

## Supporting Information

### **Theoretical Characterization of First and Second Generation Grubbs Catalysts in Styrene Cross-Metathesis Reactions: Insights From Conceptual DFT**

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## 2.1 Computed Ru-PR<sub>3</sub> bond strength in 1-2a(b)-PC

The computed ruthenium-phosphane bond strength ( $BE_{PR_3}$ ) in  $[\text{RuCl}_2(=\text{CHPh})(\text{L})(\text{PR}_3)]$  ( $\text{L}=\text{PR}_3$  or  $\text{NCH}$ ) **1-2a(b)-PC** can be done from the ground state total energy of the fully optimized species as :

$$BE_{PR_3} = E(16e - PC) - [E(14e \text{ Inact} - C) + E(PR_3)] \quad (1)$$

The reverse defines the Ru-PR<sub>3</sub> bond dissociation energy ( $BDE$ ). Either  $BDE$  or  $BE_{PR_3}$  can be divided into two hypothetical steps displayed in Scheme 1 of main text, which is also known as distortion/interaction model by Houk<sup>30</sup> or activation strain model by Bickelhaupt.<sup>31</sup>

While the first step involves the distortion (here also called as reorganization) of both isolated fragments on bringing to the complex geometry ( $\Delta E_{reorg}$ ), which is computed as the energy change between the structure of the fragment in the complex and that fully optimized in absence of the other fragment; the second step allows the interaction ( $\Delta E_{int}$ ) between the distorted fragments. This thus leads to write the bond strength in terms of the following contributions:<sup>32</sup>

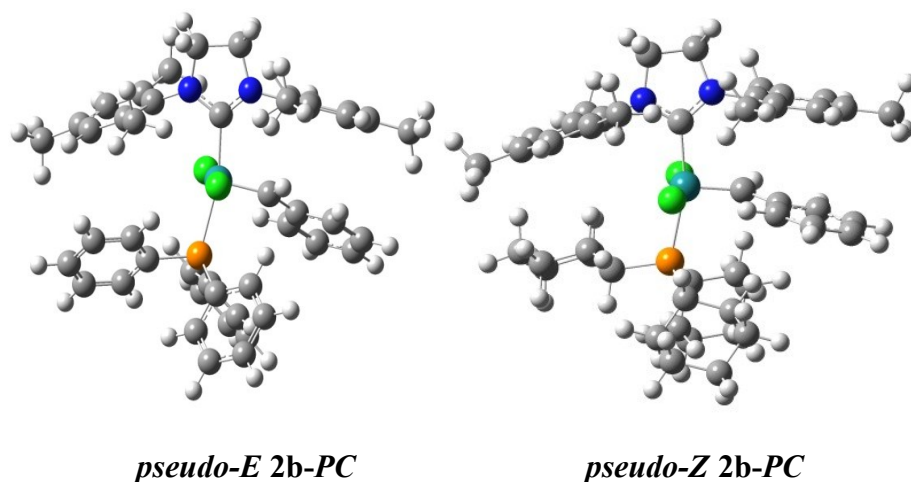
$$BE_{PR_3} = \Delta E_{reorg}(14e) + \Delta E_{reorg}(PR_3) + \Delta E_{int} = -BDE \quad (2)$$

and the interaction energy as

$$\Delta E_{int} = BE_{PR_3} - \Delta E_{reorg} \quad (3)$$

This analysis has been employed in many types of the chemical processes revealing, for instance, the origins of selectivities in the iridium-catalyzed borylation of aromatic rings

reactions<sup>33</sup> and the difference of the initiation rates among a series of ruthenium-based catalysts encompassing chelated benzylidene classified as Hoveyda-type catalysts.<sup>34</sup> One of current authors has also applied this model to approximate to sulfur-induced copper corrosion through the dibenzyl disulfide adsorption on Cu<sub>7</sub> cluster.<sup>35</sup>



**Figure S1.** Isomers for the 16e- precatalysts **2b-PC**

**Table S1.** Absolute difference energy between the conformers *pseudo-E* and *pseudo-Z* for the precatalysts **2b-PC**. Values are in kcal/mol.

Functional	<i>pseudo-E 2b-PC</i>	<i>pseudo-Z 2b-PC</i>	$\Delta E_{E-Z}$
<b>BP86</b>	-2044779.2	-2044784.0	4.8
<b>PBE</b>	-2042763.2	-2042768.3	5.1
<b>PBE0</b>	-2042983.5	-2042988.8	5.3
<b>TPSS</b>	-2044926.8	-2044931.4	4.6
<b>M06L</b>	-2044579.8	-2044584.0	4.2
<b>MPWB1K</b>	-2044108.6	-2044114.5	5.9

**Table S2.** Energy contributions in terms of the DFT-Reactivity descriptors.

( $\Delta\Lambda_{reorg}^{14}$ ,  $\Lambda=\mu, \eta, \omega$ ). Values are in kcal/mol.

$\Delta\Lambda_{reorg}^{14}$	$\Delta E_{reorg}^{14}$	$\Delta\mu$	$\Delta\eta$	$\Delta\omega$
<b>1a</b>	16.4	-5.0	-7.8	16.8
<b>2a</b>	13.0	-3.7	-8.7	13.6
<b>1b</b>	20.8	-8.4	-13.0	27.0
<b>2b</b>	14.4	-5.9	-9.6	18.3

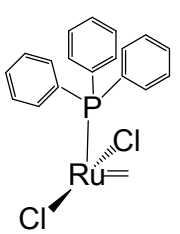
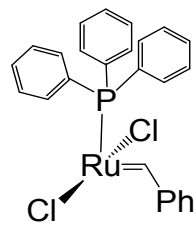
**Table S3.** Energies contributions in terms of the DFT-Reactivity descriptors.

( $\Delta\Lambda_{int}$ ,  $\Lambda=\mu, \eta, \omega$ ). Values are in kcal/mol.

$\Delta\Lambda_{int}$	$\Delta E_{int}$	$\Delta\mu$	$\Delta\eta$	$\Delta\omega$
<b>1a</b>	-43.3	4.2	-13.3	5.6
<b>2a</b>	-42.9	4.5	-15.1	6.3
<b>1b</b>	-57.1	-6.4	-31.7	24.8
<b>2b</b>	-55.7	-6.1	-30.6	23.0

**Table S4.**  $BE_{olefin}$ ,  $\Delta E_{reorg T-T(14)}$ , and  $\Delta E_{int}$  for the ruthenacyclobutanes **1a-RCB**.

