

## Electronic supplementary information

### **A comparative study of Rh<sub>2</sub>-catalyzed intermolecular nitrene transfer reactions: mechanism and chemoselectivity**

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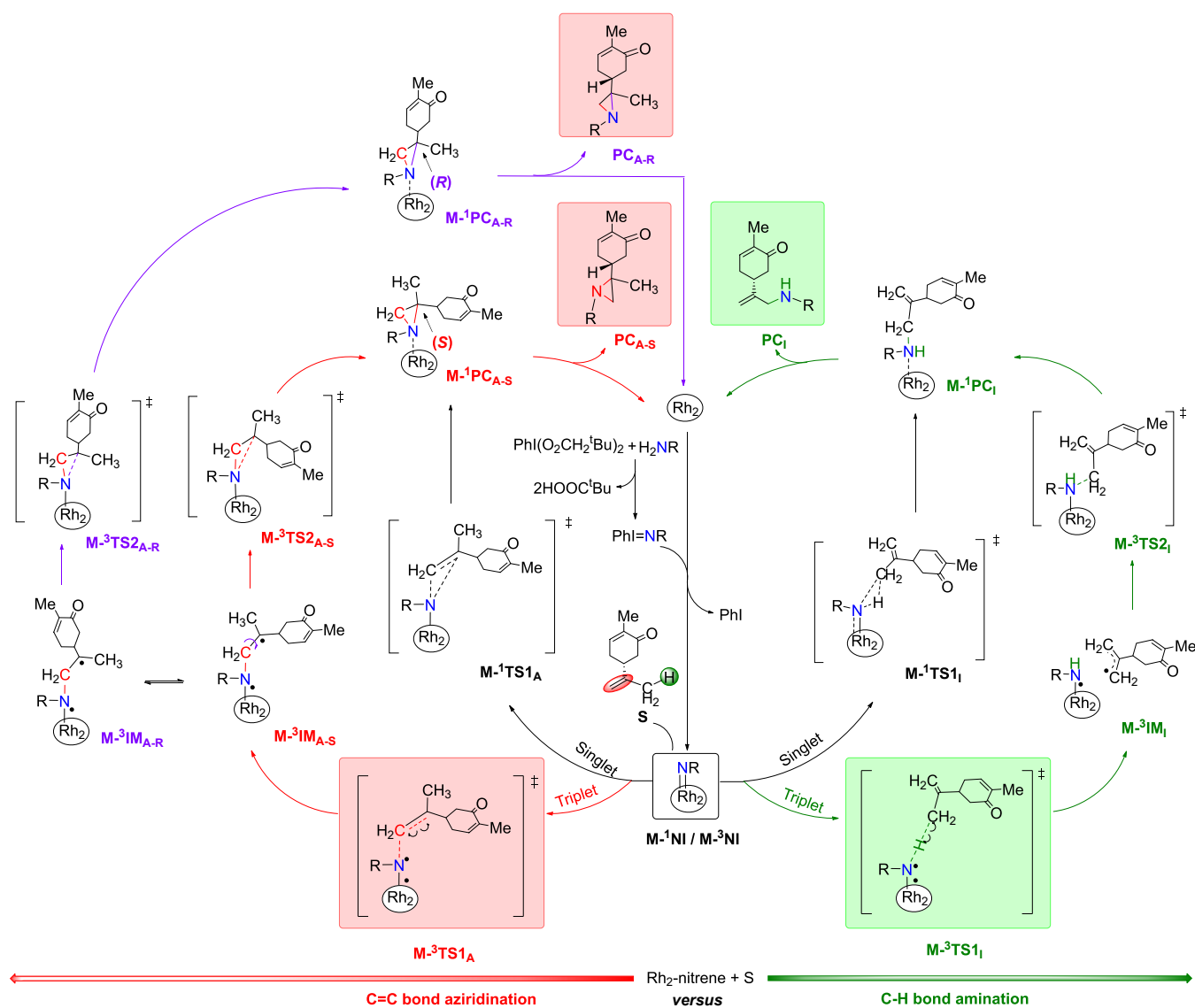
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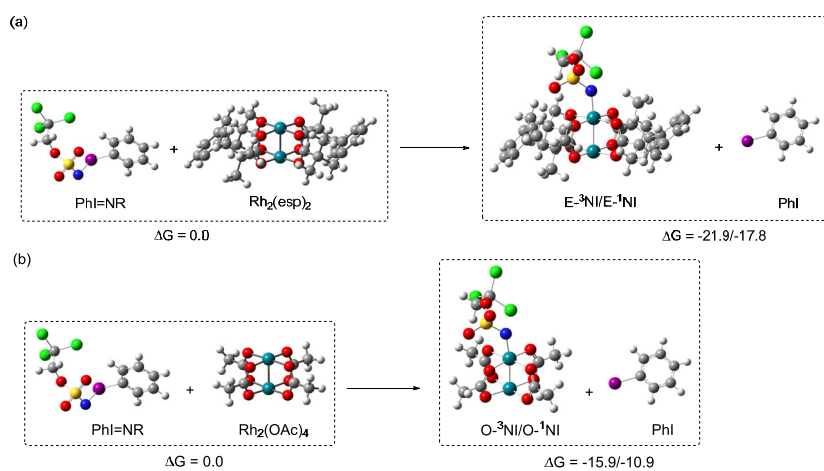
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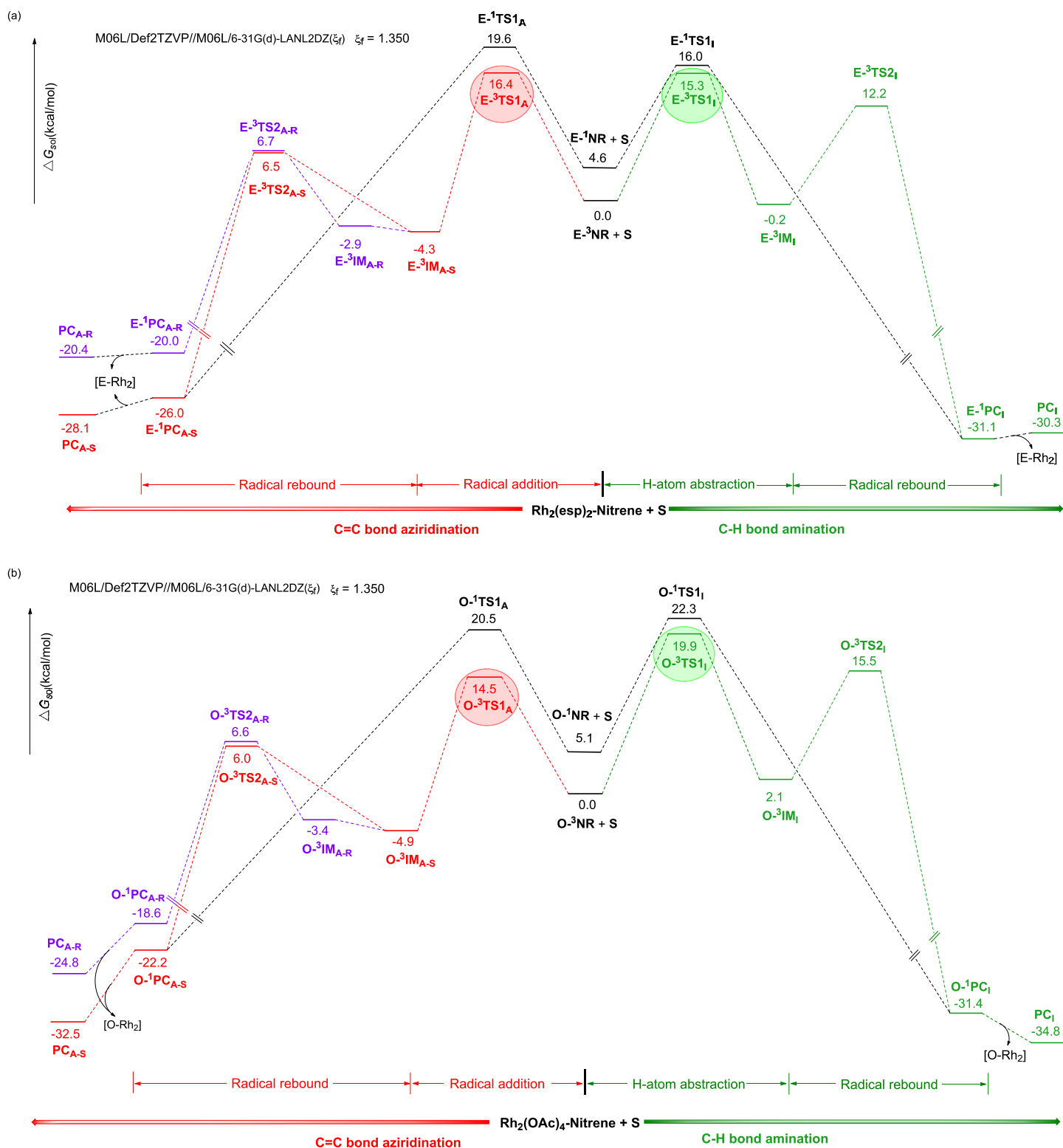
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**Scheme S1** Catalytic cycles of aziridination vs. amination for the substrate carvone (S).

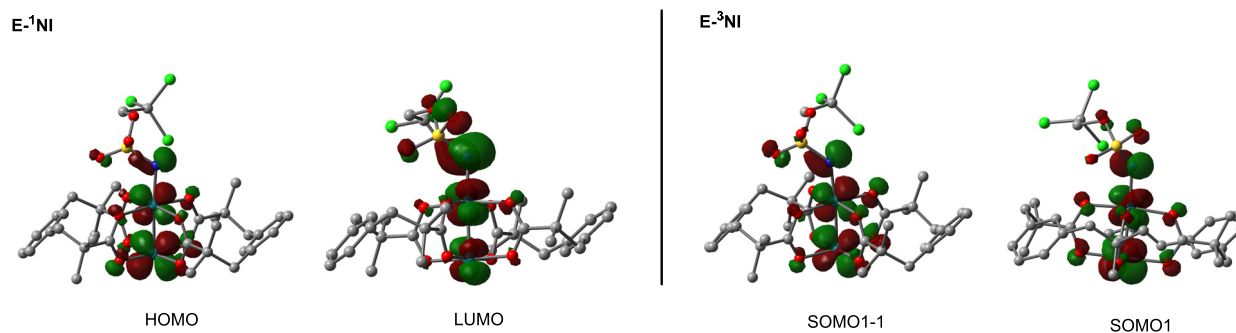


**Scheme S2** Relative free energy ( $\Delta G$ , in kcal/mol) for the  $\text{Rh}_2$ -mediated decomposition of imino phenylidines in Part I (computed at M06L/BS2//M06L/BS1 level). Obviously, the formation step of  $\text{Rh}_2$ -nitrene is exothermic.

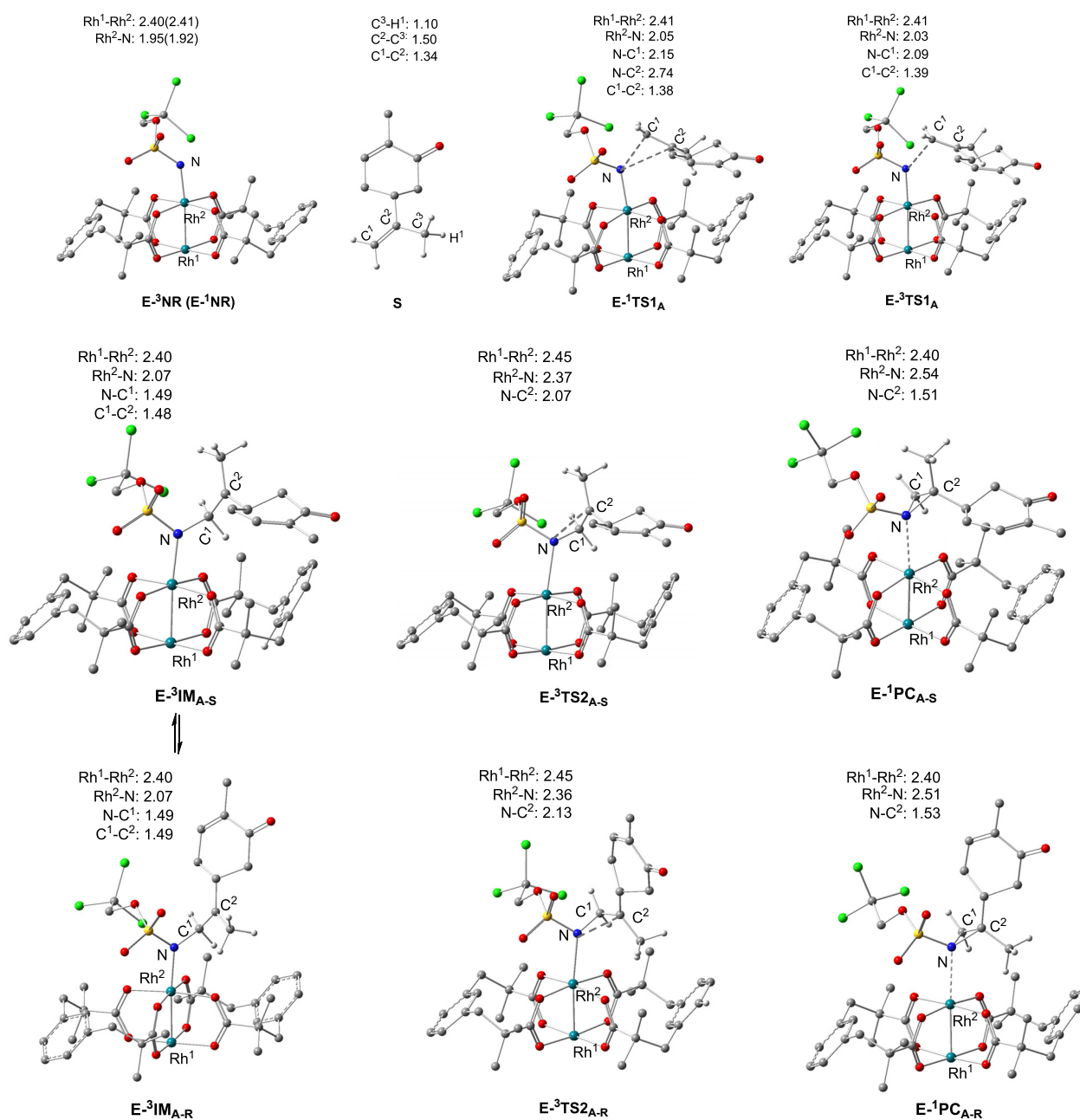


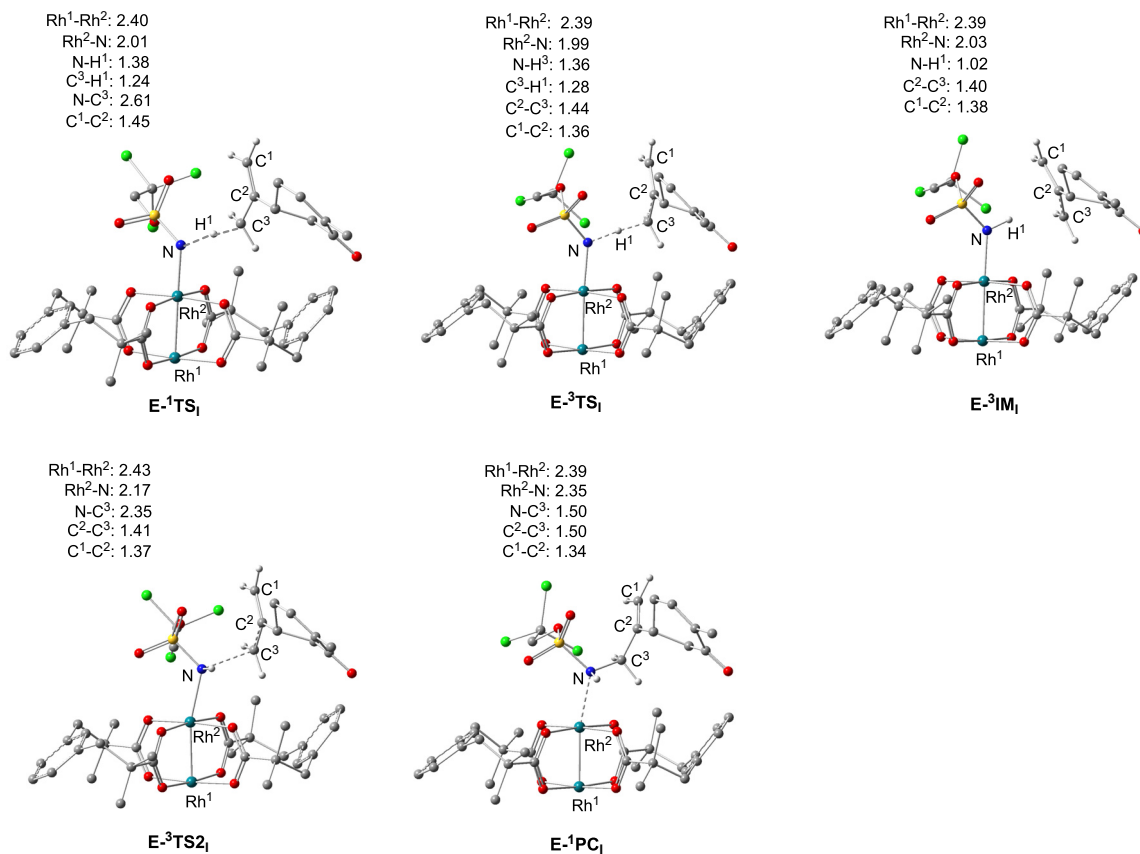
**Fig. S1** Free energy profiles of Rh<sub>2</sub>-catalyzed nitrene transfer reactions. (a) Rh<sub>2</sub>(esp)<sub>2</sub>-catalysis. (b) Rh<sub>2</sub>(OAc)<sub>4</sub>-catalysis. Energetics were computed at M06L/BS3//M06L/BS1 level. This method slightly underestimated energy of Rh<sub>2</sub>(esp)<sub>2</sub>-catalyzed amination, resulting in  $\text{E}^{-3}\text{TS1}_I$  lower in energy than  $\text{E}^{-3}\text{TS1}_A$  (13.4 vs. 14.5 kcal/mol). Relatively, computed energetics at M06L/BS2//M06L/BS1 level are more reasonable.

(a) Important Kohn Sham orbitals for singlet and triplet  $Rh_2(esp)_2$ -nitrene. SOMO: singly occupied molecular orbital

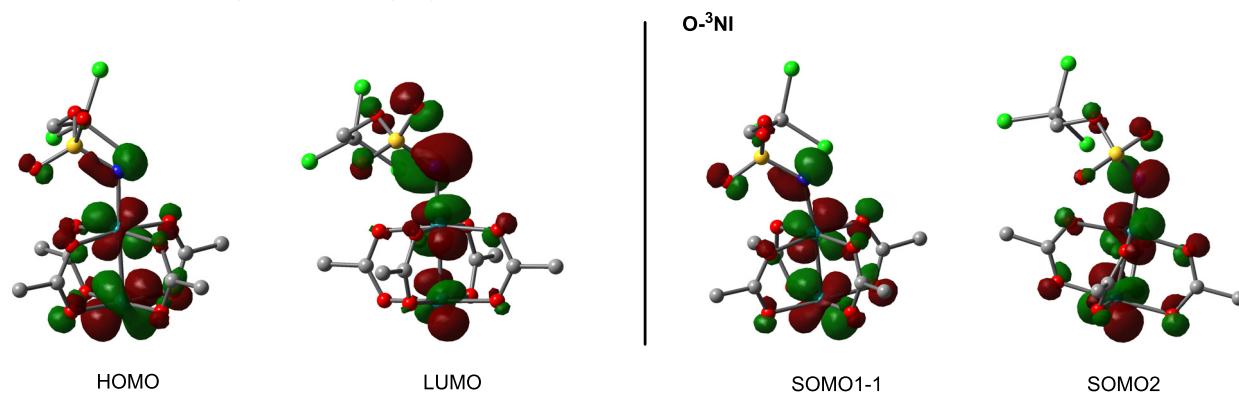


(b) Optimized structures of species with important bond lengths for  $Rh_2(esp)_2$  catalysis

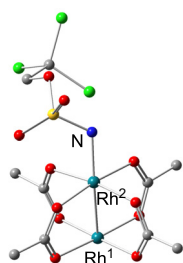




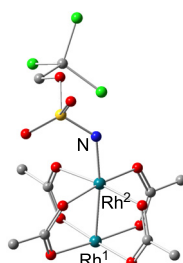
**Fig. S2** Orbitals of Rh<sub>2</sub>(esp)<sub>2</sub>-nitrene and optimized structures of Rh<sub>2</sub>(esp)<sub>2</sub>-based catalysis (bond lengths in Å). For clarity, except for H atoms related to reaction sites (i.e. –CH<sub>3</sub> and CH<sub>2</sub>=C-), other H atoms are omitted.

