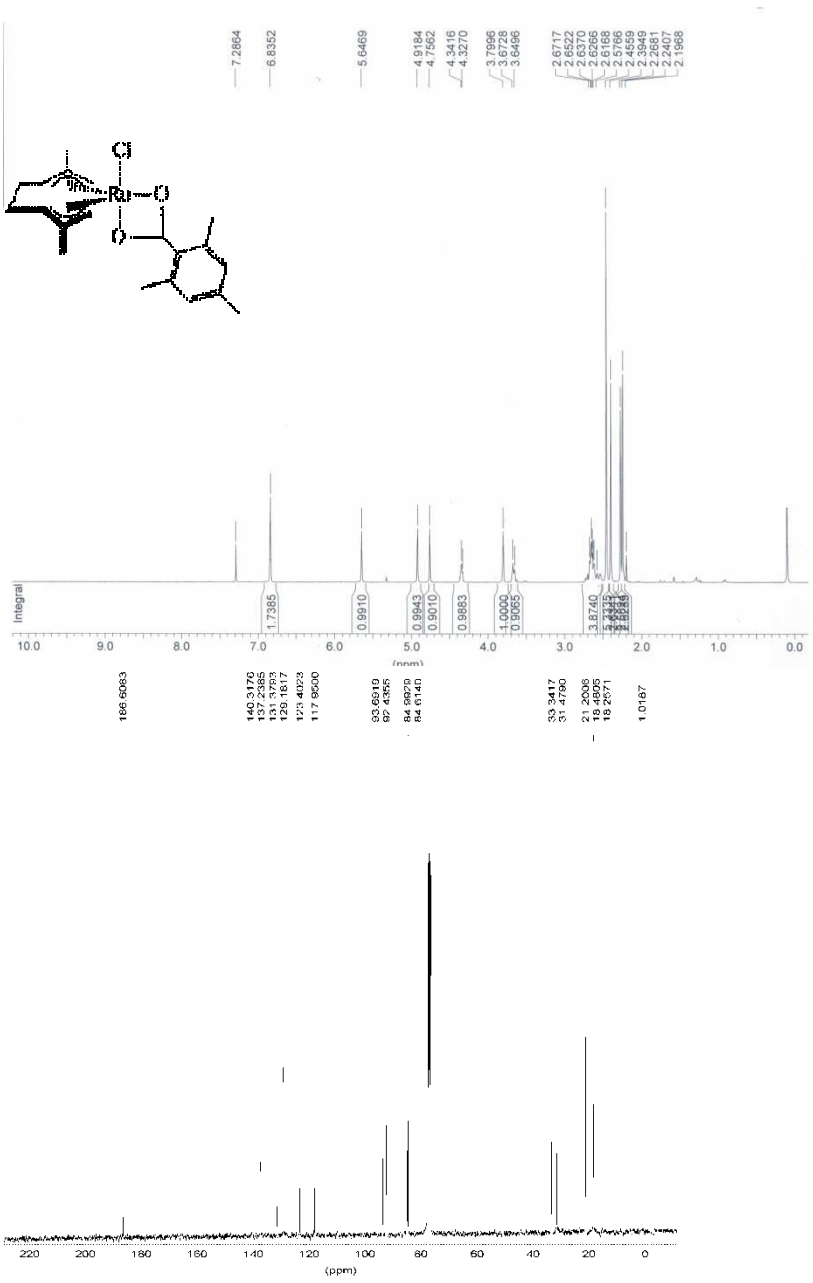
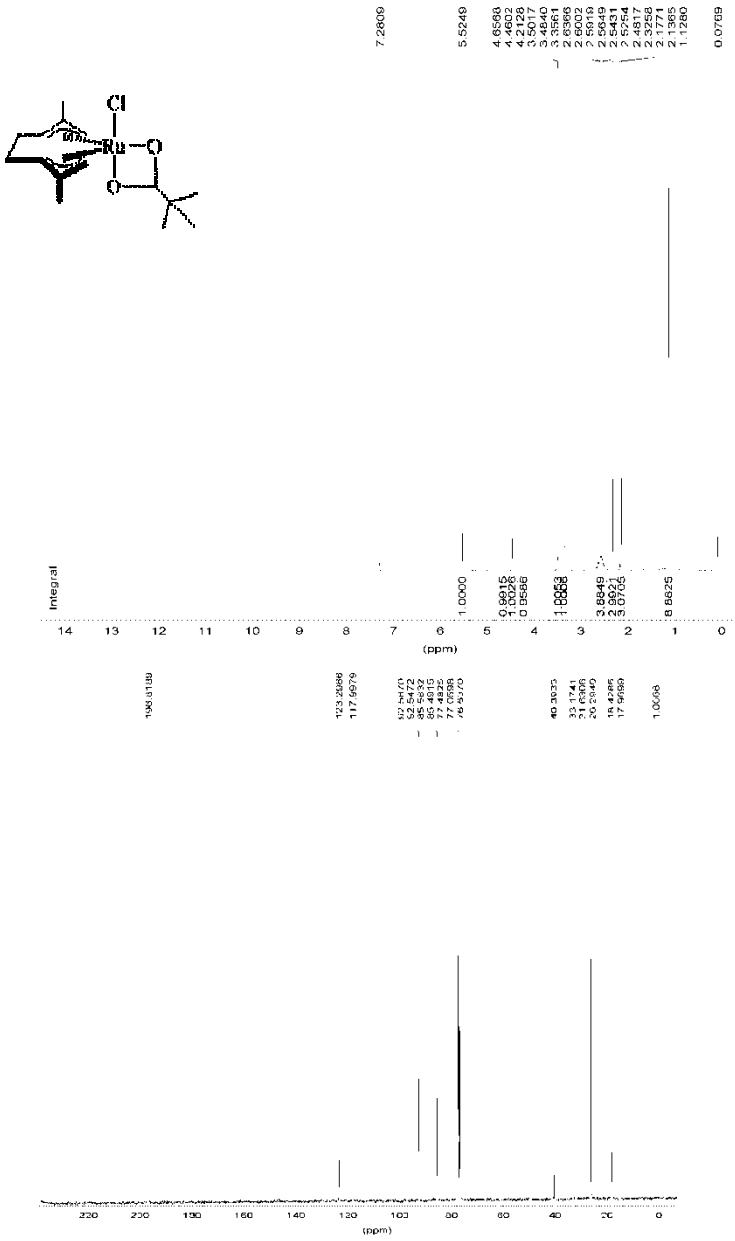



Figura S4.2. Espectros del complejo **4.1d**.