Values are in kcal/mol

Reactants		<b>1a-RCB</b>	$BE_{olefin}$	$\Delta E_{reorg T-T(14)}$	$\Delta E_{int}$
	+ ethene	<b>RCB-0</b>	-11.0	9.0	-140.1
	+ styrene	<b>RCB-1<math>\alpha</math></b>	-10.6	12.2	-134.3
	+ styrene	<b>RCB-1<math>\beta</math></b>	-2.0	12.9	-134.0
	+ <i>cis-stilbene</i>	<b><i>cis</i>-RCB-2<math>\alpha\beta</math></b>	-7.6	15.5	-143.0
	+ <i>trans-stilbene</i>	<b><i>trans</i>-RCB-2<math>\alpha\beta</math></b>	0.3	15.9	-130.6
	+ ethene	<b>RCB-1<math>\alpha</math></b>	-5.8	11.3	-137.0
	+ styrene	<b><i>trans</i>-RCB-2<math>\alpha\alpha</math></b>	-2.9	12.7	-128.3
	+ styrene	<b><i>cis</i>-RCB-2<math>\alpha\alpha</math></b>	-1.5	16.7	-128.8
	+ styrene	<b><i>trans</i>-RCB-2<math>\alpha\beta</math></b>	4.4	10.2	-120.8
	+ styrene	<b><i>cis</i>-RCB-2<math>\alpha\beta</math></b>	3.6	10.4	-120.9
	+ <i>trans-stilbene</i>	<b><i>trans,trans</i>-RCB-3</b>	6.1	18.2	-122.8
	+ <i>trans-stilbene</i>	<b><i>trans,cis</i>-RCB-3</b>	9.0	13.8	-102.2
	+ <i>cis-stilbene</i>	<b><i>cis,cis</i>-RCB-3</b>	8.7	16.4	-125.6

## Coordinate Cartesian

MO6L

1a-PC

Ru	0.00000000	0.00000000	0.00000000
Cl	0.00000000	0.00000000	2.41495696
Cl	0.97279794	0.00000000	-2.21986197
P	-0.04825118	2.41611979	-0.01089821
P	0.51349239	-2.31124994	0.11640736
C	-1.73687087	-0.31527554	-0.54472070
H	-1.85782051	-1.05066999	-1.36315665
C	-5.47552197	1.37393912	0.59293035
C	-5.29455441	0.84352196	-0.68651127
C	-4.07439785	0.28110174	-1.03562093
C	-2.99411824	0.27831428	-0.12810951
C	-3.19376534	0.81807389	1.15748322
C	-4.42857677	1.34517017	1.51427322
H	-6.43503671	1.80128526	0.87240126
H	-6.11104715	0.85720457	-1.40341886
H	-3.93220667	-0.15409838	-2.02341725
H	-2.37140372	0.79577131	1.86881536
H	-4.56915892	1.75100075	2.51273936
C	-0.58488759	-3.41412945	1.07182535
C	-0.34948684	-4.79741615	1.08430840
C	-1.69113300	-2.90318717	1.75718778
C	-1.19785356	-5.64970136	1.78305700
H	0.49809612	-5.20578288	0.53639690
C	-2.54465820	-3.76155554	2.44892178
H	-1.87371674	-1.83222321	1.75939285
C	-2.29865088	-5.13157316	2.46593904
H	-1.00452261	-6.71894803	1.78827583
H	-3.40275057	-3.35360650	2.97587079
H	-2.96443220	-5.79829223	3.00733400
C	0.66041857	-3.21639605	-1.46446078
C	1.88588499	-3.44272485	-2.09588457
C	-0.51955431	-3.62066912	-2.10439926
C	1.93219913	-4.06907169	-3.33888455
H	2.81153895	-3.13445230	-1.61833721
C	-0.47090704	-4.24197812	-3.34792060
H	-1.48177865	-3.46164731	-1.61958293
C	0.75646989	-4.46712522	-3.96940023

H	2.89299901	-4.24134613	-3.81605310
H	-1.39360413	-4.55253693	-3.83083146
H	0.79444530	-4.95199616	-4.94108047
C	2.15535043	-2.38868954	0.90800234
C	3.17055998	-1.58105908	0.37026384
C	2.40065493	-3.09931464	2.08680717
C	4.41530781	-1.51356481	0.98720440
H	2.97611885	-1.00241792	-0.53358118
C	3.64745414	-3.02267283	2.70359503
H	1.61220883	-3.69735529	2.53583049
C	4.65689170	-2.23524955	2.15503343
H	5.19347489	-0.88607299	0.56070695
H	3.82597066	-3.57513898	3.62196166
H	5.62600282	-2.17438851	2.64273942
C	1.62304997	3.00816929	0.45666017
C	2.72036241	2.32837112	-0.09205451
C	1.85364494	4.09586064	1.30670439
C	4.01891721	2.72716982	0.20879118
H	2.55209972	1.50045202	-0.78020927
C	3.15644809	4.48820737	1.60870761
H	1.01628397	4.64141365	1.73407759
C	4.24113527	3.80437709	1.06388073
H	4.85874034	2.19340381	-0.22807179
H	3.32183888	5.33361455	2.27131617
H	5.25538021	4.11137786	1.30417567
C	-0.34908753	3.21592380	-1.62899695
C	0.13724144	4.50245560	-1.89114331
C	-1.12719874	2.56908901	-2.59368015
C	-0.15768753	5.13437538	-3.09569695
H	0.75085522	5.00964078	-1.14870351
C	-1.42792657	3.20625397	-3.79493606
H	-1.47967902	1.55704824	-2.41069110
C	-0.94453045	4.48796301	-4.04792199
H	0.22851809	6.13119445	-3.29110336
H	-2.02972277	2.69245629	-4.53952167
H	-1.17356569	4.98050710	-4.98919506
C	-1.19174099	3.31383230	1.09592390
C	-2.28878181	4.01951572	0.58423062
C	-1.03682845	3.21516129	2.48860688
C	-3.20295845	4.62469891	1.44333667
H	-2.43860932	4.09172917	-0.49031338