(a) Important Kohn Sham orbitals for singlet and triplet  $\text{Rh}_2(\text{OAc})_4$ -nitrene.(b) Optimized structures of species with important bond lengths for  $\text{Rh}_2(\text{OAc})_4$  catalysis

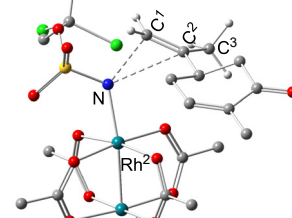
Rh<sup>1</sup>-Rh<sup>2</sup>: 2.42  
Rh<sup>2</sup>-N: 1.91



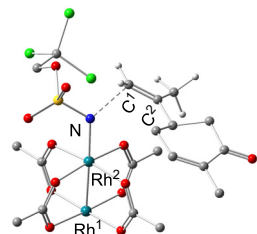
Rh<sup>1</sup>-Rh<sup>2</sup>: 2.40  
Rh<sup>2</sup>-N: 1.95



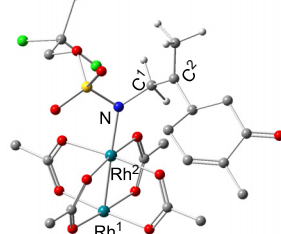
Rh<sup>1</sup>-Rh<sup>2</sup>: 2.41  
Rh<sup>2</sup>-N: 2.01  
N-C<sup>1</sup>: 2.18  
C<sup>1</sup>-C<sup>2</sup>: 1.37  
N-C<sup>2</sup>: 2.83



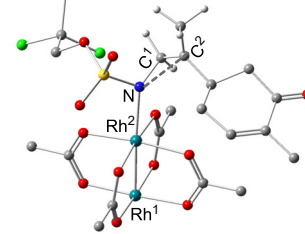
Rh<sup>1</sup>-Rh<sup>2</sup>: 2.41  
Rh<sup>2</sup>-N: 2.02  
N-C<sup>1</sup>: 2.13  
C<sup>1</sup>-C<sup>2</sup>: 1.38



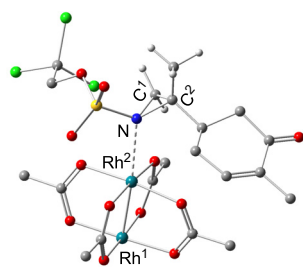
Rh<sup>1</sup>-Rh<sup>2</sup>: 2.40  
Rh<sup>2</sup>-N: 2.07  
N-C<sup>1</sup>: 1.49  
C<sup>1</sup>-C<sup>2</sup>: 1.49



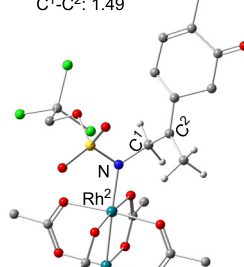
Rh<sup>1</sup>-Rh<sup>2</sup>: 2.46  
Rh<sup>2</sup>-N: 2.35  
N-C<sup>2</sup>: 2.10



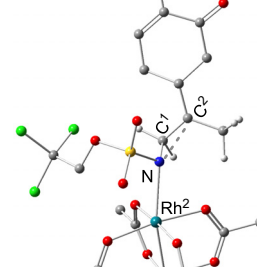
Rh<sup>1</sup>-Rh<sup>2</sup>: 2.40  
Rh<sup>2</sup>-N: 2.53  
N-C<sup>2</sup>: 1.52

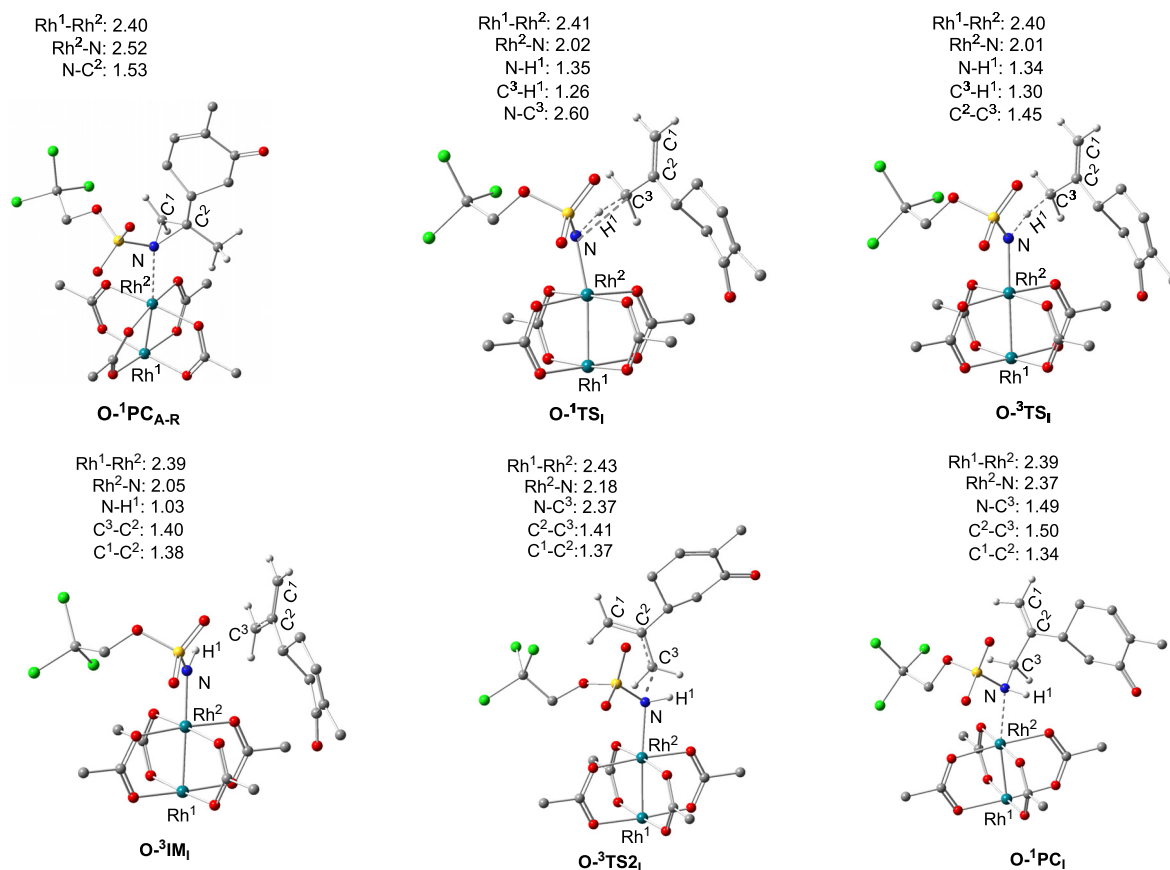


Rh<sup>1</sup>-Rh<sup>2</sup>: 2.41  
Rh<sup>2</sup>-N: 2.07  
N-C<sup>1</sup>: 1.49  
C<sup>1</sup>-C<sup>2</sup>: 1.49

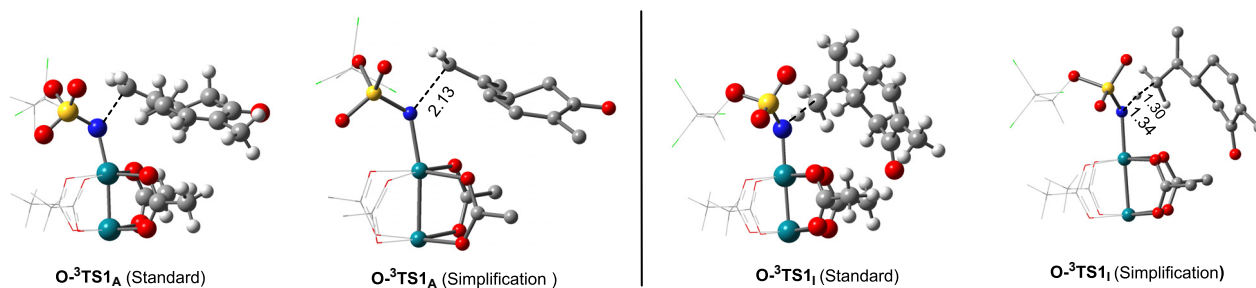


Rh<sup>1</sup>-Rh<sup>2</sup>: 2.46  
Rh<sup>2</sup>-N: 2.43  
N-C<sup>2</sup>: 2.12





**Fig. S3** Orbitals of Rh<sub>2</sub>(OAc)<sub>4</sub>-nitrene and optimized structures of Rh<sub>2</sub>(OAc)<sub>4</sub>-based catalysis (bond lengths in Å). For clarity, except for H atoms related to reaction sites (i.e. -CH<sub>3</sub> and CH<sub>2</sub>=C-), other H atoms are omitted.



**Fig. S4** Comparison of steric hindrance of O<sup>-3</sup>TS<sub>1A</sub> and O<sup>-3</sup>TS<sub>1</sub>. Steric hindrance of between OAc ligand and substrate carvone in transition states O<sup>-3</sup>TS<sub>1A</sub> and O<sup>-3</sup>TS<sub>1</sub> are very small and has no effect on chemoselectivity. The atomic radii in O<sup>-3</sup>TS<sub>1A</sub> and O<sup>-3</sup>TS<sub>1</sub> are shown in both normal (Standard) and reduced (Simplification) sizes. In the latter, other H atoms are omitted except those H atoms on reactive groups (i.e. -CH<sub>2</sub>=C and -CH<sub>3</sub>), and a smaller atomic radii and omitted H atoms make the structures clearer. Bond lengths are shown in Å.

#### Equation S1

PC<sub>A</sub>, PC<sub>1</sub>, *k<sub>A</sub>* and *k<sub>1</sub>* denote products and rate coefficients of aziridination and amination, respectively.



## Cartesian coordinates

E- <sup>1</sup> Nl			
Rh	-0.20990600	-0.15889200	-0.49762800
Rh	-0.72484900	-1.60075000	1.36753000
O	-1.33562300	1.30919500	0.49144200
C	-1.86920000	1.04950400	1.61607300
O	-1.78578800	-0.05361500	2.24236900
O	-1.93139200	-0.88629100	-1.39293900
C	-2.64824700	-1.75017700	-0.79381700
O	-2.39691700	-2.24471600	0.34898000
O	0.35437000	-3.08391800	0.42288700
C	0.87365800	-2.85713300	-0.70963600
O	0.81445900	-1.74924200	-1.34450700
O	1.45492400	0.42763700	0.61920700
C	1.67585800	-0.07587800	1.76950600
O	0.95199200	-0.94467300	2.34259200
C	-2.66484000	2.16847000	2.28985100
C	-4.07526200	1.62337800	2.63806700
H	-3.95872900	0.81430300	3.37037900
H	-4.61482300	2.43952200	3.14039400
C	-4.85037900	1.13430800	1.44747300
C	-4.72570300	-0.19421100	1.03326600
C	-5.66246500	1.99084000	0.69776400
C	-5.35293800	-0.67055400	-0.12085300
H	-4.11984200	-0.87864100	1.62631500
C	-6.31762200	1.52741400	-0.43904300
H	-5.78340600	3.02799500	1.01251600
C	-6.15762100	0.20819800	-0.85221700
H	-6.95548600	2.20027000	-1.00966600
H	-6.66593500	-0.14877200	-1.74863700
C	-3.89454100	-2.25726100	-1.51609900
C	-5.11398900	-2.08366800	-0.57156000
H	-5.98975600	-2.46882100	-1.11377300
H	-4.96248300	-2.73322700	0.30019200
C	2.91661900	0.43619000	2.49903900
C	1.63268200	-3.98832200	-1.39981900
C	4.16284500	0.12680300	1.62660200
H	4.10079800	0.73635400	0.71454000
H	5.03891700	0.47719900	2.19164500
C	3.10749700	-3.54234600	-1.58819500
C	4.31817900	-1.31834300	1.24544000
C	3.72191000	-1.77711600	0.06940800
C	5.02550300	-2.22934600	2.03548700
C	3.79921600	-3.11451800	-0.32454400
H	3.20194700	-1.06618000	-0.57104200
C	5.12060400	-3.56504100	1.65310400
H	5.51611400	-1.88620500	2.94739100
C	4.50824300	-4.00832900	0.48351500
H	5.68454600	-4.26489600	2.26795000
H	4.59394600	-5.05416500	0.18539500
O	1.18797500	0.71110600	-4.03733300
S	1.53868700	1.12636000	-2.68813900
O	2.69188300	0.55155600	-2.00554200
N	0.12394500	1.14973800	-1.86373700
O	1.86279800	2.75372700	-2.85285300
C	2.71434800	3.35475800	-1.90069400
H	3.15403400	2.61005100	-1.22589100
H	3.51716400	3.86797600	-2.44312200
C	1.96206100	4.39300300	-1.06877600
Cl	1.28822200	5.66091200	-2.11539600
Cl	3.16486200	5.10683300	0.05941400
Cl	0.65849000	3.60568000	-0.15134500
C	-4.10563300	-1.51387500	-2.82957900
H	-3.25625500	-1.65201200	-3.50594600
H	-5.00600600	-1.89792400	-3.32606500
H	-4.23094800	-0.43795500	-2.67339900
C	-3.68908400	-3.75259900	-1.78283800
H	-4.57952900	-4.16576100	-2.27237200
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H	-3.51753800	-4.30532300	-0.85300200
C	-2.76603200	3.39475200	1.38988700
H	-3.38822000	4.15622000	1.87783100
H	-1.78212100	3.83658700	1.20352800
H	-3.21000300	3.15567600	0.41870200
C	-1.93187800	2.52874700	3.58606400
H	-0.92629900	2.91471900	3.37356800
H	-2.48119400	3.31481200	4.11854500
H	-1.83737700	1.66108400	4.24744200
C	2.78759500	1.95520700	2.64443100
H	1.91374600	2.22949300	3.24917500
H	3.67814400	2.35849500	3.14204900
H	2.68765600	2.44043800	1.66777600

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C	3.03626300	-0.22160400	3.86835200
H	3.92959100	0.16020900	4.37904900
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H	-0.03238800	-4.54978000	-2.69642500
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C	1.55405800	-5.26371000	-0.56851900
H	0.51700900	-5.58890300	-0.43325500
H	2.09928200	-6.06660300	-1.08095000
H	1.99094300	-5.12938300	0.42576600
H	3.12129700	-2.71465700	-2.30997600
H	3.63564800	-4.38705600	-2.05411800

E-<sup>3</sup>NI

Rh	-0.25185400	-0.12443300	-0.47604800
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C	-1.88256500	1.10412300	1.60216600
O	-1.81210700	-0.00793900	2.21336200
O	-1.97411300	-0.79708500	-1.40492800
C	-2.69285600	-1.67302300	-0.82489500
O	-2.45356600	-2.19012400	0.31083300
O	0.27763900	-3.10017200	0.47593800
C	0.80687400	-2.87237300	-0.65531400
O	0.75548100	-1.76679400	-1.28811300
O	1.41876000	0.47235300	0.65334100
C	1.62811800	-0.05434300	1.79663900
O	0.90621100	-0.93889100	2.34872200
C	-2.66290600	2.22582700	2.28244600
C	-4.08569500	1.69892800	2.61061100
H	-3.98862900	0.88267300	3.33789300
H	-4.61685200	2.51906000	3.11516800
C	-4.85891400	1.22984800	1.41066500
C	-4.75432900	-0.09863300	0.99046100
C	-5.65310700	2.10341700	0.66152200
C	-5.38394500	-0.55946700	-0.16867300
H	-4.16389100	-0.79691400	1.58302800
C	-6.31165700	1.65568900	-0.47965600
H	-5.75893900	3.14076300	0.98105900
C	-6.17178100	0.33584900	-0.89834500
H	-6.93699100	2.34117100	-1.04909700
H	-6.68310300	-0.00858100	-1.79788200
C	-3.93932400	-2.16040800	-1.56156900
C	-5.16455500	-1.97367200	-0.62632400
H	-6.04183300	-2.34060600	-1.17846900
H	-5.03138000	-2.63147000	0.24223700
C	2.85786300	0.44304900	2.55468800
C	1.57152300	-4.00653800	-1.33434900
C	4.11737100	0.10893600	1.71099600
H	4.08922900	0.71887500	0.79711700
H	4.98758900	0.44445600	2.29374900
C	3.05173500	-3.56695800	-1.49624300
C	4.25297900	-1.34102900	1.33957100
C	3.66215200	-1.80166700	0.16147800
C	4.93692200	-2.25598600	2.14535500
C	3.72633900	-3.14279800	-0.22205200
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C	5.01608100	-3.59632800	1.77556600
H	5.42163000	-1.91236600	3.06025400
C	4.41218300	-4.04023200	0.60183600
H	5.56219400	-4.29916800	2.40300300
H	4.48812500	-5.08911600	0.31208900
O	1.38136600	0.76787500	-4.25382200
S	1.69349300	0.99162600	-2.85780600
O	2.79245200	0.28407700	-2.20995800
N	0.33119100	0.96765500	-1.97743100
O	2.06859300	2.60924400	-2.80270800
C	2.79419200	3.06086500	-1.67309600
H	2.90049700	2.27473600	-0.91301200
H	3.78993900	3.38031900	-2.00281600
C	2.08857500	4.25767200	-1.04185100
Cl	1.85287900	5.54803600	-2.24091000
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Cl	0.52850000	3.75618400	-0.35822900
C	-4.13006700	-1.40701200	-2.87247200
H	-3.27480800	-1.54849900	-3.54060800
H	-5.02837600	-1.78023900	-3.38085900
H	-4.24776500	-0.33099700	-2.71133600
C	-3.75424000	-3.65680000	-1.83603400
H	-4.64784200	-4.05429800	-2.33277300
H	-2.89961900	-3.83482300	-2.50026800

H	-3.59507600	-4.21751300	-0.90885300
C	-2.73232200	3.46473600	1.39713500
H	-3.35150600	4.22890700	1.88421700
H	-1.73834900	3.89499300	1.23689000
H	-3.16353500	3.24518600	0.41548600
C	-1.93871600	2.55742600	3.59155400
H	-0.92680400	2.93477800	3.39577200
H	-2.48517200	3.34156400	4.12958800
H	-1.86241300	1.67917000	4.24111400
C	2.74651800	1.96275300	2.69627200
H	1.87510500	2.24706000	3.29938900
H	3.64034900	2.35847800	3.19431900
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H	-0.07246900	-4.55651800	-2.66226300
H	1.00811400	-3.31071800	-3.32556300
C	1.47322500	-5.28350700	-0.50739800
H	0.43276000	-5.60463800	-0.38975000
H	2.02303500	-6.08745300	-1.01324700
H	1.89509700	-5.15386000	0.49403100
H	3.08321900	-2.73846800	-2.21621100
H	3.58311800	-4.41449600	-1.95327200

**E<sup>-1</sup>TS1<sub>A</sub>**

Rh	0.13559500	-0.30072900	0.01774300
Rh	0.53158400	-2.34032200	1.23081100
O	-0.45482700	0.53448700	1.87876500
C	-0.58567200	-0.23973400	2.87904200
O	-0.32358100	-1.48254000	2.90520100
O	-1.76886500	-0.99000000	-0.41730000
C	-2.04257500	-2.20737900	-0.14154700
O	-1.31178700	-2.98917900	0.53588800
O	1.36952500	-3.14960400	-0.46671100
C	1.21547000	-2.52271700	-1.55870500
O	0.69554200	-1.36535800	-1.68932900
O	2.12111300	0.18361700	0.58123500
C	2.75608100	-0.55739800	1.39742600
O	2.34694700	-1.66092200	1.87389900
C	-1.11512100	0.34211400	4.19327300
C	-2.45227200	-0.37928700	4.53010100
H	-2.20792900	-1.40084200	4.84841200
H	-2.88075700	0.13434800	5.40338600
C	-3.45936200	-0.44594600	3.41277400
C	-3.46086600	-1.55488700	2.56125600
C	-4.41088100	0.55683700	3.19105600
C	-4.36173400	-1.68065600	1.50041200
H	-2.73819100	-2.35259300	2.73815400
C	-5.31583400	0.45338300	2.13513200
H	-4.45074100	1.41851100	3.85943500
C	-5.28893600	-0.65412100	1.28951700
H	-6.06367500	1.22903300	1.97227200
H	-6.02006400	-0.73406700	0.48310000
C	-3.37771000	-2.76907300	-0.62244400
C	-4.29651000	-2.90267800	0.62649500
H	-5.29790100	-3.17190400	0.26028800
H	-3.93357400	-3.75168800	1.22087200
C	4.13720100	-0.06972700	1.83389000
C	1.71661500	-3.19682500	-2.83537400
C	5.04122600	0.00989600	0.57451100
H	4.69350800	0.85157200	-0.04112400
H	6.05234400	0.26722400	0.92313300
C	3.07740700	-2.54946500	-3.22273400
H	3.45739200	-3.11739000	-4.08496500
H	2.87218000	-1.52871500	-3.57191300
C	5.06750300	-1.23483800	-0.26850500
C	4.14309700	-1.36736500	-1.30550400
C	5.98088500	-2.27147400	-0.05521700
C	4.10578500	-2.49413600	-2.12801500
H	3.44023800	-0.55838800	-1.49501600
C	5.95921100	-3.40410900	-0.86588500
H	6.72611700	-2.18199300	0.73653700
C	5.02892400	-3.51780100	-1.89691500
H	6.68397700	-4.20011400	-0.70129200
H	5.03029500	-4.40028600	-2.53818300
O	0.11183700	1.87114700	-3.49170500
S	0.95066000	1.73554000	-2.31037000
O	2.13060000	0.87934100	-2.34547200
N	0.18302300	1.54393800	-0.87278000

O	1.55619100	3.30243500	-2.12758900
C	2.73152900	3.38109900	-1.34878900
H	2.92898200	2.44615800	-0.80515800
H	3.58465000	3.59662300	-2.00481300
C	2.63941300	4.50971000	-0.32583700
Cl	2.13551000	6.02774600	-1.10811000
Cl	4.28443700	4.69992400	0.36929700
Cl	1.50137900	4.10782800	0.99151700
C	-1.24405900	3.13165000	-1.12762600
C	-2.33464300	2.56506300	-0.50510900
H	-1.20185300	3.21213000	-2.20837200
H	-0.58713900	3.78965400	-0.56716800
C	-2.44119400	2.62746000	0.96852000
C	-3.41166200	1.82943400	-1.22438400
H	-3.21554700	3.34640600	1.27935700
H	-1.49385700	2.92421100	1.42425700
H	-2.74122100	1.65298300	1.37616000
C	-4.78365700	2.47487000	-0.95900600
C	-3.20524700	1.63855800	-2.72034400
H	-3.44965700	0.83162500	-0.75441100
H	-4.81229000	3.47838500	-1.41478400
H	-4.98237200	2.59707800	0.11079100
C	-5.90319200	1.64377900	-1.55199400
C	-4.40087300	1.04119300	-3.38115500
H	-2.97133800	2.60154900	-3.20745000
H	-2.31870100	1.01388600	-2.90267800
C	-5.64176500	1.00061400	-2.85278100
O	-6.98196500	1.53792800	-0.98143000
H	-4.23535200	0.58327700	-4.35956300
C	-6.79436200	0.30397500	-3.49634900
H	-7.63434100	0.98920300	-3.66215000
H	-6.51094300	-0.14459700	-4.45402000
H	-7.18049200	-0.48700300	-2.84065400
C	3.98897900	1.33324700	2.42539600
H	3.36880500	1.32243300	3.33086000
H	4.97332600	1.73396900	2.69854800
H	3.52507300	2.01950800	1.70922900
C	4.74023400	-1.01954800	2.86278100
H	5.72396900	-0.64436900	3.17359800
H	4.10752300	-1.09740300	3.75345800
H	4.86718400	-2.02855100	2.45776900
C	1.88719000	-4.69446200	-2.60161800
H	0.94072100	-5.16196700	-2.30519300
H	2.22898400	-5.17450700	-3.52773500
H	2.61763600	-4.89822200	-1.81284500
C	0.72581000	-2.93777200	-3.97052400
H	1.09731600	-3.38880000	-4.89902800
H	-0.25454200	-3.38092400	-3.75474300
H	0.58495800	-1.86490900	-4.13762700
C	-3.14556000	-4.15832300	-1.21842600
H	-4.10583800	-4.60448700	-1.50537300
H	-2.52100800	-4.10463400	-2.11883600
H	-2.65226300	-4.82217300	-0.50244700
C	-4.02129100	-1.85626300	-1.65395100
H	-3.34296700	-1.64522700	-2.48939900
H	-4.92774200	-2.32595400	-2.05806000
H	-4.31323200	-0.89832800	-1.21502100
C	-1.32718400	1.84721900	4.11058600
H	-1.56169800	2.23956800	5.10830900
H	-0.43053100	2.36007600	3.74399500
H	-2.15703900	2.10516500	3.44693600
C	-0.10030400	0.02428900	5.29555400
H	0.84943300	0.54642300	5.12332700
H	-0.48889100	0.35436100	6.26707100
H	0.10539700	-1.04898700	5.34769200

**E-<sup>3</sup>TS1<sub>A</sub>**

Rh	0.31488800	-0.27103700	-0.06675100
Rh	0.86152700	-1.96298100	1.55875600
O	-0.53479800	0.84894100	1.50748300
C	-0.49866400	0.35637700	2.68176000
O	-0.02069500	-0.77618500	2.99895400
O	-1.48922200	-1.30217000	-0.38386400
C	-1.67960800	-2.39997700	0.23451300
O	-0.91943900	-2.89752700	1.12096000
O	1.73233900	-3.10080800	0.08626100
C	1.67107300	-2.67246600	-1.10554500
O	1.15274300	-1.56807400	-1.47366000
O	2.17128800	0.58886700	0.42021800
C	2.90555500	0.04700600	1.31156500
O	2.63937500	-1.01976200	1.94226500
C	-1.08719700	1.16276500	3.84117900
C	-2.32716500	0.38714900	4.37424300

H	-1.95986100	-0.49247700	4.91874100
H	-2.81516100	1.03927200	5.11329500
C	-3.31732100	-0.06360800	3.33370800
C	-3.17167300	-1.32890200	2.75799500
C	-4.39711500	0.72807600	2.92457000
C	-4.05498800	-1.81484900	1.79010500
H	-2.34745100	-1.96395900	3.08455400
C	-5.29409800	0.26122700	1.96427700
H	-4.54987800	1.70770200	3.38069600
C	-5.12180100	-1.00006400	1.39596900
H	-6.14621900	0.86821100	1.65939400
H	-5.84445600	-1.36489400	0.66329200
C	-2.94094300	-3.20598900	-0.07199200
C	-3.82622900	-3.18120300	1.20568100
H	-4.78281700	-3.65600100	0.94351000
H	-3.34619000	-3.81980300	1.95857700
C	4.22652700	0.74555800	1.63895500
C	2.27528700	-3.54040400	-2.20971200
C	5.12462100	0.70633000	0.37440200
H	4.67472400	1.36364700	-0.38301400
H	6.08891100	1.15535900	0.65442300
C	3.52413900	-2.81056400	-2.77637600
C	5.32322300	-0.66224900	-0.21353800
C	4.42293300	-1.12275900	-1.17500700
C	6.36988500	-1.50187000	0.17784100
C	4.53901500	-2.38910200	-1.75116800
H	3.61625500	-0.46864000	-1.50106700
C	6.50167700	-2.76853500	-0.38603900
H	7.09423900	-1.15507300	0.91618400
C	5.59350700	-3.21229800	-1.34437200
H	7.32782800	-3.41106100	-0.08498400
H	5.71364500	-4.19894200	-1.79384200
O	0.26183200	1.29266200	-4.00707500
S	0.94721900	1.42027400	-2.73147400
O	2.25917200	0.82214400	-2.53387000
N	-0.07514900	1.12598000	-1.49129700
O	1.18340100	3.08752300	-2.63233800
C	2.23496700	3.55956200	-1.82286300
H	2.77590000	2.73976100	-1.33091100
H	2.93035700	4.12309100	-2.45664100
C	1.70667600	4.50904100	-0.74667000
Cl	0.65592500	5.75378400	-1.48115100
Cl	3.12693900	5.29756800	0.00806500
Cl	0.79035800	3.60584600	0.48471900
C	-1.66229300	2.41580100	-1.91937700
C	-2.74754400	2.16971500	-1.09334900
H	-1.67925800	2.09283700	-2.95527200
H	-1.04244600	3.28456700	-1.71149700
C	-2.87306700	2.87261500	0.20978300
C	-3.81666100	1.17797700	-1.42463100
H	-3.56866500	3.72292600	0.13568100
H	-1.91087100	3.26050100	0.55507400
H	-3.28363900	2.20004700	0.97533000
C	-5.21846300	1.76540400	-1.20853600
C	-3.72722900	0.56373500	-2.81728300
H	-3.70521100	0.36053400	-0.68393900
H	-5.38471500	2.58143400	-1.93185200
H	-5.33812600	2.19558700	-0.20906000
C	-6.30126300	0.72898700	-1.40669700
C	-4.91462700	-0.27674700	-3.14766200
H	-3.63300500	1.35994100	-3.57702700
H	-2.80670600	-0.03273300	-2.91061100
C	-6.09445200	-0.24674900	-2.49429500
O	-7.31488100	0.71877400	-0.71741300
H	-4.79124100	-0.98963400	-3.96740300
C	-7.22545800	-1.17506400	-2.78781800
H	-8.14129700	-0.62507600	-3.03538200
H	-6.98665100	-1.85234000	-3.61444500
H	-7.47126100	-1.77811500	-1.90415200
C	-3.69590500	-2.62350900	-1.25404300
H	-3.06800700	-2.57922400	-2.15201800
H	-4.57562300	-3.24077900	-1.48081900
H	-4.04543300	-1.61032100	-1.04253500
C	-2.53599300	-4.65241100	-0.36432800
H	-3.43226500	-5.26172400	-0.53499100
H	-1.91441600	-4.71558400	-1.26604300
H	-1.97343500	-5.08531700	0.46818000
C	-1.47970200	2.57256000	3.42570800
H	-1.79356300	3.13911100	4.31147600
H	-0.64195800	3.10829200	2.96409600
H	-2.30862600	2.57195000	2.71490700
C	-0.03842700	1.23180600	4.95518000
H	0.84341600	1.80024600	4.63332600

## ARTICLE

## Journal Name

H	-0.45991300	1.74168000	5.83049500
H	0.29054400	0.23315800	5.25695300
C	3.93455700	2.20411700	1.98944500
H	3.29751900	2.28457600	2.87963200
H	4.87102900	2.73602400	2.19943500
H	3.42548400	2.71668100	1.16780900
C	4.91856000	0.05159300	2.80734200
H	5.85818600	0.57141200	3.03547800
H	4.29356900	0.06757600	3.70670600
H	5.14759400	-0.99425100	2.58179900
C	1.25056500	-3.68533900	-3.33670100
H	1.68312400	-4.26604200	-4.16075300
H	0.35239300	-4.21460700	-2.99446400
H	0.94568600	-2.70745400	-3.72336200
C	2.66001300	-4.90766900	-1.65615800
H	1.79019500	-5.43289600	-1.24596300
H	3.08195400	-5.52276900	-2.46162800
H	3.40336900	-4.82552100	-0.85705600
H	3.17578800	-1.92422300	-3.32293100
H	3.97544600	-3.48997400	-3.51441300

E-<sup>1</sup>TS<sub>1</sub>

Rh	1.13076900	1.83906900	-1.80189500
Rh	0.42543300	0.50459400	0.06451700
O	2.98593700	0.93930900	-1.72421800
C	3.17654400	0.05865300	-0.83132100
O	2.32468400	-0.33356900	0.03067100
O	1.78151600	3.29955600	-0.51422000
C	1.61927900	3.11002200	0.73144300
O	1.09069000	2.08195400	1.26320900
O	-1.43708900	1.42487300	-0.03014000
C	-1.61078600	2.33573600	-0.90369600
O	-0.75997500	2.71108500	-1.76798300
O	0.46592200	0.28352300	-3.02543100
C	-0.04865100	-0.74814300	-2.49610700
O	-0.21568900	-0.92510800	-1.24542300
C	4.53811900	-0.63354200	-0.77121200
C	5.09640300	-0.49935500	0.67076800
H	4.42310900	-1.04267900	1.34789900
H	6.06667300	-1.01743000	0.68609300
C	5.24949900	0.91993200	1.13877900
C	4.17834600	1.56201000	1.76560500
C	6.42741000	1.64144400	0.92276700
C	4.24577400	2.90636400	2.14223000
H	3.26989300	0.99600700	1.97162500
C	6.52175200	2.97305500	1.31701200
H	7.27835600	1.15029700	0.44880400
C	5.43533300	3.60503400	1.91516300
H	7.44845600	3.52217700	1.15631600
H	5.51055900	4.65011200	2.21874200
C	2.07642700	4.20402600	1.69605100
C	3.03842200	3.57304800	2.73829800
H	3.34179900	4.38137000	3.41987000
H	2.46807600	2.84610800	3.33067800
C	-0.51098200	-1.87392100	-3.41690600
C	-2.96923400	3.03824900	-0.92232200
C	-1.57496100	-1.29549100	-4.38837000
H	-1.07938200	-0.56303500	-5.03886600
H	-1.90564200	-2.12559700	-5.02950800
C	-3.62060300	2.77990800	-2.30756900
H	-4.61084900	3.25696800	-2.28752300
H	-3.02371900	3.30411900	-3.06518700
C	-2.74813300	-0.65639300	-3.69950800
C	-2.71164800	0.70439800	-3.38270500
C	-3.87003000	-1.39814000	-3.31378500
C	-3.74262400	1.32748100	-2.67343300
H	-1.85055400	1.29733200	-3.69394000
C	-4.91070100	-0.79118200	-2.61562300
H	-3.92830900	-2.45614200	-3.57199400
C	-4.84843800	0.56179200	-2.28879500
H	-5.78537700	-1.37215800	-2.32441700
H	-5.66731400	1.01761000	-1.73057600
O	-0.22940400	-2.49745200	3.27215200
S	0.61696100	-1.68512400	2.40373400
O	1.84767700	-1.11504900	2.93575800
N	-0.21913500	-0.50201700	1.67835500
C	1.70964300	-3.87998400	1.58436800
H	2.80079600	-3.75203200	1.53522500
O	1.04831700	-2.71583100	1.13720600
H	1.42126800	-4.13926400	2.61175000
C	1.32743400	-5.05614200	0.69669800
Cl	-0.43748900	-5.32324600	0.73594500
Cl	2.16951700	-6.49578900	1.34137500

Cl	1.84791300	-4.77423800	-0.98778600
C	-5.72723500	0.57153400	3.73040200
C	-4.78174800	-0.57963500	3.63771400
C	-6.39240600	1.09825300	2.68187600
H	-5.88625100	1.00318600	4.72140300
C	-4.19908800	-0.71057100	2.23626400
H	-5.32040200	-1.50338900	3.91389500
H	-3.97899700	-0.47863500	4.38060000
C	-6.25669000	0.48557900	1.34424000
C	-7.31518300	2.26599700	2.78995200
C	-3.27684700	-1.88546500	2.02919000
C	-5.34564200	-0.71793800	1.21824700
H	-3.60119200	0.19824400	2.04599700
O	-6.88754200	0.91218800	0.38342700
H	-8.31936800	2.00833000	2.43314000
H	-7.38791300	2.62906500	3.82019600
H	-6.97637200	3.09295600	2.15356800
C	-3.23724000	-2.96511000	2.84429500
H	-5.95857700	-1.62163500	1.37563300
H	-4.98619300	-0.76819700	0.18174800
H	-3.88460000	-3.06857000	3.71261900
H	-2.52614800	-3.76836500	2.67002100
C	-2.35784900	-1.79006600	0.90855000
H	-1.41110800	-1.10103600	1.31632500
H	-1.87198000	-2.71737300	0.59127500
H	-2.67342300	-1.16615300	0.06244700
C	4.30429200	-2.11701800	-1.06528300
H	3.91302500	-2.26869200	-2.07995400
H	5.24685600	-2.67288400	-0.98357500
H	3.58189300	-2.54124300	-0.36096600
C	5.49511800	-0.03343300	-1.79346400
H	6.46535900	-0.54382200	-1.73450700
H	5.10933500	-0.14818200	-2.81166600
H	5.65732800	1.03485200	-1.61881300
C	0.83758400	4.72805500	2.42918300
H	1.13477500	5.48766900	3.16287100
H	0.13341700	5.19870500	1.73170200
H	0.31655200	3.92212100	2.95623000
C	2.75694700	5.33862600	0.93994800
H	2.07681200	5.79463900	0.21340800
H	3.07235000	6.11486700	1.64927300
H	3.64080300	4.99049400	0.39628400
C	-2.73723600	4.54186800	-0.75802100
H	-3.69267600	5.07587400	-0.83269000
H	-2.30463600	4.77126600	0.22376700
H	-2.06188900	4.92621500	-1.52903500
C	-3.86564000	2.51773000	0.19368700
H	-3.42712700	2.70276000	1.18120700
H	-4.84645200	3.00832900	0.14920100
H	-4.02769800	1.43926600	0.09488800
C	-1.08511500	-3.03296300	-2.60835900
H	-1.35981700	-3.85411100	-3.28326500
H	-0.35663900	-3.41268300	-1.88509000
H	-1.97981300	-2.73639000	-2.05127300
C	0.70174900	-2.34756200	-4.22287300
H	1.46755700	-2.77746200	-3.56423500
H	0.39690600	-3.12724400	-4.93177500
H	1.15443300	-1.52391800	-4.78445700

**E<sup>-3</sup>TS<sub>1</sub>**

Rh	1.07498900	-2.24808700	1.37988000
Rh	0.39195500	-0.36577300	0.06936700
O	2.89663300	-1.33338000	1.66252200
C	3.11655100	-0.21246500	1.11110200
O	2.28265600	0.43832700	0.39761900
O	1.79569800	-3.14457600	-0.33661100
C	1.62436200	-2.54200800	-1.44057800
O	1.04624900	-1.41648300	-1.59284900
O	-1.44306400	-1.28716600	-0.15269300
C	-1.62908200	-2.45084200	0.32809200
O	-0.78651300	-3.10918000	1.01452900
O	0.36742300	-1.24168200	3.05929300
C	-0.10326400	-0.06926900	2.92444800
O	-0.23567000	0.55696900	1.82391100
C	4.47634000	0.44597200	1.33216200
C	5.05026800	0.87894800	-0.04226800
C	5.22486000	-0.25594500	-1.01366800
C	4.16305300	-0.64703400	-1.83511500
C	6.41844700	-0.98265400	-1.07514300
C	4.25326700	-1.76331500	-2.67144900
H	3.23987000	-0.06795700	-1.83231500
C	6.53666700	-2.07674600	-1.92708100
H	7.26191100	-0.68344700	-0.45146100

C	5.45782300	-2.47201300	-2.71198400
H	7.47501700	-2.62722600	-1.97620800
H	5.54965800	-3.33619800	-3.37124200
C	2.12734400	-3.20226700	-2.72342300
C	3.05565000	-2.20186000	-3.46544000
H	3.37336400	-2.69793800	-4.39429600
H	2.45632600	-1.32807800	-3.75045600
C	-0.55888100	0.64470200	4.19632500
C	-2.99028400	-3.09155400	0.05869100
C	-1.68956400	-0.20679500	4.83401700
H	-1.24662900	-1.14512400	5.19204900
H	-2.04228700	0.34248400	5.71901600
C	-3.72780900	-3.24142200	1.41729200
H	-4.72940400	-3.63415200	1.19170600
H	-3.20471200	-4.00863800	2.00357600
C	-2.82989500	-0.50676700	3.90342500
C	-2.81887100	-1.68049500	3.14617900
C	-3.89577000	0.38250900	3.73386100
C	-3.82362400	-1.97532300	2.22063900
H	-1.99924000	-2.38872300	3.27915700
C	-4.90493300	0.10541300	2.81554100
H	-3.93705200	1.29311700	4.33255800
C	-4.87112300	-1.06243100	2.05559700
H	-5.73423900	0.80148900	2.69246700
H	-5.66508400	-1.26062600	1.33321900
O	-1.15336400	1.96560100	-3.21359200
S	0.05000400	1.80243400	-2.41581500
O	1.25276500	1.19918100	-2.97120800
N	-0.28840200	1.19358800	-0.96439600
C	1.72986800	3.60403000	-1.53413400
H	2.24147300	2.66090900	-1.29727800
O	0.43049200	3.39302900	-2.04592300
H	2.32330800	4.15518100	-2.27412100
C	1.66176800	4.43813300	-0.26004000
Cl	0.79680100	5.96696600	-0.55577800
Cl	3.36012500	4.79211000	0.20889000
Cl	0.84941900	3.52694600	1.03608400
C	-5.39317800	0.93775600	-3.69538000
C	-4.54925900	2.01385900	-3.09806300
C	-6.09417600	0.02991100	-2.98408400
H	-5.43686800	0.89134000	-4.78626500
C	-4.09746200	1.64166900	-1.69270400
H	-5.13243900	2.95197700	-3.07566200
H	-3.67867200	2.21983500	-3.73349400
C	-6.11752600	0.11399400	-1.51012800
C	-6.89859700	-1.06402900	-3.60411800
C	-3.28577500	2.68590500	-0.96760200
C	-5.32058300	1.22936300	-0.86657600
H	-3.44839000	0.75261600	-1.78804700
O	-6.78300000	-0.66704400	-0.83734500
H	-7.94648300	-1.01518000	-3.28539100
H	-6.85935600	-1.02328700	-4.69749200
H	-6.53427600	-2.04756400	-3.28115000
C	-3.23764100	3.99254100	-1.33851900
H	-5.98888700	2.10025000	-0.75578400
H	-5.05202800	0.91758000	0.15123300
H	-3.78441300	4.37916400	-2.19532900
H	-2.61505900	4.70182400	-0.79494500
C	-2.47180100	2.20417100	0.12391800
H	-1.40283800	1.75665800	-0.42796800
H	-2.07809500	2.95422100	0.81490600
H	-2.79528200	1.28164300	0.62329500
C	2.85806400	-4.50149600	-2.40677300
H	2.19843000	-5.21579500	-1.90342600
H	3.21268400	-4.96004100	-3.33901400
H	3.72274800	-4.33209500	-1.75717400
C	0.91083100	-3.48154400	-3.61224400
H	1.23915500	-3.93276300	-4.55675600
H	0.21950500	-4.18545400	-3.13202000
H	0.36591300	-2.55944300	-3.84060900
C	-2.76681200	-4.48212900	-0.53787700
H	-3.73190400	-4.98305200	-0.68243400
H	-2.27575100	-4.41959400	-1.51664100
H	-2.14722300	-5.10199600	0.11787600
C	-3.80977300	-2.22863600	-0.89369200
H	-3.31358000	-2.11613800	-1.86507700
H	-4.79624800	-2.68082200	-1.05451900
H	-3.96446100	-1.22545800	-0.48222400
C	-1.04949700	2.05445500	3.88763500
H	-1.39780400	2.53495500	4.81103000
H	-0.24499400	2.67138500	3.47226500
H	-1.87364000	2.05251000	3.16688400
C	0.62430200	0.70313800	5.16551800



H	1.43613300	1.32120000	4.76175100
H	0.30675900	1.15205700	6.11481800
H	1.02073100	-0.29658000	5.36911900
H	6.01453100	1.36983800	0.15501400
H	4.38424200	1.64325200	-0.46506400
C	4.24387500	1.69049900	2.19551200
H	3.86868200	1.41377900	3.18866500
H	5.18919700	2.23010500	2.33522800
H	3.52508400	2.37494800	1.73264700
C	5.42625100	-0.50964800	2.04557400
H	6.39824700	-0.02020000	2.18948500
H	5.03769600	-0.79354500	3.02870500
H	5.58621800	-1.42841100	1.47269300