C	-1.95314192	3.82295035	3.34154932	H	1.66650200	6.15824200	-0.78705800
H	-0.20733731	2.64666958	2.89989062	C	1.78031500	4.22787300	-1.76789000
C	-3.03772254	4.53025065	2.82271574	H	2.80405500	4.40520500	-2.13167200
H	-4.04990077	5.16539521	1.02912771	H	1.10990200	4.50203300	-2.59206800
H	-1.81821943	3.74015851	4.41670445	C	1.61839900	2.75006000	-1.43629000
H	-3.75146375	5.00298530	3.49229118	H	1.80428600	2.12007900	-2.31559600
				H	0.56425600	2.55754300	-1.16715800
				C	3.26380800	-0.26471900	-1.37964000
				H	2.49156900	-0.31948000	-2.16419900
				C	4.45365000	0.50395700	-1.96529300
				H	5.25002800	0.60680000	-1.21309600
				H	4.16149000	1.52102900	-2.25150300
				C	4.99924000	-0.22108600	-3.19516100
				H	4.22854300	-0.20745700	-3.97945700
				H	5.86074600	0.32420400	-3.59827500
				C	5.37192900	-1.66678800	-2.89003200
				H	5.73332400	-2.16754300	-3.79564400
				H	6.20676800	-1.68185600	-2.17313500
				C	4.18973500	-2.41899600	-2.29116700
				H	4.46617200	-3.45133200	-2.04617500
				H	3.37874800	-2.47993800	-3.03255700
				C	3.67194300	-1.70403800	-1.04922200
				H	2.83138900	-2.25266900	-0.60818400
				H	4.46752700	-1.69113400	-0.28931300
				C	-3.29079700	-0.77430500	-1.30344200
				H	-2.87601600	-0.36147400	-2.23613700
				C	-2.88524400	-2.25009900	-1.30022200
				H	-3.22954500	-2.74519800	-0.38168700
				H	-1.79444800	-2.32245800	-1.31223100
				C	-3.47564800	-2.96395600	-2.51153100
				H	-3.02797800	-2.53938800	-3.42244100
				H	-3.19541700	-4.02381500	-2.49501100
				C	-4.99176900	-2.80844300	-2.57024100
				H	-5.39741300	-3.30567500	-3.45906600
				H	-5.44085800	-3.31445100	-1.70190800
				C	-5.39682600	-1.33894100	-2.55195800
				H	-5.03013000	-0.84961100	-3.46670400
				H	-6.48853300	-1.23777900	-2.56268500
				C	-4.81313600	-0.61916100	-1.33913400
				H	-5.24452400	-1.05017600	-0.42308000
				H	-5.10322600	0.43999600	-1.34916600
				C	-3.25891000	0.03293100	1.62683400
				H	-2.50726800	0.46520100	2.30503100
				C	-3.40605500	-1.44300800	2.01035900
				H	-4.18608100	-1.90752000	1.38776600
<b>1b-PC</b>							
Ru	-0.03367500	0.00472300	0.07051700				
Cl	-0.08469000	-0.27271700	-2.36589600				
Cl	-0.03636300	0.82538700	2.39989700				
P	2.32578100	0.50439200	0.03068000				
P	-2.42875100	0.24812100	-0.02331500				
C	-0.00834300	-1.70964900	0.75878300				
H	-0.25970700	-1.74463800	1.83552700				
C	3.22337000	0.22911600	1.62871700				
H	2.69176000	0.92869100	2.29254700				
C	4.70608200	0.61331200	1.61127000				
H	4.84650200	1.61165000	1.17542400				
H	5.26323000	-0.08573100	0.96940900				
C	5.28389400	0.56454900	3.02403500				
H	6.34856300	0.82566700	3.00569600				
H	4.78600700	1.33067000	3.63706700				
C	5.07383300	-0.80317900	3.66241900				
H	5.47639400	-0.81436200	4.68192500				
H	5.64421100	-1.55529100	3.09633800				
C	3.59863300	-1.18788500	3.66186600				
H	3.45884800	-2.18211000	4.10182800				
H	3.03700200	-0.48538100	4.29481000				
C	3.01316200	-1.15132900	2.25439500				
H	1.94117900	-1.37103400	2.29027300				
H	3.48349100	-1.93318200	1.64307200				
C	2.50754700	2.33420600	-0.25785200				
H	3.55905600	2.50500200	-0.54012400				
C	2.21681400	3.20799500	0.96499500				
H	2.87009300	2.93766600	1.80318100				
H	1.19017100	3.02629700	1.31412800				
C	2.40379700	4.68334100	0.62386200				
H	2.19100400	5.29873200	1.50533900				
H	3.45838900	4.86647000	0.36627900				
C	1.52043900	5.09913900	-0.54476100				
H	0.46692500	4.99292400	-0.24375200				

H	-2.47805600	-1.99237900	1.80536700	C	-1.60675700	0.21698600	-0.47485300
C	-3.79897500	-1.57540200	3.47742100	H	-1.89548900	-0.02141300	-1.51563600
H	-2.99110600	-1.16336000	4.09941300	C	-2.59280100	1.07387800	0.16198000
H	-3.89691800	-2.63278600	3.75020200	Cl	0.19710100	-0.33036500	2.42968400
C	-5.09596800	-0.82666800	3.75978400	Cl	0.53828000	-0.69017200	-2.39894900
H	-5.36265600	-0.90147600	4.82032100	C	-0.40740600	-2.41221700	0.12520400
H	-5.91494900	-1.30422000	3.20063000	N	0.53764800	-3.35951900	0.32387900
C	-4.98905700	0.63438100	3.34026100	N	-1.60179600	-3.04018800	0.06042700
H	-5.93723100	1.15677100	3.51435000	C	-1.50230900	-4.49228000	0.27248000
H	-4.23729000	1.13504900	3.96761600	H	-1.99682100	-5.03047700	-0.54431000
C	-4.57595800	0.77742700	1.87613100	H	-2.00822400	-4.76917200	1.20691100
H	-4.47815000	1.84192200	1.63438900	C	0.00452400	-4.72586300	0.32394800
H	-5.37223800	0.38092900	1.22990100	H	0.32897600	-5.26188800	1.22319800
C	-2.85767400	1.99208300	-0.50376500	H	0.38081200	-5.27473000	-0.55010200
H	-3.94193400	2.09477400	-0.33466700	C	-2.88402700	-2.43270900	-0.08997500
C	-2.59420700	2.32446200	-1.97453800	C	-3.59241300	-2.02427400	1.04933100
H	-3.13545800	1.63523400	-2.63292900	C	-4.84819900	-1.44173800	0.86440900
H	-1.52805100	2.18136200	-2.20358200	H	-5.39573000	-1.08897700	1.73766600
C	-3.00832900	3.76003800	-2.28223300	C	-5.39855700	-1.26466700	-0.40596100
H	-2.80727600	3.98852200	-3.33514400	C	-4.66643500	-1.69639200	-1.51670700
H	-4.09621600	3.85904000	-2.14676600	H	-5.07773200	-1.55627000	-2.51595300
C	-2.29505600	4.75117200	-1.37278200	C	-3.40942800	-2.28681000	-1.38397100
H	-1.21541500	4.70634900	-1.58205100	C	-2.98938600	-2.15549300	2.41083500
H	-2.60902100	5.77784000	-1.59407100	H	-3.66342500	-1.76658400	3.17802600
C	-2.53250000	4.42194800	0.09650900	H	-2.03918600	-1.60935100	2.47975700
H	-3.59858900	4.56164200	0.33320200	H	-2.76499700	-3.19919700	2.66271600
H	-1.98097700	5.11489200	0.74354300	C	-6.74484200	-0.63021600	-0.57960600
C	-2.13489400	2.98567300	0.41405200	H	-6.76058600	0.04620400	-1.44017500
H	-1.04640000	2.86749300	0.28130600	H	-7.03509300	-0.05705000	0.30504600
H	-2.31138300	2.74953100	1.47132900	H	-7.52258700	-1.38301400	-0.75268600
C	0.89846700	-5.67500100	-0.53195500	C	-2.60630700	-2.69714500	-2.57727600
C	0.58270300	-5.40018100	0.79808300	H	-1.69017600	-2.09548900	-2.66517000
C	0.28359200	-4.09818900	1.18069800	H	-3.18145400	-2.58148500	-3.49892300
C	0.30197100	-3.03814000	0.24925000	H	-2.28089900	-3.74225000	-2.51210400
C	0.62263300	-3.33758400	-1.09062800	C	1.94549500	-3.11017900	0.32046500
C	0.91291700	-4.64047300	-1.47108400	C	2.60784100	-2.89202000	1.54347500
H	1.13290700	-6.69146900	-0.83695000	C	3.97204700	-2.59627900	1.50449400
H	0.56873800	-6.19963900	1.53400300	H	4.48913100	-2.39763900	2.44241100
H	0.03508000	-3.87511100	2.21725400	C	4.68902100	-2.56441800	0.30645400
H	0.63441800	-2.53014300	-1.81947100	C	4.01668700	-2.87945900	-0.87568400
H	1.15818800	-4.85375000	-2.50840700	H	4.56750100	-2.89945200	-1.81573800
				C	2.64929100	-3.16602100	-0.89685300
				C	1.92317200	-3.06067700	2.86459800
<b>2a-PC</b>				H	0.83608100	-3.05898500	2.77539900
Ru	0.06258500	-0.41418400	0.00261200	H	2.18634800	-2.25491200	3.55342400



H	2.23665400	-4.00671800	3.32442300	H	5.17642100	-0.36613300	-1.70146000
C	6.14317100	-2.20186000	0.29758300	C	-1.64496500	4.83207200	-2.40456000
H	6.28304500	-1.13023700	0.48347700	H	-1.73400400	3.29088200	-3.91149600
H	6.61138200	-2.43235200	-0.66351200	H	-1.35925500	6.16710600	-0.73848800
H	6.69712400	-2.73147000	1.07869600	H	2.51098400	4.37309700	4.77573500
C	1.99991200	-3.59885300	-2.17509800	H	5.96320100	1.57081700	-3.05077000
H	2.20652300	-4.66139000	-2.36054900	H	-2.29544500	5.51464400	-2.94514200
H	2.39012300	-3.03256200	-3.02363100	P	1.06502300	1.83216400	-0.13593500
H	0.91896600	-3.44912800	-2.16861300				
C	-2.63128500	1.35244900	1.54166300	<b>pseudo-Z</b>			
H	-1.88478300	0.89626400	2.18736100	<b>2b-PC</b>			
C	-3.62054800	2.17308700	2.06701500	Ru	0.05093200	-0.41062600	0.13675600
H	-3.64451100	2.36953100	3.13608400	C	1.75338700	0.26194100	0.37692700
C	-4.58107500	2.74870200	1.23117800	H	2.08928000	0.22988200	1.43046400
H	-5.34640000	3.39886300	1.64731900	C	2.76099500	0.89184000	-0.46603000
C	-4.55803300	2.48497900	-0.13797300	Cl	-0.28561800	-0.50787300	-2.29286400
H	-5.30429800	2.92768900	-0.79287700	Cl	-0.18501100	-0.40117400	2.59567700
C	-3.58427500	1.64437900	-0.66281800	C	0.50516000	-2.41610600	0.27495200
H	-3.56811400	1.41828700	-1.72792500	P	-1.09361900	1.75956600	0.14890600
C	1.56804000	2.67174700	1.40764600	N	-0.43443200	-3.39404800	0.32192300
C	2.60783300	1.78562400	-1.10987300	N	1.70419400	-3.00541300	0.50187800
C	0.02222000	3.06805500	-1.00376200	C	1.58768800	-4.44029300	0.80590700
C	2.89472600	3.02368800	1.67692400	H	1.78879100	-4.61542000	1.87150200
C	0.58780000	2.92778300	2.37684000	H	2.31822700	-5.01217600	0.22460200
C	3.05084300	2.86995900	-1.87337500	C	0.14602100	-4.73873000	0.42972000
C	3.38371100	0.62256100	-1.05343900	H	0.05898200	-5.25949300	-0.53541500
C	-0.51201300	2.70285000	-2.24859000	H	-0.38758600	-5.32933300	1.18123200
C	-0.28443500	4.32451200	-0.47200700	C	2.99932100	-2.41236300	0.42624700
C	3.23049500	3.63274700	2.88572200	C	3.58765800	-2.25059000	-0.83863200
H	3.67119800	2.82525100	0.94268500	C	4.87830700	-1.72413200	-0.90281800
C	0.92276800	3.54538900	3.57599600	H	5.33255400	-1.56696600	-1.88041900
H	-0.44338400	2.63995200	2.18467300	C	5.58282200	-1.36244100	0.24693300
C	4.25616700	2.79212200	-2.56816300	C	4.96598000	-1.54079600	1.48813700
H	2.44855300	3.77473000	-1.92734200	H	5.49449100	-1.24603500	2.39431200
C	4.58923100	0.54786700	-1.74392900	C	3.67852000	-2.06816400	1.60574900
H	3.03378500	-0.23902500	-0.48253700	C	2.82552500	-2.58719000	-2.07974300
C	-1.33122600	3.58481000	-2.94540900	H	3.44175100	-2.44578100	-2.97102600
H	-0.28270700	1.72017600	-2.66209600	H	1.93149700	-1.95552200	-2.18114900
C	-1.12129400	5.19757100	-1.16796700	H	2.47109200	-3.62563200	-2.07206900
H	0.12519600	4.62789900	0.48748300	C	6.96654600	-0.79563400	0.15312200
C	2.24722000	3.89773600	3.83483200	H	7.16184200	-0.07972700	0.95737600
H	4.26500200	3.90196000	3.08120400	H	7.12568100	-0.28455300	-0.80071000
H	0.15041700	3.73877100	4.31542100	H	7.72721200	-1.58117000	0.23189900
C	5.02666500	1.63250400	-2.50299800	C	3.02533300	-2.22644600	2.94223700
H	4.59117900	3.63701800	-3.16374800	H	2.00475900	-1.82342700	2.94042100