E-<sup>3</sup>IM<sub>A,S</sub>

Rh	0.72935400	-2.32849200	1.44883700
Rh	0.21315000	-0.43005900	0.07641800
O	2.56899400	-1.49234500	1.82758800
C	2.89274600	-0.41670900	1.24071200
O	2.14700300	0.24678900	0.44513600
O	1.49162400	-3.26996600	-0.21744300
C	1.32922500	-2.71733700	-1.34992300
O	0.79312200	-1.58034800	-1.55219500
O	-1.66943500	-1.25522700	-0.19552400
C	-1.90185200	-2.43222000	0.22998100
O	-1.12171300	-3.11766300	0.96344900
O	-0.04185000	-1.29075000	3.09079300
C	-0.35264200	-0.07132000	2.92305600
O	-0.31283200	0.55959800	1.81874100
C	4.27717000	0.16466000	1.51212300
C	4.98175700	0.41624800	0.15215000
H	4.43339300	1.20731900	-0.37820800
H	5.97919600	0.82057700	0.37901600
C	5.08929800	-0.80163400	-0.72392900
C	4.05067100	-1.11642700	-1.60503200
C	6.19323200	-1.65803000	-0.65945700
C	4.07972400	-2.26928500	-2.39401400
H	3.20003900	-0.44052300	-1.69125400
C	6.24692900	-2.80031700	-1.45341800
H	7.02097700	-1.41966600	0.00999700
C	5.19460800	-3.10860300	-2.31044300
H	7.11751900	-3.45263700	-1.40624700
H	5.24011600	-4.00464800	-2.93068500
C	1.80916200	-3.45750600	-2.59607500
C	2.90823800	-2.59553500	-3.27657400
H	3.23838500	-3.15137300	-4.16639200
H	2.43995900	-1.66682900	-3.62717700
C	-0.85192000	0.70875700	4.13727400
C	-3.24850600	-3.05175200	-0.13872800
C	-2.21566300	0.09330100	4.55817600
H	-2.01296900	-0.87818900	5.02797100
H	-2.62981200	0.74584200	5.34050100
C	-4.16494800	-2.94648900	1.11465700
H	-5.17558700	-3.23944400	0.79510500
H	-3.82711300	-3.69780500	1.84118300
C	-3.20959400	-0.10116600	3.44632300
C	-3.27680900	-1.34093900	2.80671500
C	-4.08009900	0.90987600	3.02297300
C	-4.17813900	-1.59573000	1.77065200
H	-2.60738800	-2.13967600	3.13213900
C	-4.98784600	0.67558300	1.99178300
H	-4.06684800	1.87746000	3.52645600
C	-5.03774600	-0.56950700	1.36770500
H	-5.68554600	1.45172900	1.67905200
H	-5.77387900	-0.74758300	0.58237800
O	-0.52070500	2.13736300	-3.37536100
S	0.40759700	1.79263100	-2.31470800
O	1.55520900	0.94118200	-2.56489000
N	-0.37183100	1.25632100	-0.97457400
C	2.29164400	3.28574100	-1.28164800
H	2.49519900	2.35516200	-0.73161000
O	0.99643700	3.29241700	-1.85411000
H	3.04861500	3.41362300	-2.06625100
C	2.39469400	4.45460200	-0.31251500
Cl	1.91914600	5.97521300	-1.10094200
Cl	4.10336600	4.55595500	0.21359100
Cl	1.34703700	4.16023700	1.10972800
C	-4.82265200	0.33781000	-3.24977400
C	-3.58962500	1.12393600	-2.96250100
C	-5.96778100	0.40636800	-2.53870800
H	-4.76547100	-0.37906000	-4.07415700
C	-3.59973200	1.70983200	-1.54238900
H	-3.47174100	1.93360500	-3.70353800

H	-2.70084200	0.49190200	-3.09979600
C	-6.08540300	1.37594200	-1.43109100
C	-7.14304900	-0.48140100	-2.78313000
C	-2.46178800	2.63622100	-1.26460100
C	-4.96032700	2.37422000	-1.29237100
H	-3.51800800	0.85585600	-0.84713200
O	-7.05048200	1.37148200	-0.67338500
H	-8.04924500	0.09992400	-2.99242900
H	-6.96316400	-1.16519000	-3.61961100
H	-7.37288200	-1.07716400	-1.89007300
H	-5.11272600	3.17902100	-2.03068100
H	-5.01480500	2.83597400	-0.29932800
C	-1.38339400	2.16411100	-0.36116900
H	-0.84272100	3.01166500	0.08728300
H	-1.80406100	1.56888500	0.45818000
C	-2.42396900	3.99541800	-1.86435400
H	-2.61138200	3.97346000	-2.94815800
H	-3.19379500	4.65497800	-1.42958600
H	-1.45193500	4.47891300	-1.71323000
C	0.62550300	-3.58022900	-3.56053400
H	0.94449300	-4.08917200	-4.47846500
H	-0.18855900	-4.16972700	-3.11973900
H	0.23070400	-2.59490700	-3.82850000
C	2.33838700	-4.83845500	-2.22934300
H	1.55729900	-5.45076400	-1.76578200
H	2.68332100	-5.35324800	-3.13539800
H	3.17331700	-4.78053500	-1.52442400
C	4.07430100	1.50056100	2.23305600
H	3.60324400	1.35380300	3.21369100
H	5.04115900	1.99311300	2.39562200
H	3.44073200	2.17788900	1.65039600
C	5.09888500	-0.78129100	2.38004100
H	6.08766500	-0.34229000	2.56529700
H	4.61500600	-0.95486900	3.34645400
H	5.23950200	-1.75469700	1.89942300
C	-3.86949900	-2.30651300	-1.31328900
H	-3.21231300	-2.32251300	-2.19190100
H	-4.82387500	-2.77340200	-1.59088100
H	-4.06388900	-1.25861300	-1.06852900
C	-3.05927700	-4.52789400	-0.48480300
H	-4.03511200	-4.98806900	-0.68278400
H	-2.44534800	-4.65124200	-1.38474000
H	-2.57793500	-5.07372400	0.33184800
C	-1.00847600	2.18865500	3.80303000
H	-1.34906500	2.73272700	4.69310200
H	-0.05504900	2.62372300	3.48240100
H	-1.73422200	2.35374400	2.99966500
C	0.14279000	0.53037000	5.28530100
H	1.11222600	0.98455100	5.04564100
H	-0.23847500	1.01956800	6.19018900
H	0.30759700	-0.52869400	5.50637600

E-<sup>3</sup>IMA-R

Rh	-0.64811400	0.36320700	-0.17122200
Rh	-2.58314500	1.55727500	0.60185900
O	0.25723100	0.78135900	1.65447000
C	-0.37974200	1.46456600	2.51824900
O	-1.56032700	1.91304700	2.38213700
O	0.05254200	2.17745600	-0.93682800
C	-0.68162200	3.21341900	-0.84750800
O	-1.81171000	3.26769900	-0.27040700
O	-3.52030500	1.13156100	-1.18271200
C	-2.86825000	0.50171900	-2.07192100
O	-1.66992800	0.08633900	-1.95596400
O	-1.49051400	-1.34203600	0.70725900
C	-2.62186500	-1.24664500	1.28942700
O	-3.30461400	-0.18369300	1.40626900
C	0.32915600	1.76388600	3.83905900
C	0.31521800	3.29945400	4.06110700
H	-0.72817000	3.61920400	4.17798300
H	0.82043500	3.48758500	5.01969800
C	0.96815700	4.08312600	2.95741100
C	0.20362100	4.52356700	1.87424000
C	2.34008700	4.35492300	2.95710400
C	0.77457900	5.19822300	0.79193600
H	-0.87059600	4.33812100	1.87377600
C	2.92411800	5.03989900	1.89548400
H	2.95108100	4.03600400	3.80221800
C	2.14859500	5.45449500	0.81633300
H	3.99064100	5.25831700	1.91214700
H	2.60950300	5.99424700	-0.01163100
C	-0.17658100	4.50702600	-1.48684200
C	-0.08449800	5.58814500	-0.37710300

H	0.29981400	6.50204400	-0.85288000
H	-1.10311800	5.80780600	-0.03189400
C	-3.18188800	-2.52176300	1.91659700
C	-3.55166300	0.20761500	-3.40537800
C	-3.25778000	-3.61744700	0.82173600
H	-2.23414200	-3.85201300	0.49636100
H	-3.65760100	-4.52268000	1.30165100
C	-3.55789700	-1.33057600	-3.61943200
C	-4.09125900	-3.23408700	-0.36952700
C	-3.50024100	-2.53897600	-1.42761000
C	-5.45828100	-3.51857200	-0.43639100
C	-4.24166100	-2.11045300	-2.53154600
H	-2.42867400	-2.34565100	-1.40359900
C	-6.20945800	-3.11021000	-1.53520100
H	-5.93390200	-4.07180100	0.37454700
C	-5.60762900	-2.40605100	-2.57460800
H	-7.27107400	-3.34755000	-1.58406100
H	-6.19926900	-2.09349300	-3.43602500
O	2.02754200	-1.89473500	-2.79950600
S	1.12319900	-1.93460200	-1.66570300
O	-0.24060800	-2.40988700	-1.80299800
N	1.10518200	-0.52827700	-0.82797600
O	1.92067800	-3.00793700	-0.64233800
C	1.13304100	-3.79522600	0.22400500
H	0.09417700	-3.43935000	0.27208300
H	1.14440200	-4.83557200	-0.12610100
C	1.72485800	-3.75580900	1.62867200
Cl	3.45651800	-4.19208500	1.59685000
Cl	0.83333300	-4.95817500	2.61074000
Cl	1.53191300	-2.12265800	2.31663200
C	2.40945700	0.06838400	-0.43035600
C	3.36026600	0.26881800	-1.55664300
H	2.83835000	-0.54733900	0.37320100
H	2.12116200	1.03003700	0.02192000
C	2.93684700	1.16435500	-2.66556300
C	4.66024900	-0.45865300	-1.69745900
H	3.33244800	2.18709000	-2.54887800
H	1.84387600	1.25095200	-2.70671600
H	3.29294700	0.79388300	-3.63629100
C	5.83909400	0.51929400	-1.82337600
C	4.97357800	-1.47627800	-0.60626100
H	4.61118100	-1.01991700	-2.65030500
H	5.93428900	1.09022000	-0.88394600
H	5.68712000	1.25667700	-2.61987900
C	7.16069100	-0.17956000	-2.07375100
C	6.32735400	-2.07796800	-0.77629700
H	4.91647200	-1.00044700	0.39070300
H	4.21305500	-2.26811200	-0.58913700
C	7.33629400	-1.51930700	-1.47504700
O	8.05950700	0.36082400	-2.70486700
H	6.49734700	-3.04488300	-0.29469400
C	8.67021700	-2.16238800	-1.66268600
H	9.47387700	-1.51908300	-1.28469800
H	8.72584600	-3.13180500	-1.15669100
H	8.88628100	-2.31211800	-2.72746100
C	1.17597400	4.29879500	-2.15536000
H	1.11140400	3.55715800	-2.95847300
H	1.52116400	5.24465500	-2.59231800
H	1.93303900	3.95267100	-1.44381000
C	-1.21027900	4.95444000	-2.52493100
H	-0.89723800	5.90512400	-2.97385700
H	-1.30294200	4.22019400	-3.33465300
H	-2.19704000	5.09327300	-2.07180600
C	1.76079000	1.23893900	3.83152800
H	2.26209900	1.52543600	4.76512900
H	1.78855400	0.14667500	3.76363600
H	2.33976700	1.64054900	2.99358500
C	-0.47030900	1.08793800	4.95696900
H	-0.47666300	-0.00259100	4.83058200
H	-0.01242700	1.30644300	5.92961000
H	-1.50737100	1.43900300	4.97444400
C	-2.20338900	-2.96211200	3.00715700
H	-2.14775300	-2.21927700	3.81308700
H	-2.53168900	-3.91151900	3.44829700
H	-1.19586800	-3.10132300	2.60447300
C	-4.55727900	-2.26835500	2.52396400
H	-4.93513800	-3.19830700	2.96842400
H	-4.51006400	-1.50971100	3.31164600
H	-5.27954700	-1.92708500	1.77619600
C	-2.71664700	0.85131400	-4.51664000
H	-3.15955500	0.62253700	-5.49375400
H	-2.69172500	1.94331000	-4.41235200
H	-1.68684600	0.47920300	-4.50773400

C	-4.96913500	0.76680100	-3.42066800
H	-4.97128700	1.85351900	-3.28479300
H	-5.44019000	0.54352700	-4.38678900
H	-5.58554000	0.33092200	-2.62832600
H	-2.51600700	-1.66508300	-3.70982000
H	-4.04496900	-1.51237600	-4.58877500

**E-<sup>3</sup>IM<sub>1</sub>**

Rh	1.11287500	-1.71102500	1.87830800
Rh	0.40543700	-0.43684500	-0.01641600
O	2.94231600	-0.77154300	1.80612000
C	3.12752500	0.12720700	0.92853400
O	2.26878900	0.50726200	0.06629500
O	1.80461100	-3.15514800	0.59189200
C	1.67091300	-2.97992500	-0.65892000
O	1.13479600	-1.95924400	-1.20169600
O	-1.42258000	-1.41163600	0.06800900
C	-1.59299500	-2.30597100	0.95971300
O	-0.74585300	-2.63520100	1.84729400
O	0.41078800	-0.18947800	3.09233400
C	-0.12674700	0.83248300	2.56050700
O	-0.29646000	1.00338600	1.31043900
C	4.48304400	0.83394400	0.89701300
C	5.07969600	0.69757200	-0.52929500
H	4.41825500	1.22680800	-1.22859200
H	6.04095500	1.23182000	-0.52206300
C	5.26689100	-0.72154200	-0.98317500
C	4.22188000	-1.37817500	-1.63824700
C	6.44739100	-1.42629200	-0.72950900
C	4.31858000	-2.72281700	-2.00758700
H	3.31799400	-0.81870600	-1.88164300
C	6.57114800	-2.75698200	-1.11788600
H	7.27801000	-0.92244100	-0.23365800
C	5.51071700	-3.40467400	-1.74507400
H	7.50033800	-3.29308700	-0.93047300
H	5.60976600	-4.44887000	-2.04484900
C	2.16780200	-4.06319300	-1.61099000
C	3.13828400	-3.41064000	-2.63280200
H	3.47041000	-4.21201700	-3.30874600
H	2.56673700	-2.69341200	-3.23590200
C	-0.60435000	1.93377500	3.50477100
C	-2.93010800	-3.04560400	0.96551100
C	-1.68535700	1.32507300	4.44046700
H	-1.19484500	0.59077900	5.09258800
H	-2.04151800	2.14175000	5.08499200
C	-3.62142400	-2.77713500	2.32904700
H	-4.60164600	-3.27281800	2.28968500
H	-3.03686600	-3.27833800	3.11159100
C	-2.83319500	0.67698300	3.71768700
C	-2.77306900	-0.68357700	3.40470300
C	-3.95484600	1.40293600	3.30347200
C	-3.77669500	-1.32195000	2.67096500
H	-1.91502700	-1.26771000	3.74057900
C	-4.96859600	0.78177500	2.57805100
H	-4.03584400	2.46049600	3.55725100
C	-4.88060800	-0.57018100	2.25231800
H	-5.83989700	1.35505000	2.26387700
H	-5.67732100	-1.03986200	1.67234400
O	-0.31109500	1.45799900	-4.00408700
S	0.46199300	1.41654800	-2.77916100
O	1.85979200	1.03188100	-2.75916200
N	-0.31310600	0.60275200	-1.61070700
C	0.90986300	3.21449800	-0.96563400
H	0.23889700	2.84604400	-0.17474900
O	0.34686200	2.99640500	-2.24545100
H	1.88247300	2.71217100	-0.86858600
C	1.10411700	4.70895700	-0.78078800
Cl	2.25111000	5.35111300	-1.97410800
Cl	1.75781200	4.95381100	0.87577800
Cl	-0.46166000	5.56021800	-0.91979300
C	-4.92373000	-0.79861100	-3.78454700
C	-4.17631700	0.46894800	-3.53704600
C	-5.76882300	-1.37563700	-2.90452800
H	-4.77018000	-1.28073800	-4.75326600
C	-4.01792800	0.74238900	-2.04655500
H	-4.72071500	1.30031500	-4.01893200
H	-3.19481900	0.44063200	-4.03184800
C	-6.04800200	-0.71447900	-1.61237800
C	-6.47792300	-2.66333400	-3.16414100
C	-3.33444800	2.05238100	-1.69631900
C	-5.38282500	0.62127700	-1.36445100
H	-3.38782300	-0.07077000	-1.64314500
O	-6.80698100	-1.21616900	-0.78957100

H	-7.56318100	-2.54458000	-3.06395000
H	-6.25566600	-3.05184900	-4.16339700
H	-6.19258300	-3.42383300	-2.42618200
C	-3.09349600	3.03152200	-2.64369500
H	-6.04918500	1.41105700	-1.75112900
H	-5.31460000	0.77878000	-0.28028000
H	-3.34296600	2.90983100	-3.69390900
H	-2.57424900	3.94754200	-2.36821600
C	-2.91477200	2.21607400	-0.37523300
H	-1.28964600	0.90151200	-1.54171300
H	-2.41470600	3.13140100	-0.05940300
H	-3.05029700	1.43424600	0.37429000
C	4.25176000	2.31913900	1.18478100
H	3.76960800	2.47430600	2.15856100
H	5.21247000	2.84812700	1.19997400
H	3.62498800	2.78538800	0.41765600
C	5.41641000	0.24099400	1.94671100
H	6.38960300	0.74621200	1.89844700
H	5.01320900	0.37314600	2.95614900
H	5.57653900	-0.83000200	1.79049100
C	0.95450100	-4.61265800	-2.36877400
H	1.28349400	-5.36798200	-3.09289200
H	0.24494700	-5.09653500	-1.68609600
H	0.42898100	-3.82008500	-2.91126400
C	2.85356700	-5.18233900	-0.83662200
H	2.16682600	-5.64927000	-0.12319200
H	3.19819300	-5.95439300	-1.53644500
H	3.71956200	-4.81590200	-0.27653900
C	-2.65037300	-4.54488400	0.83719700
H	-3.59309800	-5.10235500	0.89590200
H	-2.18543000	-4.78109300	-0.12806400
H	-1.98781900	-4.89691600	1.63445900
C	-3.81582100	-2.56981600	-0.17662300
H	-3.35298400	-2.74928600	-1.15398600
H	-4.78165000	-3.08941200	-0.14728900
H	-4.01511800	-1.49666200	-0.09312800
C	-1.17000800	3.12041900	2.73410900
H	-1.46155400	3.90921800	3.43921200
H	-0.42837800	3.54466800	2.04791000
H	-2.05174400	2.84384300	2.14909700
C	0.59253200	2.38227100	4.34811800
H	1.36371700	2.84798900	3.72111800
H	0.26913700	3.12913100	5.08332400
H	1.04373700	1.54002200	4.88204400

**E<sup>-3</sup>TS<sub>2A-s</sub>**

Rh	0.58415400	-2.29942500	1.56278600
Rh	0.14912200	-0.41340700	0.05625200
O	2.47488900	-1.54747900	1.86299400
C	2.85545300	-0.50554600	1.24695300
O	2.13384100	0.19277100	0.46394600
O	1.25979100	-3.36717800	-0.07663700
C	1.15816900	-2.84151600	-1.22960500
O	0.72305800	-1.67559400	-1.48846800
O	-1.77861500	-1.23854100	-0.19631000
C	-2.06122900	-2.35254000	0.34205900
O	-1.31956800	-2.99250300	1.15385000
O	-0.10215100	-1.07899100	3.12821300
C	-0.40444300	0.12835500	2.88128600
O	-0.38837300	0.68494900	1.73780200
C	4.28773300	-0.02765000	1.47974200
C	4.97281700	0.16865000	0.10169600
H	4.44315400	0.96871400	-0.43428900
H	5.99069100	0.53655900	0.29893000
C	5.01493800	-1.07167200	-0.74750400
C	3.93875600	-1.38117800	-1.58361900
C	6.09767400	-1.95502600	-0.69629500
C	3.91190900	-2.55400200	-2.34357600
H	3.10553200	-0.68319200	-1.65862100
C	6.09536400	-3.11842400	-1.46044000
H	6.95224700	-1.72171900	-0.05960400
C	5.00692400	-3.42038700	-2.27391000
H	6.94943700	-3.79311200	-1.42396300
H	5.00891800	-4.33294700	-2.87154600
C	1.59695500	-3.66307500	-2.44157600
C	2.70567300	-2.86805200	-3.18320300
H	2.99375200	-3.46408200	-4.06190600
H	2.26097200	-1.93396500	-3.55102800
C	-0.86838600	0.98814500	4.05797000
C	-3.42745100	-2.96724600	0.03705900
C	-2.24408300	0.43553500	4.52333600
H	-2.06342000	-0.51311600	5.04552500
H	-2.63659500	1.14155300	5.26985600