H	3.59576700	-1.71185900	3.71932500	H	0.93371800	3.37807100	-3.42142200
H	2.95559500	-3.28046600	3.23822800	C	0.44228100	3.60014500	-1.34061600
C	-1.79837100	-3.26213400	-0.08999500	H	0.32549700	4.41964400	-0.61525100
C	-2.12211700	-3.37004200	-1.45251000	H	1.27784100	2.98768000	-0.98486800
C	-3.47043100	-3.28559000	-1.81499400	C	-0.79592300	2.81824300	1.64491700
H	-3.73046800	-3.33703700	-2.87155000	H	-1.18610700	2.17146500	2.44539400
C	-4.48474800	-3.16541300	-0.86660700	C	0.67471900	3.04759500	2.00294500
C	-4.12619200	-3.12406100	0.48498200	H	1.19684200	2.08580200	2.02131100
H	-4.90606100	-3.06127600	1.24331100	H	1.16916200	3.67163200	1.24661800
C	-2.79556000	-3.16728200	0.89904900	C	0.78614800	3.72234500	3.36650200
C	-1.08890900	-3.65445600	-2.49827900	H	0.39341600	3.03638600	4.13132900
H	-0.09222400	-3.32149100	-2.20342000	H	1.83996400	3.89396200	3.61592400
H	-1.32914200	-3.14513300	-3.43383900	C	0.00597100	5.03139300	3.40782900
H	-1.04897300	-4.73161600	-2.70897800	H	0.07959200	5.49493700	4.39850200
C	-5.92596600	-3.11926000	-1.27523100	H	0.45630600	5.74300900	2.69902700
H	-6.45888900	-2.29820300	-0.78301500	C	-1.45434200	4.81126000	3.03069700
H	-6.44796000	-4.04219700	-0.99870600	H	-2.00349100	5.76033900	3.03324000
H	-6.03392700	-2.99065400	-2.35536700	H	-1.93211600	4.17336100	3.78939400
C	-2.44415400	-3.15241700	2.35242300	C	-1.58135500	4.13396600	1.66827800
H	-3.34515500	-3.09892800	2.96889000	H	-1.19339100	4.80957700	0.89137700
H	-1.79635600	-2.30548800	2.60587300	H	-2.63990400	3.96579300	1.42971300
H	-1.89534400	-4.05678900	2.64100400	C	-2.93293100	1.50123400	0.20717300
C	2.72835700	0.93178100	-1.87372100	H	-3.37607000	2.48620800	-0.01023000
H	1.88977900	0.47397600	-2.39163700	C	-3.39026900	0.52754300	-0.88418400
C	3.74533600	1.55419000	-2.58459700	H	-2.95179000	0.77917000	-1.85810100
H	3.70557800	1.57333200	-3.67098400	H	-3.00546700	-0.47954000	-0.64961300
C	4.80795000	2.16756400	-1.91580100	C	-4.91292300	0.49683700	-0.96374800
H	5.59526200	2.66185000	-2.47941000	H	-5.27039200	1.48287000	-1.29959600
C	4.85403900	2.14540400	-0.52249700	H	-5.23442600	-0.22304900	-1.72720500
H	5.67890100	2.61723900	0.00559000	C	-5.54310800	0.16124700	0.38415000
C	3.84836700	1.50429600	0.19149300	H	-6.63676100	0.22415300	0.32277700
H	3.88731000	1.46549000	1.27927500	H	-5.30188000	-0.87999000	0.63440600
C	-0.85176500	2.77972200	-1.39489600	C	-5.01858900	1.05486100	1.50155200
H	-0.71034400	2.00022100	-2.16006500	H	-5.43369600	0.74090100	2.46649400
C	-2.01334100	3.66633600	-1.85892100	H	-5.36330900	2.08812100	1.33975300
H	-2.94064300	3.08906200	-1.94486300	C	-3.49279500	1.05470900	1.55990000
H	-2.20491100	4.45965700	-1.12060500	H	-3.11193300	0.05139100	1.80431500
C	-1.69403200	4.29298100	-3.21586400	H	-3.15881400	1.71185600	2.37058800
H	-1.62257300	3.48898000	-3.96291900				
H	-2.52245900	4.93728900	-3.53347300				
C	-0.38454600	5.07211900	-3.19584300	<i>pseudo-E 2b-PC</i>			
H	-0.16657000	5.47941300	-4.18998000	Ru	0.01240400	-0.33005600	0.17989500
H	-0.48825200	5.93709600	-2.52316700	C	-0.39977200	-2.35452200	0.29724200
C	0.76241200	4.19657700	-2.70642000	N	0.56556500	-3.30208300	0.30804100
H	1.69747300	4.76767500	-2.65892000	N	-1.56122400	-2.95462800	0.66112500
				C	0.09519500	-4.59118700	0.83111600

H	0.49428400	-4.74797800	1.84284500	C	5.98531200	-2.83207100	-1.47251500
H	0.44454200	-5.41265000	0.19646700	H	6.67525200	-2.63091200	-0.64850500
C	-1.41386700	-4.41058700	0.81921100	H	6.31752800	-3.74938800	-1.97024900
H	-1.89759900	-4.74695500	1.74140600	H	6.09379500	-2.02176700	-2.20249700
H	-1.89860300	-4.92624500	-0.02341800	C	-1.68761500	0.37036500	0.36275000
Cl	0.46012200	-0.40008300	-2.23853800	H	-1.99453900	0.48461900	1.42008800
Cl	0.04315700	-0.53585700	2.64669100	C	-2.72600000	0.86646000	-0.53092300
C	-2.87838900	-2.43112800	0.47916300	C	-2.73660500	0.70965600	-1.93111400
C	-3.64983700	-2.09277200	1.60176300	C	-3.82486800	1.51747600	0.06959300
C	-3.39618300	-2.34739600	-0.82332600	C	-3.79555500	1.18771200	-2.68916500
C	-4.94371300	-1.61348500	1.38515800	H	-1.90049000	0.20545800	-2.40697100
C	-4.69987700	-1.87694100	-0.98580200	C	-4.87821200	2.00870000	-0.69274400
C	-5.48471500	-1.49313900	0.10309900	H	-3.83645200	1.62268600	1.15357300
H	-5.54296400	-1.32201000	2.24713100	C	-4.86753400	1.84174400	-2.07665800
H	-5.10034400	-1.78033000	-1.99446700	H	-3.78620600	1.05404900	-3.76821800
C	1.92347700	-3.14236700	-0.10971600	H	-5.71229600	2.50956800	-0.20785700
C	2.93641000	-2.88913800	0.82642700	H	-5.69284200	2.21692400	-2.67711600
C	2.21723000	-3.37019700	-1.46976700	H	3.06563400	3.63470900	3.95574500
C	4.24990000	-2.78577000	0.35356700	C	2.61970400	2.63754400	4.09761700
C	3.53911100	-3.24943900	-1.88832400	C	1.29839900	2.78808600	4.83937500
C	4.57096300	-2.95010600	-0.99170700	C	2.42848300	1.96720300	2.73988700
H	5.04418900	-2.57149900	1.06884600	H	3.33780900	2.06196000	4.69343900
H	3.77286800	-3.40775500	-2.94053200	C	0.32119900	3.60853900	4.00897000
C	-2.54826500	-2.69303400	-2.00584900	H	0.87004300	1.79278300	5.02402400
H	-2.10644400	-3.69331000	-1.92138000	H	1.45800700	3.25347400	5.81915000
H	-3.12987400	-2.65671000	-2.93051400	C	1.38841800	2.71060000	1.89225000
H	-1.70530700	-1.99522100	-2.10897800	H	2.11413500	0.92736300	2.88300500
C	-3.10052800	-2.23174500	2.98489000	H	3.38895600	1.94711100	2.20997900
H	-3.79054300	-1.81622400	3.72332200	C	0.07838300	2.96523600	2.64760200
H	-2.93558400	-3.28414800	3.24764300	H	0.73044500	4.62178100	3.86860100
H	-2.13198800	-1.72816800	3.08043200	H	-0.63282700	3.73167700	4.53500600
C	2.66683700	-2.79309900	2.29549100	P	1.07110800	1.92367900	0.22915000
H	1.63119900	-2.53221800	2.52001700	H	1.83742800	3.68871200	1.65084400
H	2.90201600	-3.74456400	2.78946800	H	-0.44689300	2.01105100	2.78163400
H	3.29960900	-2.03113300	2.76131100	H	-0.58022500	3.61119100	2.05195600
C	1.13871200	-3.76791800	-2.42660100	C	2.79513300	1.92167100	-0.48096800
H	0.42039900	-2.95423700	-2.56871100	C	0.03014900	3.25337800	-0.57797300
H	1.55813100	-4.02230100	-3.40290700	C	2.90219300	2.29990100	-1.95968400
H	0.57823600	-4.63832200	-2.06260400	C	3.45175200	0.55439800	-0.23246600
C	-6.87893600	-0.98334800	-0.09837400	H	3.35009400	2.67910300	0.10022200
H	-7.60741900	-1.80271200	-0.11123800	C	-0.35134000	2.99629400	-2.03835900
H	-7.17633500	-0.30147700	0.70388600	C	0.49833600	4.70478600	-0.41677600
H	-6.97590500	-0.45009900	-1.04891400	H	-0.90501900	3.14619200	-0.00037700

C	4.34996500	2.25383800	-2.44189100	H	-4.21376900	-2.21453200	-1.29613500
H	2.28647900	1.60901300	-2.55019500	H	-1.91142500	1.26195300	-0.23709400
H	2.50108200	3.30650200	-2.12276800	H	-3.92584500	2.32403600	0.67100600
C	4.90824600	0.56548800	-0.68226600	C	2.34470000	-0.22591600	0.75035800
H	2.90225600	-0.20863700	-0.80637300	C	3.38523300	-0.18664700	-0.18906600
H	3.37010300	0.26254100	0.82267700	C	2.60324600	-0.66314700	2.05253700
C	-1.47641700	3.93457800	-2.45932800	C	4.67194500	-0.56202500	0.18086900
H	0.51479200	3.17112900	-2.68744400	H	3.18037000	0.13524100	-1.20980100
H	-0.62472600	1.95145300	-2.18505900	C	3.89417600	-1.03900000	2.41607400
C	-0.59513100	5.67016400	-0.87401600	H	1.79611400	-0.71841000	2.77902700
H	1.40919300	4.86284700	-1.01438200	C	4.92822800	-0.98765000	1.48413100
H	0.76191000	4.93668000	0.62032900	H	5.47405500	-0.52820100	-0.55103200
C	5.00133200	0.90480200	-2.16434300	H	4.08960200	-1.37767100	3.42976300
H	4.92629600	3.03861900	-1.92804700	H	5.93295200	-1.28599200	1.77046100
H	4.39056700	2.49267600	-3.51104200	C	0.84353700	1.87322300	-0.49794200
H	5.46489200	1.31604300	-0.09908900	C	1.78538300	2.75652300	0.04836600
H	5.37503000	-0.40207200	-0.46848000	C	0.03814300	2.30754100	-1.55646400
C	-1.05583100	5.39028600	-2.29909600	C	1.90407300	4.05314300	-0.44482500
H	-2.36550400	3.73251000	-1.84121900	H	2.43353700	2.42500600	0.85722200
H	-1.77133900	3.72610600	-3.49496100	C	0.15727700	3.60502300	-2.04595100
H	-1.45333600	5.56722200	-0.19239100	H	-0.66115800	1.61765200	-2.02070900
H	-0.24572200	6.70477200	-0.77445700	C	1.08857700	4.47977800	-1.49150000
H	4.48338600	0.12229900	-2.74037600	H	2.64041600	4.72658600	-0.01515500
H	6.04566400	0.90629800	-2.50002300	H	-0.46697100	3.92419700	-2.87549400
H	-0.22900100	5.60221000	-2.99352400	H	1.18836000	5.48886700	-1.88184500
H	-1.87232300	6.06783200	-2.57566800	C	-0.33575600	0.36791200	1.69728600