C	-4.31857300	-2.75515100	1.29487200
H	-5.34438100	-3.03538700	1.01412600
H	-3.98946500	-3.46741600	2.06318600
C	-3.24856500	0.20483300	3.42851300
C	-3.36417100	-1.07219100	2.87541300
C	-4.07737400	1.21866000	2.93379500
C	-4.27772400	-1.36428400	1.86012000
H	-2.72288000	-1.86994700	3.25444000
C	-4.99642300	0.94820500	1.92179000
H	-4.02476400	2.21741100	3.36922000
C	-5.09865100	-0.33524500	1.38844900
H	-5.66438700	1.72717600	1.55594100
H	-5.84553200	-0.54010200	0.62014800
O	-0.11089600	2.26380200	-3.68886600
S	0.52626700	1.87895600	-2.44251800
O	1.59015600	0.89168500	-2.45850800
N	-0.55565400	1.41940900	-1.27304100
C	2.47556000	3.23558300	-1.30388700
H	2.63133800	2.27317300	-0.79563200
O	1.18760300	3.32312900	-1.88655000
H	3.24507900	3.36874400	-2.07562300
C	2.62103400	4.35402000	-0.28190300
Cl	2.17755800	5.92544000	-0.99386100
Cl	4.33524000	4.38747800	0.22755600
Cl	1.57734000	4.02345500	1.13559400
C	-4.65078800	0.25469400	-3.28434100
C	-3.36104800	0.95024600	-3.02192400
C	-5.79682600	0.44452800	-2.59856300
H	-4.63847700	-0.49771100	-4.07759400
C	-3.33506200	1.66313800	-1.66550000
H	-3.14819700	1.65644400	-3.84205600
H	-2.53188100	0.22823300	-3.05212500
C	-5.85835900	1.47235900	-1.54471000
C	-7.03527500	-0.35681600	-2.82641200
C	-2.21400500	2.63442400	-1.52301200
C	-4.66550900	2.39959400	-1.42862200
H	-3.22580700	0.89112800	-0.88639300
O	-6.84237800	1.60693800	-0.82720400
H	-7.88869900	0.28442200	-3.07700200
H	-6.89745500	-1.08987500	-3.62809600
H	-7.32310900	-0.89267900	-1.91276000
H	-4.78943900	3.19009000	-2.18684200
H	-4.69307600	2.88746100	-0.44671600
C	-1.23804900	2.45378100	-0.45715700
H	-0.62188300	3.32453600	-0.21175700
H	-1.60599300	1.96827600	0.45096700
C	-2.13545600	3.82349500	-2.40293400
H	-2.37279000	3.61530500	-3.45091200
H	-2.87853700	4.55269600	-2.03665500
H	-1.15993900	4.31505800	-2.35876200
C	0.38962000	-3.79998500	-3.37461400
H	0.67184700	-4.36294500	-4.27304700
H	-0.42996100	-4.34325300	-2.88669900
H	0.01551000	-2.81787400	-3.68266500
C	2.09515200	-5.03818900	-2.01594400
H	1.30544500	-5.60898600	-1.51589600
H	2.41852300	-5.60429500	-2.89923700
H	2.93948200	-4.96569700	-1.32351900
C	4.20664400	1.32019000	2.20064400
H	3.76671100	1.20787600	3.19974700
H	5.21035100	1.74654700	2.32250800
H	3.59807400	2.03673400	1.63967300
C	5.06375800	-1.02575300	2.33149100
H	6.08602900	-0.65707500	2.48847700
H	4.59396500	-1.15909900	3.31099500
H	5.12304200	-2.00936100	1.85496100
C	-4.04997700	-2.28768800	-1.17321600
H	-3.40553500	-2.37753300	-2.05687400
H	-5.02032300	-2.74590100	-1.40747400
H	-4.21084500	-1.22188400	-0.99043500
C	-3.27671900	-4.46729600	-0.21198400
H	-4.26473800	-4.91964300	-0.36387500
H	-2.67884800	-4.66584200	-1.11010200
H	-2.79287600	-4.96548700	0.63322400
C	-0.99014000	2.45215200	3.64904200
H	-1.30920200	3.05085200	4.51181400
H	-0.02840800	2.84561400	3.30139400
H	-1.71824500	2.59566700	2.84365400
C	0.13097600	0.84902400	5.20684500
H	1.10760100	1.26880700	4.93550600
H	-0.23119600	1.39344200	6.08786600
H	0.27493600	-0.20054400	5.48068500

E-<sup>3</sup>TS<sub>2A-R</sub>

Rh	-0.34769000	0.53267300	-0.13804300
Rh	-1.88121500	2.37877600	0.35384500
O	0.44832800	0.78777700	1.76142700
C	-0.03414300	1.68146700	2.53023800
O	-0.97349600	2.48436700	2.24680500
O	0.93944900	2.05291000	-0.95772300
C	0.57348500	3.26357800	-0.95467900
O	-0.51307600	3.70333700	-0.45615800
O	-2.70189700	2.13056200	-1.52863200
C	-2.19993500	1.24192400	-2.28688300
O	-1.24290800	0.45634500	-1.99808600
O	-1.85208900	-0.71989400	0.74926700
C	-2.94921700	-0.20973900	1.14136400
O	-3.23024600	1.02766300	1.11303500
C	0.58803700	1.80117000	3.92242300
C	1.17619100	3.23072400	4.06237000
H	0.33633300	3.93742400	4.07757500
H	1.66144500	3.28547700	5.04790200
C	2.13949800	3.62286500	2.97691400
C	1.66373700	4.26543600	1.83092600
C	3.50897600	3.35088000	3.06553400
C	2.50764700	4.62756400	0.77700700
H	0.60085700	4.49825900	1.75965500
C	4.36766600	3.71182900	2.03052900
H	3.90555200	2.87343200	3.96262300
C	3.87221400	4.34217400	0.89184800
H	5.43543200	3.51404200	2.11818700
H	4.55293400	4.63646400	0.09196600
C	1.50126600	4.31291400	-1.57092500
C	1.92770800	5.28959100	-0.44121300
H	2.65005500	5.99363300	-0.87981800
H	1.04465400	5.87350800	-0.15098700
C	-4.00172200	-1.15843800	1.71421100
C	-2.77572100	1.07753900	-3.69356600
C	-4.27285300	-2.27514600	0.67335600
H	-3.34744500	-2.85097000	0.54248700
H	-5.00923200	-2.96080000	1.11898300
C	-3.22812900	-0.39822900	-3.86432400
C	-4.75783300	-1.77117600	-0.65708500
C	-3.83842300	-1.40166100	-1.64314100
C	-6.12207700	-1.61810100	-0.92329200
C	-4.25011100	-0.85527600	-2.86284700
H	-2.77211900	-1.54774900	-1.46461500
C	-6.55007200	-1.09946900	-2.14164300
H	-6.85186800	-1.91473400	-0.16865800
C	-5.62031200	-0.71243600	-3.10178400
H	-7.61522600	-0.99635700	-2.34369000
H	-5.95743300	-0.30229300	-4.05459400
O	2.09413500	-2.89163500	-2.17963400
S	0.94684200	-2.43548000	-1.41054900
O	-0.31943100	-2.16388700	-2.06127200
N	1.27439400	-1.16398800	-0.41235100
O	0.71474000	-3.74056700	-0.37948200
C	-0.59103400	-3.91167000	0.13822500
H	-1.12812600	-2.95754900	0.24517700
H	-1.16744700	-4.58187800	-0.51300300
C	-0.47472900	-4.55308700	1.51631000
Cl	0.57806300	-5.98829000	1.46583300
Cl	-2.11600200	-5.04095300	2.02878600
Cl	0.19384900	-3.37011800	2.68558000
C	2.21691500	-1.46979500	0.70124000
C	3.32812700	-0.80370000	0.01410500
H	2.33545100	-2.53843700	0.90026800
H	1.86825700	-0.95596700	1.60117400
C	3.42100100	0.66312500	0.14248200
C	4.31264200	-1.54577400	-0.82600400
H	4.36483500	0.92069300	0.65051400
H	2.59491100	1.08498500	0.72087000
H	3.45450600	1.16681900	-0.83242700
C	5.63805300	-0.79786600	-0.99996300
C	4.58335800	-2.97691600	-0.34973500
H	3.85732900	-1.64017900	-1.82879800
H	6.13352900	-0.68286200	-0.02095200
H	5.50436300	0.21180000	-1.40062700
C	6.60374100	-1.52815700	-1.91659600
C	5.63927200	-3.64205500	-1.16531700
H	4.88159600	-2.97163600	0.71416000
H	3.66724300	-3.57739400	-0.40080100
C	6.54776100	-3.00228700	-1.92799300
O	7.42909100	-0.91082100	-2.57471400
H	5.65391500	-4.73383200	-1.13788100
C	7.55720100	-3.70042000	-2.77618100

H	8.57595400	-3.40317400	-2.50064500
H	7.47032400	-4.78837400	-2.69381800
H	7.44001400	-3.42086900	-3.82997500
C	2.72170800	3.66152000	-2.20799000
H	2.43097500	2.91689900	-2.95683900
H	3.33607000	4.42519900	-2.70208200
H	3.34430400	3.15887800	-1.46027600
C	0.71801300	5.09856600	-2.62528700
H	1.34313200	5.90350800	-3.03171900
H	0.42148300	4.45447000	-3.46211500
H	-0.18658800	5.54320300	-2.19908300
C	1.67137200	0.74756300	4.12896200
H	2.10273700	0.85028700	5.13308300
H	1.26113500	-0.26489500	4.03800100
H	2.48152400	0.84738600	3.39704600
C	-0.52171100	1.61992300	4.96097200
H	-0.95276500	0.61222600	4.90661700
H	-0.11697000	1.75582800	5.97166200
H	-1.32722800	2.34504500	4.80849700
C	-3.41887000	-1.77936500	2.98685900
H	-3.25707600	-1.01427600	3.75693500
H	-4.11393700	-2.52330000	3.39633600
H	-2.46301700	-2.27674000	2.79176300
C	-5.28706700	-0.40918300	2.04786800
H	-6.02570200	-1.11083500	2.45748400
H	-5.10742100	0.37228700	2.79289900
H	-5.72049200	0.06838600	1.16354600
C	-1.64739100	1.35013000	-4.69348200
H	-2.01265500	1.20269300	-5.71762000
H	-1.28822300	2.38407700	-4.61547000
H	-0.80145600	0.67546900	-4.52545500
C	-3.93006200	2.04422900	-3.92529700
H	-3.59712000	3.08431100	-3.84182300
H	-4.33895900	1.89695600	-4.93362700
H	-4.73694900	1.89802800	-3.20062600
H	-2.33515900	-1.03272300	-3.80083600
H	-3.62609200	-0.49216200	-4.88553200

E<sup>-3</sup>TS2:

Rh	1.40803300	-1.64127400	1.87147000
Rh	0.53262400	-0.42711100	-0.03786800
O	3.16275800	-0.56639200	1.67732400
C	3.24321900	0.32497200	0.77549800
O	2.32719200	0.64184000	-0.05152600
O	2.12894300	-3.03825800	0.53405100
C	1.94241700	-2.89176800	-0.71335100
O	1.29686100	-1.92876100	-1.24032200
O	-1.20554800	-1.55354300	0.11339500
C	-1.29106700	-2.43389000	1.03031400
O	-0.40977800	-2.68189700	1.91033300
O	0.64440800	-0.15320800	3.10480600
C	0.02501400	0.83350400	2.59060300
O	-0.19736300	0.98716200	1.35159600
C	4.54545100	1.12021000	0.66992100
C	5.04876500	1.05241600	-0.79653400
H	4.29729700	1.53309800	-1.43760600
H	5.96131500	1.66403100	-0.84903300
C	5.31992100	-0.34115500	-1.28694000
C	4.28804900	-1.08518600	-1.86663500
C	6.57502100	-0.93980700	-1.13715200
C	4.47279300	-2.41566200	-2.25284400
H	3.32035400	-0.60951900	-2.02811000
C	6.78547200	-2.25173300	-1.54991600
H	7.39404700	-0.36705200	-0.70009000
C	5.73869700	-2.98897000	-2.09480600
H	7.77046000	-2.70345400	-1.44325100
H	5.90299300	-4.02103700	-2.40770200
C	2.49473500	-3.94138200	-1.67255100
C	3.31471800	-3.21758700	-2.77491800
H	3.66766200	-3.99445400	-3.46869900
H	2.63102500	-2.56781300	-3.33615500
C	-0.50235500	1.90233900	3.54559200
C	-2.57688300	-3.25916600	1.08594900
C	-1.52383900	1.22689500	4.50097200
H	-0.97511700	0.52817100	5.14585000
H	-1.92484500	2.01857900	5.15061000
C	-3.23905500	-3.01572100	2.46833400
H	-4.18764200	-3.57119200	2.46938300
H	-2.59735500	-3.46826700	3.23530300
C	-2.63718000	0.50014700	3.79897100
C	-2.49661100	-0.85767600	3.50087900
C	-3.80758500	1.14995400	3.39262200
C	-3.47324800	-1.56834600	2.79767800



H	-1.59717000	-1.38223900	3.82616400
C	-4.79458800	0.45565100	2.69806600
H	-3.94940100	2.20403100	3.63429300
C	-4.63116700	-0.89426200	2.39419000
H	-5.70730600	0.96779500	2.39479700
H	-5.41069900	-1.42197100	1.84142200
O	-0.96203300	1.50212100	-3.88492800
S	-0.04760700	1.48380100	-2.75796700
O	1.36497200	1.17841900	-2.92841500
N	-0.68413400	0.65662700	-1.47566900
C	0.65767300	3.26450900	-1.01411200
H	0.27462900	2.70519800	-0.14500200
O	-0.13718700	3.02970500	-2.16318000
H	1.70381900	2.97844200	-1.19064000
C	0.59380400	4.75234100	-0.70979700
Cl	1.26901300	5.70523100	-2.04690800
Cl	1.55477500	5.03468400	0.77790300
Cl	-1.09991700	5.25356900	-0.41061500
C	-5.55705600	-0.90204500	-3.69560200
C	-4.78908100	0.36207800	-3.49481700
C	-6.14381400	-1.60449400	-2.70400900
H	-5.64282600	-1.27263800	-4.72002500
C	-4.25898200	0.46609900	-2.07144400
H	-5.44932400	1.21909500	-3.71633400
H	-3.96616300	0.43575100	-4.21950600
C	-6.11337300	-1.08805200	-1.31949500
C	-6.87773800	-2.88584200	-2.92109700
C	-3.49544900	1.73419900	-1.75573300
C	-5.40940900	0.23261700	-1.08976900
H	-3.55363000	-0.37502000	-1.93379700
O	-6.66353500	-1.69046900	-0.40387900
H	-7.90863100	-2.81615600	-2.55454800
H	-6.89622500	-3.16671800	-3.97899400
H	-6.41538600	-3.70306600	-2.35355100
C	-3.57542000	2.86947600	-2.51537500
H	-6.15150200	1.04059700	-1.20712500
H	-5.07509900	0.27219500	-0.04482400
H	-4.18626600	2.93635900	-3.41216000
H	-2.97694300	3.74261600	-2.26437300
C	-2.62795200	1.68588100	-0.64983800
H	-1.27405700	-0.07644500	-1.88388300
H	-2.07937500	2.56947600	-0.33108700
H	-2.62869700	0.84465600	0.04378300
C	4.22315700	2.57845700	1.00616600
H	3.81710400	2.67835800	2.02160700
H	5.13446200	3.18640900	0.94951600
H	3.49160200	2.99550200	0.30660200
C	5.59103300	0.58036000	1.63833600
H	6.51556600	1.16454700	1.54319100
H	5.24617400	0.65277700	2.67476900
H	5.82712900	-0.46947100	1.43840100
C	1.30043400	-4.64001800	-2.33203000
H	1.65911600	-5.38433000	-3.05360200
H	0.68889500	-5.16667700	-1.58884900
H	0.66298500	-3.92528900	-2.86361200
C	3.34844700	-4.95935300	-0.92608500
H	2.76045400	-5.49649700	-0.17475600
H	3.74952900	-5.69479900	-1.63546400
H	4.19058400	-4.48483000	-0.41238600
C	-2.20622000	-4.73942000	0.96875700
H	-3.10698600	-5.35738300	1.06847300
H	-1.75898600	-4.96022300	-0.00847800
H	-1.49515600	-5.03394500	1.74724200
C	-3.52908900	-2.86272100	-0.03540900
H	-3.08880500	-3.04362600	-1.02331300
H	-4.45940500	-3.43917000	0.03972100
H	-3.79226700	-1.80130600	0.02607500
C	-1.16105300	3.03872600	2.77159500
H	-1.52786200	3.80166400	3.47043100
H	-0.45032500	3.52253200	2.09208900
H	-2.00724100	2.68503600	2.17337400
C	0.67354600	2.43889500	4.36542400
H	1.40708100	2.94022000	3.72046700
H	0.31532900	3.17637100	5.09424100
H	1.18390800	1.63542100	4.90603200
<b>E-<sup>1</sup>PC<sub>A,S</sub></b>			
Rh	-0.52633200	-2.50964900	1.02796300
Rh	-0.22756500	-0.45111400	-0.16304500
O	1.27967000	-2.15907200	1.96823600
C	1.91389900	-1.09071300	1.72245200
O	1.57273600	-0.19090700	0.88294600
O	0.40748400	-3.49708800	-0.50708700

C	0.76913100	-2.83224900	-1.52752600
O	0.63971900	-1.57723500	-1.68736700
O	-2.05969400	-0.80809600	-1.08796100
C	-2.68345500	-1.88240800	-0.81145000
O	-2.31629800	-2.77053400	0.02116400
O	-1.45458000	-1.46413600	2.57186600
C	-1.58499700	-0.20938300	2.44295100
O	-1.20001000	0.47626400	1.44211500
C	3.21851900	-0.85764700	2.48617500
C	4.38710900	-0.89798200	1.46504100
H	4.31813600	0.00130500	0.83836300
H	5.32102100	-0.80729500	2.03983100
C	4.42131800	-2.11132500	0.57878900
C	3.71741100	-2.09464300	-0.62753600
C	5.13201600	-3.26482100	0.92163300
C	3.70354900	-3.19222100	-1.49074200
H	3.16888800	-1.19768600	-0.91296100
C	5.13100300	-4.36866700	0.07275800
H	5.70177200	-3.29050000	1.85155000
C	4.42309800	-4.33427000	-1.12568600
H	5.69726300	-5.25887800	0.34210800
H	4.43901900	-5.19700100	-1.79294100
C	1.44281800	-3.59846600	-2.66554600
C	2.91404500	-3.11060400	-2.76719200
H	3.39331800	-3.70961800	-3.55569900
H	2.89798600	-2.06941500	-3.11600400
C	-2.26120400	0.53903800	3.59126800
C	-4.00236900	-2.15515400	-1.53560300
C	-3.68167700	-0.05572900	3.78063400
H	-3.57003700	-1.08793000	4.13713200
H	-4.16416300	0.51361800	4.58852300
C	-5.11925200	-2.29858400	-0.46634200
H	-6.06392300	-2.45589000	-1.00747500
H	-4.91942400	-3.21303900	0.10697400
C	-4.53183100	-0.03641800	2.54153100
C	-4.50200700	-1.12220200	1.66181700
C	-5.33590400	1.06038800	2.21883500
C	-5.23729200	-1.13127400	0.47352700
H	-3.88785200	-1.98826200	1.90895000
C	-6.09535600	1.05968400	1.05284500
H	-5.37804100	1.91823100	2.89102200
C	-6.04263700	-0.02518600	0.18232000
H	-6.71780100	1.92214100	0.82267500
H	-6.64051900	-0.02228000	-0.73087600
O	1.26587600	2.43653600	-3.33056200
S	1.70442400	1.85919100	-2.08299600
O	2.33484300	0.56358500	-2.00328100
N	0.37729100	1.86853100	-1.00601500
C	3.72034600	2.36874200	-0.53844500
H	3.21609200	1.80240700	0.25941900
O	2.77171100	2.95184900	-1.43175300
H	4.39124900	1.69230500	-1.08108200
C	4.54308500	3.49031800	0.07335100
Cl	5.35395700	4.43316700	-1.19321000
Cl	5.75539600	2.71233000	1.13184100
Cl	3.50575900	4.56961500	1.05475200
C	-3.77814100	2.31860700	-2.66115700
C	-2.31446000	2.31847600	-2.39897600
C	-4.71907000	2.87735900	-1.87367900
H	-4.10017300	1.80815400	-3.57260700
C	-1.95040800	2.75486900	-0.97740600
H	-1.82531000	2.96745200	-3.14591300
H	-1.90676000	1.31434800	-2.58702000
C	-4.31638500	3.62609000	-0.66668400
C	-6.17900400	2.80934900	-2.17859100
C	-0.47204000	3.10801400	-0.90161100
C	-2.83473800	3.91231400	-0.51804500
H	-2.13177200	1.89802200	-0.30775300
O	-5.13754900	4.06458100	0.12803500
H	-6.59939200	3.80940800	-2.34342900
H	-6.37392400	2.19802700	-3.06678800
H	-6.73723200	2.38568000	-1.33622000
H	-2.63760500	4.80149800	-1.13886800
H	-2.63103300	4.20185900	0.52024500
C	0.37445400	2.68309200	0.23038800
H	1.26479300	3.28190400	0.41696800
H	-0.03876900	2.15478900	1.08601900
C	-0.05312800	4.38109700	-1.60030200
H	-0.37130200	4.41436100	-2.64615600
H	-0.51083400	5.22660000	-1.07432300
H	1.02806700	4.53594300	-1.57497200
C	0.73234500	-3.25598500	-3.97677100
H	1.23053100	-3.75984100	-4.81452900

H	-0.31268000	-3.59009100	-3.96242400
H	0.74504000	-2.17733600	-4.16238800
C	1.38667500	-5.10043200	-2.411173700
H	0.35144200	-5.44954900	-2.32982900
H	1.86249800	-5.63332100	-3.24543700
H	1.90020400	-5.37729600	-1.48574700
C	3.17399300	0.52894600	3.13292500
H	2.37585900	0.59334600	3.88317800
H	4.12497100	0.74277800	3.63690900
H	3.00021800	1.31774800	2.39044800
C	3.41267600	-1.92580000	3.55663500
H	4.34140000	-1.73129900	4.10879000
H	2.58249700	-1.92588200	4.27110000
H	3.47151600	-2.92791000	3.12106200
C	-4.33319000	-1.03344800	-2.50968000
H	-3.54634900	-0.91455600	-3.26375700
H	-5.27532700	-1.25505800	-3.02949500
H	-4.44437500	-0.07615900	-1.99055400
C	-3.86702600	-3.48353100	-2.28493900
H	-4.81308800	-3.73067200	-2.78306900
H	-3.09027600	-3.42528000	-3.05775700
H	-3.60986800	-4.29978600	-1.60251100
C	-2.33729100	2.03455800	3.30308500
H	-2.81751000	2.55147000	4.14380400
H	-1.33799600	2.46594300	3.17040900
H	-2.91965100	2.24725900	2.39947400
C	-1.44949100	0.28998500	4.86580900
H	-0.43455600	0.69867800	4.77849200
H	-1.93244800	0.78087500	5.71991800
H	-1.36916900	-0.78035300	5.08089800