**1a-Inact-C**  
PPh<sub>3</sub>Cl<sub>2</sub>Ru=CHPh

Ru	0.06241700	-1.41072000	-1.24848700
Cl	0.48931600	-3.17768100	0.21540300
Cl	0.93745600	-0.41745600	-3.16161500
P	0.66164600	0.17690900	0.17091800
C	-1.76040100	-1.29214400	-1.33677600
H	-2.05622600	-2.15674800	-1.97124000
C	-5.21577200	0.65469500	0.22183900
C	-5.29249500	-0.62111700	-0.33685500
C	-4.15378800	-1.22098700	-0.85717800
C	-2.90011500	-0.57178100	-0.81298300
C	-2.85033800	0.72080900	-0.25727100
C	-3.99171600	1.32408900	0.25062400
H	-6.10689300	1.12900000	0.62371800
H	-6.24309100	-1.14599300	-0.37210800

H	-4.21376900	-2.21453200	-1.29613500
H	-1.91142500	1.26195300	-0.23709400
H	-3.92584500	2.32403600	0.67100600
C	2.34470000	-0.22591600	0.75035800
C	3.38523300	-0.18664700	-0.18906600
C	2.60324600	-0.66314700	2.05253700
C	4.67194500	-0.56202500	0.18086900
H	3.18037000	0.13524100	-1.20980100
C	3.89417600	-1.03900000	2.41607400
H	1.79611400	-0.71841000	2.77902700
C	4.92822800	-0.98765000	1.48413100
H	5.47405500	-0.52820100	-0.55103200
H	4.08960200	-1.37767100	3.42976300
H	5.93295200	-1.28599200	1.77046100
C	0.84353700	1.87322300	-0.49794200
C	1.78538300	2.75652300	0.04836600
C	0.03814300	2.30754100	-1.55646400
C	1.90407300	4.05314300	-0.44482500
H	2.43353700	2.42500600	0.85722200
C	0.15727700	3.60502300	-2.04595100
H	-0.66115800	1.61765200	-2.02070900
C	1.08857700	4.47977800	-1.49150000
H	2.64041600	4.72658600	-0.01515500
H	-0.46697100	3.92419700	-2.87549400
H	1.18836000	5.48886700	-1.88184500
C	-0.33575600	0.36791200	1.69728600
C	-0.43936900	1.60410000	2.34909100
C	-1.01987600	-0.73852500	2.21543600
C	-1.20867100	1.72565300	3.50356900
H	0.07070400	2.47798900	1.95147900
C	-1.78112200	-0.61235400	3.37421000
H	-0.95575300	-1.69744500	1.70740800
C	-1.88062400	0.61882200	4.01857300
H	-1.28541600	2.69060700	3.99742400
H	-2.30705900	-1.47879600	3.76560400
H	-2.48549600	0.71790100	4.91582800

**1b-Inact-C**  
PCy<sub>3</sub>Cl<sub>2</sub>Ru=CHPh

Ru	0.00000000	0.00000000	0.00000000
Cl	0.00000000	0.00000000	2.34143617
Cl	1.21525049	0.00000000	-1.99870591
P	-0.85184383	-2.05107803	-0.15369689
C	-1.49673117	0.96541885	-0.44654639
H	-2.48916250	0.52969034	-0.62089690