E-<sup>1</sup>PC<sub>A-R</sub>

Rh	-0.68737000	0.46538100	-0.16496700
Rh	-2.92788000	1.01500100	0.49449400
O	-0.08644800	1.25107400	1.67948700
C	-0.93962500	1.78127200	2.46051400
O	-2.18237500	1.88778000	2.23608300
O	-0.60822400	2.29205900	-1.12809000
C	-1.64125700	3.03155100	-1.15223700
O	-2.74715900	2.79693800	-0.57010300
O	-3.63559700	0.12920500	-1.21245500
C	-2.78644600	-0.28189900	-2.06473800
O	-1.52250200	-0.25245000	-1.93648900
O	-0.86981300	-1.35039300	0.84675800
C	-1.96673200	-1.56823800	1.46387900
O	-2.97181600	-0.79848700	1.49634000
C	-0.41653400	2.36180900	3.77391900
C	-0.69001700	3.89029400	3.75391100
H	-1.77373300	4.03791500	3.84671500
H	-0.22905700	4.31356100	4.65855600
C	-0.19525400	4.59961600	2.52459800
C	-1.05084500	4.75405900	1.43036600
C	1.10684800	5.09984900	2.42605200
C	-0.64335000	5.38624800	0.25282600
H	-2.07081700	4.37372100	1.50122800
C	1.53186600	5.73333400	1.26109400
H	1.78406500	5.00948700	3.27645100
C	0.66491900	5.87533200	0.18094600
H	2.54354600	6.13214200	1.19885300
H	0.99811000	6.39029200	-0.72080200
C	-1.53448200	4.34519600	-1.92697900
C	-1.60640200	5.50383200	-0.89474000
H	-1.43693600	6.43930400	-1.44804200
H	-2.63197500	5.54340400	-0.50472700
C	-2.05423800	-2.88768900	2.22884200
C	-3.31923900	-0.88430900	-3.36466400
C	-1.89548000	-4.04519900	1.20829500
H	-0.86165500	-4.02866000	0.83990200
H	-2.01414100	-4.98737600	1.76426900
C	-2.90338500	-2.38053600	-3.40697100
C	-2.83791700	-3.99604800	0.03852900
C	-2.47898500	-3.28589500	-1.11078700
C	-4.08196000	-4.63237400	0.06958200
C	-3.33106300	-3.18838600	-2.21397300
H	-1.50485000	-2.79725800	-1.15590700
C	-4.93961400	-4.55428700	-1.02415900
H	-4.37197900	-5.20470400	0.95175900
C	-4.56927800	-3.83558400	-2.15753200
H	-5.90138800	-5.06445200	-0.99611500
H	-5.24065500	-3.78701000	-3.01577800
O	2.85886600	-1.15148300	-2.62954200
S	1.91461000	-1.45073300	-1.57862400
O	0.58804800	-1.94421300	-1.85913300

## ARTICLE

## Journal Name

N	1.73532500	-0.09614100	-0.53057500
O	2.65608300	-2.59772600	-0.64031900
C	1.76843400	-3.46975000	0.06005400
H	1.02546000	-2.90248800	0.64189500
H	1.24399400	-4.12377300	-0.64700400
C	2.61341700	-4.32331100	0.99334400
Cl	3.89534700	-5.16299100	0.09198200
Cl	1.51638200	-5.51351500	1.74582400
Cl	3.35497300	-3.30528300	2.26805800
C	2.42319300	-0.08335800	0.78396700
C	2.87492400	0.88674500	-0.23161000
H	3.05581300	-0.94226700	0.99266500
H	1.77020800	0.23015300	1.59709300
C	2.34631900	2.29547600	-0.15369900
C	4.25491700	0.74838900	-0.90041200
H	2.99727300	2.89720000	0.49020900
H	1.34150700	2.33491200	0.26793600
H	2.31940400	2.76390700	-1.14438400
C	5.13326300	1.97976000	-0.64683900
C	5.06646200	-0.48219400	-0.49048100
H	4.08890600	0.69452500	-1.98474700
H	5.33953700	2.07890400	0.43290100
H	4.66019100	2.91462500	-0.95860400
C	6.47081600	1.91330100	-1.36447900
C	6.41118400	-0.50756600	-1.13872900
H	5.19757400	-0.48577500	0.60710300
H	4.55221700	-1.41891800	-0.72316300
C	7.06555000	0.58192600	-1.58369900
O	7.04713400	2.93736700	-1.70535700
H	6.88036800	-1.48764400	-1.24909300
C	8.39570500	0.54131900	-2.25731300
H	9.13085800	1.14341400	-1.71021500
H	8.77273400	-0.48260100	-2.34648600
H	8.33895700	0.98072100	-3.26036500
C	-0.22926700	4.40638000	-2.71208300
H	-0.15181900	3.57178300	-3.41753200
H	-0.18262200	5.34357200	-3.28192600
H	0.64211000	4.36144400	-2.05095100
C	-2.72746300	4.46390300	-2.87637100
H	-2.69843900	5.43025300	-3.39546500
H	-2.70702800	3.67619600	-3.63939200
H	-3.67522300	4.38822100	-2.33463500
C	1.07450600	2.08632200	3.93580100
H	1.43464500	2.52457700	4.87558100
H	1.27795300	1.00916700	3.96818300
H	1.65726900	2.51329900	3.11159100
C	-1.19718100	1.73685900	4.93190000
H	-1.02751200	0.65396000	4.98815400
H	-0.87310100	2.17409400	5.88462300
H	-2.27270400	1.90582600	4.81950300
C	-0.89047800	-2.94042500	3.22339500
H	-0.96255200	-2.13202100	3.96248300
H	-0.89548200	-3.89376700	3.76694200
H	0.07755700	-2.84469300	2.71563200
C	-3.38243300	-3.00024900	2.96729300
H	-3.42098500	-3.94889100	3.51869600
H	-3.50880100	-2.18202700	3.68425500
H	-4.23048100	-2.96676000	2.27623900
C	-2.65175900	-0.16541600	-4.53956300
H	-2.98924600	-0.60259900	-5.48764200
H	-2.91331000	0.90019000	-4.55383900
H	-1.56175400	-0.24963400	-4.48471800
C	-4.83425800	-0.74051100	-3.44734400
H	-5.13456200	0.31269600	-3.42911500
H	-5.19674700	-1.18195600	-4.38511400
H	-5.33559100	-1.23949600	-2.61242800
H	-1.81033100	-2.42277100	-3.50301300
H	-3.32733100	-2.80263900	-4.33027000

E-<sup>1</sup>PC<sub>1</sub>

Rh	1.04405600	-2.47766600	1.09627100
Rh	0.34633600	-0.45052400	0.03420200
O	2.85300200	-1.58004800	1.51656500
C	3.05217900	-0.38783300	1.13610700
O	2.21474400	0.35392700	0.51972400
O	1.80686100	-3.10952900	-0.72314200
C	1.63153400	-2.37335800	-1.74061300
O	1.03132400	-1.24913500	-1.75767500
O	-1.47340600	-1.32341800	-0.39032900
C	-1.64788800	-2.55181800	-0.08791100
O	-0.82091100	-3.28172400	0.53436100
O	0.27844300	-1.71482300	2.88224900
C	-0.21265900	-0.54357400	2.88727500

O	-0.32314900	0.22649200	1.88068000
C	4.40356400	0.24810600	1.45904600
C	4.97821800	0.87626900	0.16210900
H	4.30151000	1.67962500	-0.15951700
H	5.93260000	1.35446700	0.42917100
C	5.18172100	-0.10628600	-0.95803700
C	4.12874400	-0.42099300	-1.82243600
C	6.40598500	-0.75855700	-1.13341800
C	4.26136100	-1.39125300	-2.82040400
H	3.17706900	0.10068300	-1.72034900
C	6.56342200	-1.70975000	-2.13692800
H	7.24260900	-0.51154200	-0.47842100
C	5.49544300	-2.03126200	-2.96933600
H	7.52485200	-2.20324700	-2.27093300
H	5.61860400	-2.78159700	-3.75139800
C	2.16825400	-2.85701300	-3.08812600
C	3.08140000	-1.74945100	-3.67949700
H	3.42183500	-2.10577300	-4.66300400
H	2.46181000	-0.85963200	-3.85044300
C	-0.73378900	-0.02138600	4.22791400
C	-2.98371600	-3.17688600	-0.48743900
C	-1.88023900	-0.96055200	4.69187200
H	-1.43701300	-1.93396300	4.93882000
H	-2.28143800	-0.54235400	5.62702100
C	-3.73010400	-3.54812300	0.82235800
H	-4.71568000	-3.93996900	0.53210400
H	-3.18206100	-4.37141600	1.29908900
C	-2.97767700	-1.15012300	3.68338500
C	-2.90764800	-2.21375900	2.78016300
C	-4.06358400	-0.27219400	3.59523000
C	-3.87809300	-2.41187100	1.79444200
H	-2.06994700	-2.90917600	2.84813200
C	-5.03902400	-0.45514200	2.61876100
H	-4.14877900	0.55093600	4.30607900
C	-4.94842400	-1.51534600	1.71981500
H	-5.88533100	0.22858600	2.55267000
H	-5.71641100	-1.63444800	0.95587400
O	-1.05475800	2.85446700	-3.12461600
S	-0.07105200	2.27118500	-2.24003600
O	1.09713100	1.58590500	-2.74505300
N	-0.82876400	1.23755300	-1.09189400
C	1.75661100	3.41458900	-0.78714400
H	2.04417800	2.41705000	-0.42378400
O	0.38793700	3.44878300	-1.21599400
H	2.41110600	3.71893100	-1.61159500
C	1.88200800	4.41517600	0.35043400
Cl	1.26340200	6.01274000	-0.13335400
Cl	3.62113100	4.53887500	0.73775800
Cl	0.97858300	3.82190100	1.77361500
C	-5.62835800	2.00076300	-3.31158000
C	-4.55841400	2.79093700	-2.63518600
C	-6.29554200	0.97538700	-2.74234500
H	-5.88107100	2.28379700	-4.33636300
C	-3.90294900	1.99161200	-1.51569200
H	-4.99872000	3.71884900	-2.23071600
H	-3.80051700	3.11941000	-3.35810100
C	-6.04451500	0.63077500	-1.32794500
C	-7.34518800	0.17947300	-3.44395500
C	-2.85322300	2.73377800	-0.72756000
C	-4.98747700	1.42823300	-0.59120400
H	-3.41843700	1.12212900	-1.99968700
O	-6.70094600	-0.23686100	-0.76232700
H	-8.30102200	0.23249600	-2.90967200
H	-7.49486300	0.52551300	-4.47178800
H	-7.07797700	-0.88414800	-3.47004700
C	-2.86753800	4.04852000	-0.49430800
H	-5.49323300	2.26754400	-0.08445200
H	-4.57509700	0.79875300	0.20897500
H	-3.63670600	4.70777700	-0.89229500
H	-2.08589600	4.52130300	0.09845300
C	-1.77547600	1.88371000	-0.12366800
H	-1.33099000	0.53523900	-1.64779900
H	-1.16020900	2.44310800	0.58544400
H	-2.19362500	1.02361900	0.42031900
C	4.14678100	1.35416100	2.48748400
H	3.78651500	0.93225400	3.43411600
H	5.07516100	1.90127700	2.69605800
H	3.40147400	2.07083500	2.12698400
C	5.36779500	-0.78095000	2.03718800
H	6.32747500	-0.29936400	2.26694300
H	4.97292600	-1.21565400	2.96062000
H	5.55444300	-1.60202400	1.33793700
C	0.97057600	-3.04657000	-4.02485500

## ARTICLE

## Journal Name

H	1.31554700	-3.37696300	-5.01263400
H	0.28354400	-3.81083300	-3.64026900
H	0.41382800	-2.11142200	-4.14888200
C	2.92248200	-4.17148200	-2.93154700
H	2.26556000	-4.96094000	-2.55189400
H	3.31553200	-4.49238100	-3.90528300
H	3.76096400	-4.07766800	-2.23449400
C	-2.71487400	-4.45756800	-1.27962900
H	-3.66292400	-4.95731500	-1.51458900
H	-2.20947700	-4.24121600	-2.22910700
H	-2.08858600	-5.15078500	-0.70941600
C	-3.81258200	-2.20374600	-1.31940400
H	-3.29638700	-1.93411600	-2.24907400
H	-4.77731700	-2.65692400	-1.58224900
H	-4.01876000	-1.28136700	-0.76640200
C	0.40208100	-0.08981300	5.25098600
H	1.23136200	0.57043600	4.96642500
H	0.04125800	0.23422000	6.23523300
H	0.79282800	-1.10826100	5.34185600
C	-1.23322400	1.41341700	4.10030400
H	-1.61979900	1.75885900	5.06803100
H	-0.42283300	2.08770400	3.80230600
H	-2.03378700	1.50428600	3.35843700

O<sup>-1</sup>NR

Rh	2.42143500	-0.98941200	0.72082900
Rh	0.83444600	0.41470700	-0.43802500
O	2.89303600	0.68810400	1.85893100
C	2.38620900	1.80759200	1.55522700
O	1.56758400	2.02436800	0.59749600
O	3.81551800	-0.44318500	-0.69469400
C	3.45674600	0.27835300	-1.67197300
O	2.28653900	0.76175900	-1.84517200
O	0.29339300	-1.35367800	-1.46243900
C	0.92689100	-2.43680600	-1.25332200
O	1.88452100	-2.60488100	-0.43493700
O	1.00574600	-1.53693800	2.10147000
C	-0.11000600	-0.93911100	2.03023000
O	-0.43315800	-0.05599100	1.17010900
C	2.75164000	3.00336000	2.37755600
C	4.47195600	0.62345900	-2.71471100
C	-1.16757400	-1.29741700	3.02697000
C	0.47121300	-3.63106800	-2.03674100
O	-1.61654900	3.38132600	-1.61861900
S	-1.59330300	2.33392100	-0.60860400
O	-1.33806300	2.63603200	0.79104800
N	-0.69367400	1.15477300	-1.31732500
C	-3.57542800	0.96576900	0.44492700
H	-2.77290000	0.82031500	1.17862800
O	-3.12932500	1.69528900	-0.68207400
H	-4.40307700	1.51033900	0.91555000
C	-4.09024000	-0.40131100	0.00282800
Cl	-5.43931500	-0.22397400	-1.14231000
Cl	-4.67671100	-1.22623200	1.49427300
Cl	-2.78141500	-1.33981000	-0.74022200
H	5.38728800	0.04851100	-2.56407500
H	4.06460100	0.43450200	-3.71189000
H	3.56875800	2.76724900	3.06129200
H	1.87524300	3.32372100	2.95089200
H	1.24203100	-4.40410500	-2.04556600
H	-1.61855900	-0.39076600	3.44217700
H	0.20386500	-3.34094600	-3.05576100
H	-0.75339500	-1.91373700	3.82693800
H	3.02877800	3.83773600	1.72733500
H	4.70141100	1.69278900	-2.65954400
H	-0.42942500	-4.04346900	-1.56691400
H	-1.96656000	-1.85083700	2.51919700

O<sup>-3</sup>NR

Rh	2.51264100	-0.86707100	0.72229400
Rh	0.76956400	0.28901700	-0.44930100
O	2.77662600	0.79321400	1.91895900
C	2.19864900	1.86227000	1.55089900
O	1.44040900	1.98783000	0.53471800
O	3.84093100	-0.10778300	-0.67044900
C	3.37488000	0.46937200	-1.69913700
O	2.13993400	0.68459300	-1.94189900
O	0.31828900	-1.51700100	-1.36253600
C	1.13522600	-2.48837000	-1.23750300
O	2.16646400	-2.49521600	-0.49772700
O	1.12481100	-1.60592000	2.05658300
C	-0.04262500	-1.11261600	2.00349200

O	-0.44205300	-0.22399600	1.18062100
C	2.40858900	3.09934100	2.36536400
C	4.34442700	0.96731800	-2.72502900
C	-1.06488600	-1.61911900	2.97269900
C	0.84192400	-3.70836300	-2.05294600
O	-1.80989300	3.54651500	-1.41589000
S	-1.68604700	2.43448500	-0.49717900
O	-1.40411300	2.64250800	0.91640600
N	-0.72070200	1.30925200	-1.17889800
C	-3.54407700	0.85912500	0.48754700
H	-2.70173500	0.66782600	1.16288100
O	-3.17151700	1.69310700	-0.59485800
H	-4.35522900	1.34381300	1.04392100
C	-4.05636800	-0.47508200	-0.04330200
Cl	-5.43181300	-0.22825500	-1.14280500
Cl	-4.59944100	-1.40949100	1.39981200
Cl	-2.75695800	-1.34883200	-0.87658000
H	5.30515800	0.45781600	-2.62871000
H	3.93679100	0.83489300	-3.73017200
H	3.07708000	2.90367100	3.20565700
H	1.43964400	3.45849800	2.72725600
H	1.05780300	-3.49903100	-3.10621300
H	-1.82717900	-2.18692300	2.42561900
H	-0.22088900	-3.95877500	-1.98689300
H	-1.57699300	-0.78080900	3.45533600
H	2.82573300	3.89114200	1.73540000
H	4.50025200	2.04152600	-2.57525300
H	1.45137200	-4.55145800	-1.72307700
H	-0.60328400	-2.26054100	3.72552800

**O-<sup>1</sup>TS1<sub>A</sub>**

Rh	-0.24752000	0.78311000	0.17481400
Rh	-0.71676200	2.98330000	-0.68052300
O	-0.19503600	0.09645900	-1.80030800
C	-0.56024100	0.90701900	-2.71600500
O	-0.89258500	2.12062400	-2.56291900
O	-2.28381300	0.45904200	0.26665700
C	-3.07199300	1.44439500	0.05227500
O	-2.72060400	2.60349100	-0.30825000
O	-0.47353500	3.70873900	1.24814300
C	-0.41988900	2.85864600	2.19014800
O	-0.44724000	1.59036900	2.06648800
O	1.77339200	1.40982700	-0.01444300
C	2.07854400	2.48355200	-0.62041000
O	1.26150800	3.35246700	-1.05833200
O	0.79490900	-1.99540900	3.09162100
S	1.42087100	-1.06859700	2.16242900
O	1.89905100	0.23406300	2.60779000
N	0.67593000	-0.92213500	0.70104700
O	2.80264500	-1.92392300	1.70050000
C	3.81526900	-1.13925100	1.10795500
H	3.48392500	-0.10747500	0.92801400
H	4.68702500	-1.12591300	1.77454500
C	4.26897100	-1.72646900	-0.22642600
Cl	4.69334700	-3.44741200	-0.04860100
Cl	5.72510900	-0.79085400	-0.71904800
Cl	3.01384200	-1.54320600	-1.47889400
C	0.22373600	-3.01622800	0.28067000
C	-0.77293000	-2.92914800	-0.65962300
H	-0.01338000	-3.17597000	1.32673400
H	1.24679200	-3.23135700	-0.01750000
C	-0.46309700	-3.04726300	-2.10937800
C	-2.18913200	-2.64802300	-0.28744100
H	-0.58848400	-4.08843500	-2.44454100
H	0.57187100	-2.76142500	-2.31973700
H	-1.13335000	-2.43404400	-2.72305200
C	-3.16813100	-3.67930600	-0.86891400
C	-2.45497800	-2.47932200	1.20227900
H	-2.42710200	-1.68137200	-0.76978500
H	-2.98163800	-4.66171300	-0.40436900
H	-3.04767000	-3.81662800	-1.94932000
C	-4.61444300	-3.30046300	-0.60326800
C	-3.89696400	-2.21634700	1.46790900
H	-2.14358500	-3.38541900	1.75176000
H	-1.84356900	-1.66516200	1.61305100
C	-4.90438000	-2.55135100	0.63502300
O	-5.50446400	-3.63899900	-1.37165800
H	-4.13852400	-1.71584000	2.40927300
C	-6.33956000	-2.23980700	0.90392400
H	-6.94179500	-3.15512600	0.94192300
H	-6.46422500	-1.69820900	1.84770900
H	-6.77077200	-1.63659800	0.09506600
C	-4.53289600	1.16742000	0.23554200

## ARTICLE

## Journal Name

H	-4.84615000	0.37337100	-0.45148800
H	-4.72075300	0.79679900	1.24862900
H	-5.12318700	2.06648000	0.05086300
C	-0.62289200	0.34988400	-4.10878700
H	0.15768400	-0.40116200	-4.25824400
H	-1.59198600	-0.14032800	-4.26046900
H	-0.52837600	1.14845900	-4.84741100
C	-0.30281100	3.36888000	3.59352000
H	-1.09329800	2.93754500	4.21522000
H	0.65061800	3.03113800	4.01359100
H	-0.35845300	4.45838600	3.62172400
C	3.54202100	2.72401800	-0.83754100
H	4.07490200	2.65921900	0.11678000
H	3.94924500	1.93961100	-1.48556400
H	3.71336300	3.70124000	-1.29245900

O-<sup>3</sup>TS1A

Rh	-0.04935500	0.79888700	0.24863800
Rh	-0.36387900	2.95688000	-0.77766700
O	-0.03486700	-0.01043300	-1.67879300
C	-0.19981100	0.76934000	-2.67481300
O	-0.39605900	2.01975700	-2.62344900
O	-2.12669800	0.63008800	0.31662700
C	-2.83813000	1.60206000	-0.10900100
O	-2.40079800	2.68961600	-0.58813400
O	-0.28978700	3.81687400	1.09725700
C	-0.21290900	3.04292500	2.10090600
O	-0.15333300	1.77156700	2.06968000
O	1.99385000	1.18469800	0.10175400
C	2.40634200	2.24485800	-0.47418900
O	1.67962700	3.16916100	-0.94820900
O	0.71668400	-2.21995900	3.23981200
S	1.32714300	-1.26835600	2.32666500
O	1.93134900	-0.03797000	2.81109200
N	0.33318200	-1.00885600	1.05396800
O	2.56906800	-2.17925300	1.65239900
C	3.65796900	-1.46107500	1.10973400
H	3.44463100	-0.38640500	1.04144300
H	4.54175600	-1.62058000	1.74019800
C	3.97714400	-1.98093500	-0.28783700
Cl	4.27471600	-3.73822400	-0.25570200
Cl	5.46567600	-1.13210400	-0.82715600
Cl	2.63839300	-1.61991000	-1.40718200
C	-0.19338300	-2.96421000	0.40133300
C	-1.16390100	-2.84208900	-0.57692000
H	-0.46624400	-3.15986600	1.43333400
H	0.81390700	-3.26530700	0.12123700
C	-0.82988300	-3.02954800	-2.01618800
C	-2.56370400	-2.43013600	-0.24415400
H	-1.20922900	-3.99695500	-2.37908700
H	0.25121500	-3.01401700	-2.18705500
H	-1.29713500	-2.25843300	-2.64290400
C	-3.63829000	-3.28676600	-0.92339600
C	-2.86455000	-2.31842800	1.24556100
H	-2.66335700	-1.40841400	-0.65896900
H	-3.60896100	-4.30861000	-0.50906900
H	-3.48493800	-3.38171700	-2.00410600
C	-5.02908200	-2.72522000	-0.69587800
C	-4.27912800	-1.92098800	1.49066000
H	-2.66731100	-3.28283500	1.74726000
H	-2.18591300	-1.59595400	1.71902800
C	-5.28408500	-2.06681500	0.60245500
O	-5.90957900	-2.83852600	-1.53834100
H	-4.50099000	-1.47307400	2.46305100
C	-6.68024700	-1.59983100	0.84826600
H	-7.39610400	-2.42604600	0.76525500
H	-6.78467000	-1.14193200	1.83763900
H	-6.98576400	-0.86690100	0.09080000
C	-4.32463700	1.41641300	-0.04953200
H	-4.63074000	0.67072600	-0.79359600
H	-4.62387600	1.02790600	0.92857900
H	-4.83761900	2.35700800	-0.25871800
C	-0.17851300	0.13007600	-4.03257700
H	0.42562500	-0.78116800	-4.02316300
H	-1.20027900	-0.14103000	-4.32359400
H	0.20259500	0.83233300	-4.77746600
C	-0.20788700	3.66454600	3.46431500
H	-1.18087600	3.50301400	3.94110000
H	0.54571200	3.18124500	4.09197900
H	-0.02179100	4.73813500	3.39764900
C	3.89236400	2.37838600	-0.60972700
H	4.37957600	2.18118900	0.35045400
H	4.25838100	1.62470300	-1.31659800



H 4.16227800 3.37282200 -0.96979400

**O<sup>-1</sup>TS1<sub>1</sub>**

Rh -0.74798500 -3.04196600 -0.04071000  
 Rh -0.14854500 -0.71582900 0.08711600  
 O -2.04903600 -2.70260900 1.52568400  
 C -2.19814300 -1.53057800 1.97753800  
 O -1.53155600 -0.50440800 1.59825600  
 O 0.80318000 -3.47397700 1.27011900  
 C 1.49281400 -2.50667600 1.71759700  
 O 1.32508600 -1.27045000 1.45961200  
 O 1.21127000 -1.19191700 -1.42678200  
 C 1.24955300 -2.34959100 -1.95115000  
 O 0.53394500 -3.34237400 -1.61639200  
 O -2.24925300 -2.48134100 -1.35010600  
 C -2.42682000 -1.25215900 -1.60985200  
 O -1.69979900 -0.28251600 -1.20894900  
 C 2.24446200 -2.53230500 -3.05599400  
 C 2.62513000 -2.82782100 2.64788600  
 C -3.62225600 -0.89608200 -2.43545700  
 C -3.25190200 -1.28904700 3.00882200  
 H 3.79448900 1.08854600 -2.03565100  
 C 3.36674400 1.21327900 -1.03211500  
 H 2.78553100 0.31738800 -0.77759100  
 O 2.57950800 2.38800900 -0.97545800  
 C 4.50520200 1.32583700 -0.02908300  
 S 0.93903900 2.09603100 -1.10549700  
 Cl 5.55694700 2.70881500 -0.42683800  
 Cl 5.44889200 -0.20297400 -0.15616000  
 Cl 3.88209000 1.50053500 1.62581100  
 O 0.37637800 3.42457600 -0.92059800  
 O 0.75416700 1.37296700 -2.35337800  
 N 0.70148100 1.11162700 0.18876400  
 H 0.28491700 1.86923400 1.22729100  
 C -0.34251400 2.45759600 2.14824200  
 C -1.18449300 3.46368900 1.53089500  
 H 0.45456600 2.82882800 2.79837200  
 H -0.84108200 1.56877900 2.54565900  
 C -2.28291900 2.96368200 0.62566100  
 C -0.89803000 4.77397100 1.70878700  
 C -2.92247100 4.04155600 -0.23778700  
 C -3.37497100 2.17807800 1.36023700  
 H -1.79827400 2.24781200 -0.06187600  
 H -1.47855700 5.57184700 1.25301400  
 H -0.05346600 5.08018900 2.32199600  
 C -4.07913500 3.53018500 -1.02453600  
 H -3.28325800 4.87414300 0.39301500  
 H -2.16898800 4.48225600 -0.90534700  
 C -4.33265000 1.54464600 0.37380100  
 H -3.94886300 2.86465500 2.00526800  
 H -2.95761100 1.39205400 1.99710500  
 C -4.74113900 2.38191300 -0.77253400  
 H -4.41074000 4.14905700 -1.86201900  
 O -4.78028400 0.41182300 0.53157500  
 C -5.90521600 1.91566100 -1.58421400  
 H -6.79602700 1.78764400 -0.95672900  
 H -6.14322700 2.62445200 -2.38396500  
 H -5.71700000 0.93637400 -2.03767800  
 H -4.49188900 -0.86971300 -1.76785500  
 H -3.80129600 -1.65703300 -3.19882900  
 H -3.50232200 0.08969700 -2.89112900  
 H 2.17450500 -3.53442100 -3.48257000  
 H 3.25580500 -2.36999900 -2.66684100  
 H 2.07456600 -1.77887100 -3.83149100  
 H 2.73618700 -3.90642600 2.77104700  
 H 3.55308700 -2.39588400 2.25934100  
 H 2.44343800 -2.36426800 3.62298400  
 H -4.09563700 -0.79456900 2.50898900  
 H -2.88207800 -0.61524400 3.78794600  
 H -3.58903700 -2.22931600 3.44890800

**O<sup>-3</sup>TS1<sub>1</sub>**

Rh -0.35654900 -3.09339200 0.10745600  
 Rh 0.01542300 -0.72400700 -0.01999100  
 O -1.62733100 -2.74836900 1.69846100  
 C -1.81823000 -1.55948300 2.09172200  
 O -1.24376800 -0.51618100 1.62682900  
 O 1.25762000 -3.22436800 1.39010300  
 C 1.90457700 -2.16886500 1.66646700  
 O 1.64246000 -1.00072300 1.22753900  
 O 1.27984200 -1.12885500 -1.61975500  
 C 1.46542900 -2.33295900 -1.99320500  
 O 0.91734200 -3.36346900 -1.49845300

O	-1.96769700	-2.86815500	-1.14705100
C	-2.30353800	-1.69365500	-1.49693000
O	-1.66006300	-0.62556500	-1.23355500
C	2.43202000	-2.51844600	-3.12320100
C	3.07840300	-2.27836600	2.58952600
C	-3.58372200	-1.53295600	-2.24997900
C	-2.82384900	-1.33760400	3.17621700
H	3.65594900	1.39705100	-2.03684300
C	3.12789400	1.47940600	-1.07809200
H	2.58457600	0.54539600	-0.89377800
O	2.26757300	2.60211200	-1.08636400
C	4.16128300	1.64238000	0.02728400
S	0.66072600	2.22366700	-1.35676200
Cl	5.21541200	3.04192600	-0.29808500
Cl	5.14917300	0.13432700	0.01226700
Cl	3.38438900	1.83552900	1.61338000
O	0.01222200	3.51676400	-1.22983000
O	0.60436600	1.46704500	-2.59607800
N	0.30259600	1.26738000	-0.09301200
H	-0.01261700	2.00311100	0.98105800
C	-0.55363600	2.62546100	1.99081700
C	-1.53128300	3.51377400	1.39798200
H	0.25846900	3.10392000	2.54323100
H	-0.92315500	1.71463000	2.47127500
C	-2.61843400	2.86391400	0.57430000
C	-1.38533600	4.85839100	1.49856100
C	-3.51210000	3.83036400	-0.18935600
C	-3.49179500	1.88943400	1.36930000
H	-2.08747500	2.25839800	-0.18201200
H	-2.07613600	5.56221200	1.04135100
H	-0.54731900	5.28700800	2.04432300
C	-4.61691400	3.13013800	-0.90353900
H	-3.95258700	4.57113100	0.50282200
H	-2.91382500	4.41561300	-0.90234800
C	-4.39673800	1.10760600	0.44513500
H	-4.12216600	2.45479300	2.07653000
H	-2.89758100	1.17877900	1.94886500
C	-5.02478500	1.86806300	-0.65495700
H	-5.12204500	3.69325900	-1.69230100
O	-4.63333200	-0.08609900	0.61855500
C	-6.11866900	1.19718000	-1.41953600
H	-6.89006100	0.80496500	-0.74597100
H	-6.58947700	1.88589400	-2.12853200
H	-5.74515800	0.33463400	-1.98394600
H	-4.38055000	-1.37332400	-1.51181100
H	-3.81222300	-2.43317900	-2.82450900
H	-3.54037200	-0.65617000	-2.90131700
H	2.12386100	-1.90656500	-3.97643400
H	2.49351900	-3.56776200	-3.41669700
H	3.42241900	-2.16399800	-2.81639400
H	3.22997100	-3.31260000	2.90381900
H	3.97851600	-1.90236800	2.09186400
H	2.91506400	-1.64393800	3.46656900
H	-3.74779400	-0.98611300	2.69925700
H	-2.48360400	-0.56204200	3.86903300
H	-3.02720900	-2.26618800	3.71338800

**O-<sup>3</sup>IM<sub>A-S</sub>**

Rh	-0.01320200	-3.18019100	-0.28453100
Rh	-0.02599100	-0.80868500	0.07911500
O	-2.04197300	-3.21482200	0.09174800
C	-2.59409900	-2.14243700	0.48701000
O	-2.01092100	-1.02381900	0.66894600
O	0.36935300	-3.42716200	1.72908600
C	0.65865600	-2.39675500	2.41320100
O	0.67798100	-1.19746800	1.98547800
O	1.94484600	-0.77786200	-0.56959800
C	2.54564900	-1.89069500	-0.74297200
O	2.01574200	-3.03945900	-0.66014500
O	-0.41655900	-2.83306800	-2.28572000
C	-0.67757300	-1.64597300	-2.64671100
O	-0.63473800	-0.60984000	-1.90384600
O	0.16395400	3.09107000	2.04846600
S	-0.67345200	1.97970900	1.64005100
O	-1.11588000	0.96806200	2.57714600
N	-0.05378400	1.24560100	0.30025300
C	-3.25458000	2.05313900	1.10647200
H	-3.09919200	0.99389300	1.34749300
O	-2.03309800	2.76630300	1.05692000
H	-3.90049200	2.51103800	1.86570600
C	-3.96737900	2.14698700	-0.23761300
Cl	-4.18672300	3.84743700	-0.71479000
Cl	-5.57470700	1.37095500	-0.01599700

Cl	-3.04942500	1.28010500	-1.49165000
C	4.47386400	1.25738400	1.11614800
C	3.11732100	1.86254700	0.99979200
C	5.49395200	1.49282500	0.26480800
H	4.63331700	0.55913700	1.94374500
C	2.84105800	2.35593200	-0.43341900
H	3.00731500	2.70181800	1.70800100
H	2.35829900	1.12897000	1.30155200
C	5.32701600	2.47480300	-0.82875700
C	6.82544900	0.82439100	0.36186700
C	1.50753800	3.01836000	-0.56673700
C	4.01499400	3.22852700	-0.87877400
H	2.83319400	1.44982800	-1.06136000
O	6.22442300	2.68602500	-1.63497100
H	7.63101600	1.55913100	0.47849700
H	6.86514000	0.12465700	1.20397700
H	7.05716300	0.27651100	-0.56040100
H	4.10170300	4.10088100	-0.20948400
H	3.88339200	3.62481200	-1.89254700
C	0.32529600	2.14557500	-0.82244500
H	-0.55541400	2.74782000	-1.09365500
H	0.51758300	1.45045500	-1.65128800
C	1.35269100	4.47418100	-0.31270300
H	1.75551100	4.76272400	0.67053300
H	1.89387500	5.07912900	-1.05800700
H	0.30139600	4.78128700	-0.32747800
C	-4.06851500	-2.16674800	0.74828700
H	-4.44513700	-3.19100900	0.76530000
H	-4.29492800	-1.66466100	1.69401900
H	-4.58146000	-1.60713600	-0.04306500
C	0.99204200	-2.58812700	3.86025700
H	0.15448700	-2.22963800	4.46846000
H	1.17382600	-3.64106000	4.08292500
H	1.86330800	-1.98539800	4.13048400
C	4.01135600	-1.81337900	-1.04307100
H	4.55685900	-1.61883200	-0.11186200
H	4.36952100	-2.75108400	-1.47194300
H	4.22421000	-0.97702000	-1.71554400
C	-1.10334100	-1.43546500	-4.06821400
H	-0.50764400	-2.06029400	-4.73865700
H	-2.14903600	-1.74537800	-4.17707200
H	-1.02124600	-0.38427600	-4.35241000

**O<sup>-3</sup>IMA-R**

Rh	1.39766800	-0.50330900	-0.12192700
Rh	3.71697600	-0.69789500	0.48281900
O	1.03546400	0.04656800	1.85612900
C	2.01224800	0.13356700	2.67131100
O	3.22491400	-0.13298000	2.41334200
O	1.15110900	-2.47881400	0.46177000
C	2.17336800	-3.12743800	0.86360500
O	3.35450900	-2.67536500	0.95834500
O	4.12466000	-1.23428700	-1.45990800
C	3.15789300	-1.34773800	-2.27716000
O	1.92893400	-1.14833400	-2.01386500
O	1.80410700	1.47431700	-0.60376500
C	2.97647700	1.94180200	-0.42523500
O	3.98264700	1.29189700	-0.00722100
O	-2.34437000	-0.32095000	-2.43173400
S	-1.20498300	0.39424300	-1.88784000
O	-0.09443000	0.81561300	-2.71591000
N	-0.61787800	-0.35393700	-0.54453300
O	-1.94023100	1.78061500	-1.28417100
C	-1.13517600	2.93923100	-1.18056800
H	-0.06839900	2.70655000	-1.29201600
H	-1.43880600	3.65681700	-1.95319200
C	-1.34490700	3.58490400	0.18288600
Cl	-3.07392900	3.92370100	0.46158300
Cl	-0.42096000	5.12479900	0.17578600
Cl	-0.72383400	2.51683800	1.46101100
C	-1.61107700	-0.78319300	0.47332100
C	-2.56621100	-1.81694400	-0.01120900
H	-2.12273400	0.11062500	0.85809900
H	-0.98429000	-1.17101500	1.28949300
C	-1.98708000	-3.10192100	-0.48614000
C	-4.03954500	-1.59326600	-0.14423700
H	-1.57878500	-3.70474500	0.34150800
H	-1.14009500	-2.92326200	-1.16565300
H	-2.72663200	-3.71450500	-1.01448500
C	-4.83465400	-2.58853000	0.71650300
C	-4.53146600	-0.18184500	0.16051100
H	-4.30430700	-1.79902500	-1.19887500
H	-4.62409300	-2.38690500	1.78068700

## ARTICLE

## Journal Name

H	-4.54158200	-3.62902500	0.53463400
C	-6.33194100	-2.47391600	0.51104100
C	-6.01851200	-0.08558600	0.08824900
H	-4.20641000	0.12853600	1.17116400
H	-4.07425200	0.54416200	-0.52492800
C	-6.86441300	-1.12850500	0.21278700
O	-7.07089900	-3.44267700	0.62874200
H	-6.43673500	0.91040300	-0.07806800
C	-8.34815100	-1.01094100	0.09887100
H	-8.84250700	-1.36907400	1.01007800
H	-8.65827200	0.02224000	-0.08893500
H	-8.72924900	-1.64234400	-0.71283500
C	3.15151300	3.39927100	-0.72335800
H	4.20581200	3.67994400	-0.69951100
H	2.71852900	3.63918000	-1.69946000
H	2.60432900	3.98504100	0.02434300
C	3.48158800	-1.73285200	-3.68754200
H	3.38821600	-0.85010900	-4.32928700
H	4.49978800	-2.11976200	-3.75992000
H	2.76406500	-2.47215900	-4.05275200
C	1.68881800	0.63118300	4.04742100
H	1.80072800	1.72191300	4.06298100
H	0.65541000	0.39769900	4.31399100
H	2.38082700	0.21345200	4.78185200
C	1.93654700	-4.55545200	1.25215100
H	1.16530100	-4.60590300	2.02739800
H	1.55884100	-5.11438200	0.38962200
H	2.85627400	-5.01705300	1.61533700

O-<sup>3</sup>IM<sub>1</sub>

Rh	-0.21107800	-3.06074400	-0.09645500
Rh	0.03831700	-0.69501700	0.17488100
O	-1.79814600	-2.99287700	1.21396200
C	-2.14211300	-1.87657000	1.70798200
O	-1.54442200	-0.76331600	1.51588900
O	1.11533000	-3.35559100	1.45491900
C	1.61141000	-2.33586100	2.02503700
O	1.34569900	-1.12294200	1.74333600
O	1.61048300	-0.79792000	-1.17758700
C	1.95383000	-1.93156800	-1.64665000
O	1.38005400	-3.03898600	-1.41077300
O	-1.52821700	-2.68831900	-1.61981400
C	-1.84836500	-1.48602200	-1.88016500
O	-1.35200100	-0.45132300	-1.32754500
C	3.16517000	-1.94886000	-2.52675000
C	2.62629900	-2.56576300	3.10246100
C	-2.92367900	-1.26756000	-2.89139000
C	-3.36926400	-1.84223800	2.56000200
H	3.58273400	2.81067700	-1.94489100
C	3.14925200	2.17585300	-1.16197600
H	2.73392200	1.26900500	-1.61729500
O	2.16541700	2.91250800	-0.46477700
C	4.26757000	1.76741100	-0.21030100
S	0.57145200	2.45505700	-0.69830100
Cl	4.99779000	3.19499400	0.56229500
Cl	5.50973200	0.93575600	-1.21773700
Cl	3.64817400	0.65323500	1.02367000
O	-0.13085500	3.68199300	-0.36788400
O	0.49114400	1.84250100	-2.00927400
N	0.29326100	1.32216700	0.43172500
H	0.16820200	1.74046900	1.35971700
C	-1.70599700	2.30638900	2.91333700
C	-2.30945900	3.17688600	2.00531400
H	-1.23998500	2.69130200	3.81910000
H	-1.69809500	1.22802400	2.76229100
C	-2.95094500	2.58622100	0.75938500
C	-2.29348100	4.54031300	2.23735600
C	-3.55909300	3.61352600	-0.18718400
C	-4.00421100	1.52572700	1.09628100
H	-2.15285200	2.06776000	0.20455200
H	-2.69820000	5.26542100	1.53803200
H	-1.81659400	4.93832400	3.13110100
C	-4.36708200	2.99969100	-1.27703100
H	-4.22006600	4.29828100	0.37494700
H	-2.77144600	4.25098000	-0.61227800
C	-4.51467500	0.84438800	-0.15127900
H	-4.85943200	2.00912700	1.59897800
H	-3.61273100	0.76804900	1.77969000
C	-4.81839900	1.72857000	-1.29437400
H	-4.61843600	3.64958800	-2.11937000
O	-4.70704400	-0.36947800	-0.20553100
C	-5.64866500	1.17245700	-2.40499900
H	-6.58172000	0.74210900	-2.02086700

H	-5.89916300	1.94548700	-3.13892400
H	-5.13887000	0.35948500	-2.93290000
H	-3.88306500	-1.29914800	-2.35931200
H	-2.91275900	-2.06267600	-3.64032800
H	-2.81970700	-0.28699700	-3.36233700
H	3.17220200	-2.84033400	-3.15713000
H	4.06106800	-1.96276700	-1.89468200
H	3.21110900	-1.04506500	-3.14005400
H	2.43851100	-3.51267400	3.61367500
H	3.62134700	-2.62092100	2.64510300
H	2.63095500	-1.73721100	3.81433700
H	-4.20280800	-1.52717300	1.91815200
H	-3.26467400	-1.10962500	3.36554000
H	-3.58626600	-2.83203700	2.96715900

**O<sup>-3</sup>TS<sub>A-s</sub>**

Rh	-0.38892700	-3.15235600	0.31661300
Rh	-0.13412300	-0.76024200	-0.17319200
O	1.61926600	-3.40596500	-0.10490600
C	2.30910400	-2.39146100	-0.43526200
O	1.87730800	-1.20252900	-0.56280400
O	-0.85238400	-3.42295100	-1.67831400
C	-0.89439600	-2.41409000	-2.45272100
O	-0.66929800	-1.20652700	-2.12817900
O	-2.18423100	-0.58740200	0.29125600
C	-2.84208100	-1.61920900	0.64305500
O	-2.38508500	-2.79928800	0.73353900
O	0.10539800	-2.73138600	2.28975000
C	0.35848200	-1.53352900	2.62036800
O	0.30954300	-0.51653000	1.85362100
O	0.54890300	3.29493700	-2.36451800
S	1.03383800	2.07408800	-1.74643600
O	1.32226900	0.90525800	-2.55268700
N	0.08921400	1.56299000	-0.48354100
C	3.53951500	1.66035600	-0.99495400
H	3.20575700	0.64263700	-1.23372900
O	2.47513100	2.58952400	-1.04348400
H	4.31467400	1.97106800	-1.70709800
C	4.15841600	1.65301000	0.39828800
Cl	4.64726100	3.30068000	0.87887600
Cl	5.60738600	0.59825300	0.32001200
Cl	3.00627500	0.99786300	1.58746200
C	-4.34618500	1.73087600	-1.09574000
C	-2.93443500	2.20117900	-1.13157700
C	-5.20697600	1.94142300	-0.07896800
H	-4.68600100	1.15165000	-1.95877100
C	-2.41254400	2.54458600	0.27119500
H	-2.84557000	3.07466200	-1.80105000
H	-2.29146200	1.42709000	-1.57062500
C	-4.79141600	2.76208600	1.07595600
C	-6.59381200	1.39018600	-0.03999400
C	-1.05815100	3.16543800	0.25389000
C	-3.43717100	3.44162000	0.98219800
H	-2.35147100	1.59351100	0.81728300
O	-5.51785900	2.92148100	2.04746100
H	-7.33747300	2.19013400	0.05658900
H	-6.82133300	0.80716200	-0.93889700
H	-6.73576800	0.74754100	0.83815200
H	-3.56946100	4.37828400	0.41604100
H	-3.12145900	3.72138400	1.99411600
C	0.08625200	2.39613100	0.74611500
H	1.00741400	2.96865300	0.90383300
H	-0.09826700	1.73599200	1.59990700
C	-0.88174000	4.53598100	-0.27070500
H	-1.39592800	4.70692200	-1.22425300
H	-1.32785100	5.23207700	0.46012300
H	0.16809400	4.80818000	-0.39400000
C	3.77479600	-2.60204900	-0.67142500
H	3.99816600	-3.65998400	-0.82227300
H	4.11260800	-2.01575200	-1.53090100
H	4.33135700	-2.24547100	0.20337000
C	-1.24344400	-2.68140200	-3.88665600
H	-0.52567500	-3.38994700	-4.31152700
H	-2.23005600	-3.15190200	-3.94642500
H	-1.23594300	-1.75871400	-4.46904100
C	-4.29415100	-1.41458300	0.96331100
H	-4.84471000	-1.19903200	0.04019100
H	-4.71870100	-2.30397800	1.43276000
H	-4.41995900	-0.54538300	1.61759700
C	0.78329700	-1.29353100	4.03876700
H	0.20071800	-1.91602900	4.72261800
H	1.83469200	-1.58372600	4.14816800
H	0.68743600	-0.23905900	4.30698400

**O<sup>-3</sup>TS<sub>2A,R</sub>**

Rh	-3.70752400	-0.67676800	-0.58411100
Rh	-1.42981000	-0.52429800	0.32307800
O	-3.24404600	-2.52087500	-1.40334500
C	-2.05264300	-2.94550200	-1.30791400
O	-1.08760100	-2.34018500	-0.74180300
O	-3.02634100	0.28090200	-2.30287100
C	-1.83970300	0.72281200	-2.32491000
O	-0.95855700	0.56600700	-1.41477100
O	-2.06753000	1.27555700	1.20057200
C	-3.22497300	1.73575200	0.95428600
O	-4.11585700	1.16685100	0.24912000
O	-4.23012700	-1.60733800	1.18921800
C	-3.33021200	-1.86509500	2.04973100
O	-2.08869100	-1.60192800	1.94908400
C	-1.74905000	-4.28896700	-1.90524900
C	-1.40739700	1.50658700	-3.52915300
C	-3.77377200	-2.52725000	3.31959500
C	-3.57032900	3.07528400	1.53380000
O	2.81659100	-0.20575000	2.29896200
S	1.53113300	0.18318800	1.74786200
O	0.38147700	0.37159800	2.61535900
N	0.98020600	-0.75627300	0.51767400
C	0.75260400	2.39562800	0.65856200
H	0.07581700	1.76906400	0.06592800
O	1.90259900	1.67387000	1.06660700
H	0.20524600	2.78452500	1.52601500
C	1.18517300	3.55676500	-0.21352700
C	2.06841700	-3.16602900	-0.42162200
H	2.39613300	-3.67410800	-1.34393100
H	0.97542000	-3.18272100	-0.39618000
H	-4.58489400	-3.23214100	3.12173000
H	-2.93679400	-3.02939600	3.80864000
H	-2.76696200	3.44359900	2.17497700
H	-4.50159200	3.00633900	2.10422000
H	-2.18786800	1.51519000	-4.29181600
H	-1.17437000	2.53549700	-3.23233400
H	-2.58112500	-4.64344300	-2.51601400
H	-1.56446900	-5.00959700	-1.10066400
Cl	2.25902300	4.66442000	0.66761900
Cl	-0.31457600	4.41745900	-0.69760800
Cl	2.02354600	2.96463600	-1.68437800
C	2.57766600	-1.77527700	-0.42412200
C	1.64979300	-0.70430100	-0.79975500
H	2.09411900	0.26453000	-1.05203900
H	0.90675000	-0.98119500	-1.55422200
C	3.99605900	-1.52217400	-0.03682400
C	4.92168600	-2.55201400	-0.71237600
C	4.51610500	-0.11786900	-0.33913400
H	4.07846200	-1.68216700	1.05209400
H	4.86303500	-2.43743200	-1.80778600
H	4.63881700	-3.58550100	-0.49036400
C	5.97110400	0.00935600	-0.03954200
H	4.34394300	0.12444100	-1.40387800
H	3.95914900	0.63875000	0.22577900
C	6.84046100	-1.01939000	0.01526500
H	6.34267700	1.01953900	0.14501200
H	2.46770500	-3.75323600	0.41464600
C	6.37808000	-2.38008700	-0.30988700
O	7.13646100	-3.33910700	-0.31042600
C	8.28687900	-0.86689100	0.34887800
H	8.91956200	-1.24193300	-0.46446200
H	8.54638900	0.17818100	0.54510900
H	8.55030400	-1.46233000	1.23100800
H	-3.74299700	3.78957200	0.72182200
H	-4.15854400	-1.76222600	4.00339200
H	-0.83643500	-4.23881600	-2.50733000
H	-0.48558300	1.08228300	-3.94041800

**O<sup>-3</sup>TS<sub>2</sub>**

Rh	3.79096300	-1.05158300	0.35531700
Rh	1.46391400	-0.65896700	-0.22403100
O	4.12511100	-1.53203800	-1.62047800
C	3.16415100	-1.51193200	-2.45310600
O	1.96040100	-1.21453100	-2.17659400
O	3.25546100	-3.02155400	0.74546800
C	2.05067300	-3.38710300	0.58666800
O	1.07824800	-2.65401000	0.20916400
O	1.19392300	-0.12082600	1.82083900
C	2.17883900	-0.18690200	2.61836900
O	3.36020200	-0.53955200	2.30469200
O	4.17893100	0.93681300	-0.06892100

C	3.21235300	1.67178500	-0.44056700
O	2.00379500	1.30757400	-0.60670400
C	3.48396500	-1.83816700	-3.87939000
C	1.74125500	-4.83157500	0.84755100
C	3.50582800	3.12181200	-0.69066100
C	1.92623300	0.15519000	4.05641900
O	-2.75278300	0.70908900	-1.45988000
S	-1.32599400	0.87647900	-1.22711800
O	-0.49192700	1.46235300	-2.26673300
N	-0.68702400	-0.48902200	-0.55430500
C	-0.40086600	2.98975700	0.06720100
H	0.25484600	3.00865100	0.94635900
O	-1.17107100	1.81471200	0.14097000
H	0.21080000	3.01154200	-0.84121100
C	-1.29225600	4.22975400	0.10357000
Cl	-2.35844300	4.27495700	-1.31203900
Cl	-0.19772000	5.65303900	0.10002000
Cl	-2.27626200	4.24526200	1.59679400
H	0.67307900	-4.97944200	1.01904500
H	2.31967800	-5.19516300	1.70049600
H	3.86004600	-0.93548300	-4.37408300
H	4.26868500	-2.59651500	-3.93232000
H	1.52490300	-0.72650200	4.56926500
H	1.18084200	0.95046700	4.13654300
H	2.93637300	3.48403200	-1.55107800
H	4.57483200	3.27937500	-0.84701100
C	-6.50159700	-1.22775700	-0.71609500
C	-5.49261900	-0.41994200	0.02931800
C	-6.62634100	-2.56768200	-0.62614200
H	-7.18208700	-0.68195300	-1.37424500
C	-4.29725500	-1.26529400	0.44536300
H	-5.98047800	0.01402200	0.92051400
H	-5.15604100	0.43429400	-0.57262500
C	-5.76815700	-3.32623600	0.30799100
C	-7.62566600	-3.35950000	-1.40231500
C	-3.25513200	-0.53337000	1.26199100
C	-4.79750800	-2.52598800	1.15475100
H	-3.80111700	-1.58385100	-0.48641700
O	-5.86467800	-4.54122100	0.42153600
H	-8.28318200	-3.92693900	-0.73289100
H	-8.24143000	-2.71769200	-2.04075900
H	-7.12917800	-4.10639100	-2.03361300
C	-3.49808100	0.65271900	1.90208500
H	-5.31818400	-2.23360400	2.08242900
H	-3.97979100	-3.19002300	1.46049800
H	-4.45324000	1.16964500	1.85139700
H	-2.70880100	1.14549900	2.46468600
C	-1.97394100	-1.10484800	1.34287900
H	-0.98058800	-1.26443000	-1.16072100
H	-1.18227700	-0.63760500	1.92239700
H	-1.78357100	-2.11883200	0.99736500
H	2.59071700	-2.16985300	-4.41235300
H	2.03618900	-5.42453100	-0.02543100
H	2.85249400	0.44713600	4.55560400
H	3.19513400	3.71024100	0.18098100

**O-<sup>1</sup>PC<sub>A-S</sub>**

Rh	0.98100200	-2.97277900	-0.29552900
Rh	0.45810200	-0.67499900	0.15917600
O	-0.96815100	-3.46260200	0.17443300
C	-1.79883000	-2.52147400	0.35073000
O	-1.53710800	-1.27539800	0.33816600
O	1.51531300	-3.17676800	1.69124200
C	1.34325400	-2.18712000	2.47015900
O	0.89850200	-1.03879400	2.15055300
O	2.50506400	-0.30723500	-0.10313500
C	3.25722900	-1.23318900	-0.54890200
O	2.91764800	-2.43554100	-0.76385700
O	0.40708900	-2.66252700	-2.26608800
C	0.09760500	-1.48779200	-2.62636200
O	0.10124500	-0.44742700	-1.88782600
O	-1.29219900	2.96263600	2.61706300
S	-1.51655100	1.77158600	1.83033100
O	-1.57849500	0.47298600	2.45325900
N	-0.37052800	1.68633000	0.53753600
C	-3.84159700	0.94923300	0.89763200
H	-3.32394700	-0.01092100	1.01014400
O	-2.93108100	2.04073800	1.01435600
H	-4.62110100	1.05746800	1.66103400
C	-4.50385700	0.99282500	-0.47397000
Cl	-5.19402700	2.60684100	-0.78552400
Cl	-5.81548000	-0.22791900	-0.44278100
Cl	-3.33684300	0.58185200	-1.75652000

## ARTICLE

## Journal Name

C	3.99099600	2.25166200	1.01019100
C	2.51905800	2.39884100	1.18237500
C	4.68709700	2.67677400	-0.06361200
H	4.53032200	1.75288300	1.82019800
C	1.81354600	2.65468600	-0.14713200
H	2.31471300	3.22076600	1.89253100
H	2.10892900	1.49220300	1.65008500
C	3.99621500	3.39640700	-1.15420700
C	6.15733900	2.47518000	-0.22848400
C	0.33880900	2.94144800	0.05498200
C	2.53883300	3.74979700	-0.92327400
H	1.89262900	1.72740100	-0.73032500
O	4.58627600	3.73469000	-2.17140900
H	6.67579400	3.43341400	-0.35343100
H	6.59181500	1.95156600	0.63013100
H	6.37759500	1.89966200	-1.13627100
H	2.52413200	4.69369200	-0.35348800
H	2.07238900	3.95892600	-1.89402200
C	-0.66801100	2.28181800	-0.78838300
H	-1.63262300	2.77694000	-0.88933900
H	-0.39262900	1.62412800	-1.61108800
C	-0.01164700	4.30907600	0.58345900
H	0.46543400	4.53004800	1.54272800
H	0.33597400	5.04455100	-0.15178300
H	-1.08720600	4.44711500	0.70802000
C	-3.23101100	-2.90015100	0.59069600
H	-3.34216900	-3.98396900	0.65521300
H	-3.59187900	-2.43865200	1.51685500
H	-3.85667900	-2.52277000	-0.22670500
C	1.66689400	-2.39977700	3.91988700
H	2.00248400	-1.46816900	4.38158000
H	0.76018300	-2.72178600	4.44454900
H	2.42110700	-3.18109600	4.03723900
C	4.67599900	-0.84839000	-0.85091000
H	5.13925600	-0.40524600	0.03698800
H	5.25453800	-1.71340600	-1.17993900
H	4.69071100	-0.07721800	-1.62961600
C	-0.34426400	-1.30637500	-4.04896300
H	0.24139700	-1.94326300	-4.71652200
H	-1.39258600	-1.61511900	-4.13834000
H	-0.26653800	-0.26094200	-4.35612300

O-<sup>1</sup>PC<sub>A-R</sub>

Rh	-1.50392300	-0.54297700	0.10975700
Rh	-3.83815500	-0.13795300	-0.24378400
O	-1.33334500	-0.74525300	-1.97818900
C	-2.40342200	-0.80208400	-2.67125600
O	-3.58236400	-0.64794400	-2.23703500
O	-1.98101600	-2.56577800	0.27977300
C	-3.20969500	-2.89136600	0.35424100
O	-4.20564100	-2.11486900	0.22171600
O	-4.02251300	0.35702200	1.74931800
C	-3.04234300	0.06471800	2.50622800
O	-1.92115300	-0.40414100	2.13795400
O	-1.17909200	1.50328600	-0.12811200
C	-2.16193400	2.22450300	-0.50647100
O	-3.35309900	1.83371300	-0.68674700
O	2.61162200	-0.40683100	2.30288800
S	1.59467300	0.33126000	1.58796500
O	0.45548100	0.89833600	2.26518200
N	1.00868600	-0.60696200	0.26247100
O	2.39148800	1.58323900	0.84643300
C	1.70472000	2.83561600	0.83469200
H	0.63880200	2.69950400	0.61103900
H	1.82321600	3.33204400	1.80489800
C	2.34188500	3.70505100	-0.23736000
Cl	4.10281200	3.81662500	0.00491500
Cl	1.60370000	5.32604700	-0.09847000
Cl	2.01097300	3.03335800	-1.86230800
C	1.53316400	-0.36606700	-1.10205800
C	1.85269500	-1.65543900	-0.46370700
H	2.32180500	0.37710800	-1.17584400
H	0.74697100	-0.29332400	-1.85182500
C	0.98927100	-2.83899100	-0.81277800
C	3.29371400	-1.98682300	-0.04115200
H	1.39173300	-3.34789800	-1.69548200
H	-0.02903500	-2.52396000	-1.04369000
H	0.94520100	-3.56057400	0.01107400
C	3.82114600	-3.21572000	-0.79051900
C	4.31121100	-0.85941400	-0.23203100
H	3.27608900	-2.24468500	1.02639400
H	3.85575700	-3.00836000	-1.87403100
H	3.18663700	-4.09705500	-0.66434200



C	5.21935500	-3.62515300	-0.35977900
C	5.69566900	-1.28916700	0.12510800
H	4.30168600	-0.53002500	-1.28687600
H	4.05841300	0.02950400	0.35393300
C	6.13075000	-2.56342900	0.10429300
O	5.58053100	-4.79122900	-0.44081400
H	6.39156200	-0.49865700	0.41504200
C	7.51158900	-2.97906000	0.48630600
H	8.00791700	-3.50066200	-0.34052500
H	8.12383000	-2.12071400	0.78090600
H	7.48950900	-3.69340400	1.31800700
C	-1.86377800	3.67713700	-0.74209200
H	-2.71677900	4.18346300	-1.19759500
H	-1.63323300	4.16316600	0.21345700
H	-0.98056500	3.78645200	-1.38111000
C	-3.21300700	0.29119500	3.97922300
H	-2.42091300	0.95382400	4.34253400
H	-4.19192600	0.72116800	4.19931400
H	-3.10225900	-0.65859700	4.51256900
C	-3.50010200	-4.33472500	0.64512200
H	-3.27943000	-4.54307300	1.69795500
H	-4.54838800	-4.56910900	0.45087300
H	-2.85101100	-4.98004300	0.04658700
C	-2.23465700	-1.07051000	-4.13840000
H	-3.20320300	-1.20049700	-4.62423900
H	-1.70739800	-0.23306000	-4.60799900
H	-1.61885500	-1.96267400	-4.28944800

**O-<sup>1</sup>PC<sub>i</sub>**

Rh	-1.41862400	-3.05461600	-0.36209000
Rh	-0.45644300	-0.92835700	0.17041000
O	-3.11017800	-2.52134800	0.69956400
C	-3.13392400	-1.38059900	1.25485700
O	-2.20554600	-0.50961000	1.23460400
O	-0.55546500	-3.79347300	1.37002000
C	0.17269900	-3.02379900	2.06915200
O	0.40835900	-1.79119700	1.84156200
O	1.23459000	-1.48297100	-0.89943400
C	1.27435400	-2.65137400	-1.42166400
O	0.34218800	-3.50477300	-1.38409400
O	-2.24087900	-2.17340100	-2.06077400
C	-2.04994500	-0.93808500	-2.26526500
O	-1.34608800	-0.15165600	-1.54446200
C	-4.39122900	-1.00438900	1.98318300
C	0.84397000	-3.61988500	3.27063600
C	-2.71839800	-0.31843400	-3.45731100
C	2.53967500	-3.00112400	-2.14471500
O	1.60616100	3.08041700	1.91999200
S	0.50054400	2.17816200	1.69825800
O	-0.13355800	1.44106000	2.76559600
N	0.86569800	1.01988500	0.47239600
C	-1.85440500	2.41305600	0.66309000
H	-1.72767000	1.48018200	0.10275900
O	-0.59113000	3.05964200	0.87580700
H	-2.33645400	2.19653600	1.62211700
C	-2.72530400	3.34357400	-0.15645800
Cl	-2.96976500	4.89640400	0.66761700
Cl	-4.29029700	2.49591700	-0.35751200
Cl	-1.99095000	3.62515400	-1.76305200
H	1.87549100	-3.88473500	3.01172600
H	0.32760500	-4.52685400	3.59112200
H	-5.09281400	-0.54671600	1.27596300
H	-4.87199800	-1.89139000	2.40242200
H	2.56822300	-4.06515700	-2.38659800
H	3.41515300	-2.71900000	-1.54697900
H	-2.01567800	0.32426100	-3.99564900
H	-3.54249900	0.32119400	-3.12017200
C	6.17746100	1.92535100	0.15501400
C	4.97059500	2.65786700	-0.32795100
C	6.31652600	0.58339700	0.15224000
H	7.00202900	2.53362800	0.53479900
C	3.73281300	1.77280200	-0.32765200
H	5.15995400	3.03611600	-1.34829400
H	4.79755300	3.55220400	0.28676400
C	5.25082500	-0.26028400	-0.42519500
C	7.52245000	-0.12252200	0.67645500
C	2.49414600	2.42147400	-0.89025900
C	4.05521600	0.44656100	-1.02607700
H	3.52741400	1.54040700	0.73403700
O	5.34825300	-1.48240300	-0.45444400
H	7.98514500	-0.74327100	-0.09983400
H	8.26913100	0.58285700	1.05509800
H	7.25206000	-0.81085600	1.48618100

## ARTICLE

## Journal Name

C	2.45791100	3.64071400	-1.43290700
H	4.27943000	0.64771500	-2.08760600
H	3.21268900	-0.25543700	-1.01722700
H	3.33932700	4.27175800	-1.52019600
H	1.52539600	4.06379300	-1.80297400
C	1.24163900	1.59024200	-0.85595600
H	1.62876900	0.45099700	0.85460200
H	0.37528200	2.15406300	-1.21127300
H	1.32767000	0.70630300	-1.49902200
H	0.88502000	-2.89339100	4.08610200
H	-4.18179000	-0.27537000	2.76974100
H	2.59186600	-2.42672500	-3.07749700
H	-3.11578200	-1.08575600	-4.12413700