C	4.98128835	0.03901303	0.79861775	Cl	-3.06233800	-0.95337200	-0.58493800
H	4.74561802	2.17299891	0.70790988	P	0.11066000	0.16452300	0.03381400
H	4.95237418	-2.08989156	1.12984319	C	-0.52687300	-0.58416900	-2.76039000
C	-1.92941297	-2.59392784	2.54376756	H	-0.04107000	0.38669100	-2.92767900
H	-1.24584544	-2.55863900	3.39910083	C	1.93159800	0.07614700	0.13480000
H	-2.47115777	-3.54151267	2.58417393	C	2.60617300	0.42615300	1.31019400
H	-1.29602599	-2.60636967	1.64573467	C	2.66741600	-0.28479400	-0.99943000
C	-2.64793693	2.37935523	2.46116529	C	3.99862800	0.41781500	1.34674200
H	-3.43489154	3.13542587	2.41470462	H	2.04368500	0.70390600	2.19863500
H	-2.04657493	2.56779120	3.35724516	C	4.05776100	-0.28758800	-0.96027100
H	-1.97801445	2.52934446	1.60458759	H	2.14547600	-0.58602200	-1.90538000
C	2.42611990	2.57995047	2.00671065	C	4.72529100	0.06267200	0.21255900
H	1.35202783	2.50851724	2.18876095	H	4.51475300	0.68544100	2.26464500
H	2.90162889	2.98815996	2.90810211	H	4.62053900	-0.57772900	-1.84272600
H	2.56201203	3.31003063	1.20566306	H	5.81122600	0.05067900	0.24434700
C	2.59120331	-2.45115219	2.41839065	C	-0.22129500	1.88082000	-0.50404000
H	1.60676107	-2.65452383	1.98677659	C	-1.53305500	2.24243600	-0.84289200
H	3.23941350	-3.29989037	2.18905971	C	0.79568900	2.84192500	-0.57435800
H	2.47169975	-2.40697050	3.50827828	C	-1.82245900	3.54853000	-1.22447100
C	-6.56032919	-0.74218706	1.84938952	H	-2.32448600	1.49642500	-0.80386500
H	-7.09900546	-0.95318358	2.78024495	C	0.49949000	4.14630800	-0.96611700
H	-7.02788823	0.13679326	1.39791198	H	1.81965000	2.57825600	-0.32367700
H	-6.72935617	-1.59586591	1.18626701	C	-0.80729400	4.50228900	-1.28924100
C	6.29545393	0.02688515	0.08011958	H	-2.84322100	3.81808800	-1.47996900
H	6.73644881	1.02546297	0.02704366	H	1.29593300	4.88325000	-1.02108100
H	7.01566496	-0.63825441	0.56596135	H	-1.03411700	5.51976700	-1.59562500
H	6.17674737	-0.33304876	-0.94808382	C	-0.44741700	0.05739700	1.76407400
C	-1.76947329	-0.25632737	-0.43675198	C	-0.27780900	-1.17108500	2.41879700
H	-2.55869955	-0.48006237	0.28644794	C	-1.06223600	1.12056400	2.43090200
C	-2.20455017	-0.23157946	-1.81577518	C	-0.70935800	-1.32454900	3.73114800
C	-1.32750940	0.09454570	-2.87203264	H	0.19262200	-2.00282100	1.89419900
C	-3.54053926	-0.55426222	-2.13012143	C	-1.49744500	0.95782800	3.74472200
C	-1.76670247	0.08872134	-4.18597696	H	-1.20253600	2.07351700	1.92659700
H	-0.29546528	0.36857729	-2.65044258	C	-1.32200500	-0.26114800	4.39475400
C	-3.97791853	-0.55967371	-3.44849635	H	-0.57552600	-2.27820200	4.23370200
H	-4.22331087	-0.80225479	-1.31895247	H	-1.97725300	1.78605500	4.25839300
C	-3.09307813	-0.23957929	-4.47844086	H	-1.66676600	-0.38565200	5.41760100
H	-1.07990810	0.34392452	-4.98758842	H	-0.86368500	-1.10937800	-3.66934400
H	-5.00987222	-0.81200455	-3.67694653				
H	-3.43588600	-0.24243915	-5.50959115				

**PPh<sub>3</sub>Cl<sub>2</sub>Ru=CH<sub>2</sub>**

Ru	-0.86673600	-1.40314000	-1.18138200
Cl	0.72307200	-3.04529000	-0.80330100

**PCy<sub>3</sub>Cl<sub>2</sub>Ru=CH<sub>2</sub>**

Ru	1.17767900	-1.09122200	-1.42309900
C	-0.14771500	-1.92763800	-2.31418300
P	-0.01692900	-0.01211300	0.12865700

C	-1.14898800	1.28730300	-0.57595700	H	-1.47268800	-1.02767200	3.36185500
C	-1.78167300	2.25822600	0.43090200	H	-3.78431100	-0.08618700	2.91495800
C	-2.49154200	3.39523000	-0.30148600	H	-3.46218000	-0.19899900	1.19885400
C	-3.54919500	2.85858300	-1.25704700	H	-3.87210900	-2.44999700	3.19305800
C	-2.93512100	1.87948600	-2.24792600	H	-4.57772800	-2.23677900	1.60442100
C	-2.20999000	0.74165500	-1.53596100	H	-2.99298200	-3.91565400	1.11136200
C	1.06589600	0.97328300	1.28386000	H	-1.88899000	-3.39721800	2.36507600
C	1.73996900	2.17399600	0.61060500	H	-1.01925400	-2.92845900	0.03195200
C	2.49087800	3.01779100	1.63631800	H	-2.36954400	-1.82269800	-0.19947200
C	3.51323300	2.18704000	2.40087200	Cl	1.99288400	-2.71441900	0.04450400
C	2.85475700	0.97666500	3.04945800	Cl	1.67121100	0.81774100	-2.66997000
C	2.11194400	0.13031300	2.02055000	H	-1.22716800	-1.94709200	-2.13014200
C	-0.89464800	-1.17457700	1.28281400	<b>NHC-Cl<sub>2</sub>Ru=CH<sub>2</sub></b>			
C	-1.72036500	-0.52163700	2.41878500	Ru	0.12295300	-0.05684200	-1.38958300
C	-3.21846600	-0.65540800	2.16954800	C	-1.55420700	-0.08063000	-2.04844400
C	-3.64510200	-2.12736400	2.17009100	C	-0.10451700	-0.03768700	0.53121500
C	-2.55183600	-3.02590700	1.57178300	N	-1.21395700	0.08625400	1.30414400
C	-1.70754100	-2.26185200	0.56023800	C	-0.92147200	-0.04033100	2.73655900
H	0.19502400	-2.53130600	-3.17361600	C	0.59860700	0.02807100	2.77836800
H	-0.44019800	1.86056400	-1.19390700	N	0.96411100	-0.15645500	1.37282800
H	-1.02827400	2.66987300	1.11258400	C	2.33203300	-0.05141600	0.96468500
H	-2.51648600	1.72925900	1.05179600	C	2.90778500	1.22403800	0.81404200
H	-2.93654100	4.08413600	0.42548400	C	4.23078600	1.29714000	0.37852800
H	-1.74874100	3.97633400	-0.86752500	C	4.98963000	0.15241100	0.12604800
H	-4.04568600	3.68117300	-1.78365000	C	4.41010300	-1.09356400	0.36885000
H	-4.33103000	2.34522800	-0.67671800	C	3.09084800	-1.22407300	0.80637500
H	-3.70065600	1.47238000	-2.91798500	C	-2.56984500	0.05722100	0.86889000
H	-2.21398600	2.40964800	-2.88644500	C	-3.22258800	1.27476900	0.63589100
H	-1.74230500	0.08490800	-2.27573600	C	-4.55440900	1.23258700	0.21957100
H	-2.94260000	0.13732500	-0.97838900	C	-5.22881500	0.02234300	0.03318600
H	0.36513900	1.36357500	2.04072300	C	-4.53449400	-1.17035700	0.25824900
H	1.00991700	2.79588700	0.07979700	C	-3.20142900	-1.17918800	0.67235600
H	2.43725100	1.81390300	-0.15738300	C	2.17666400	2.48041600	1.17992500
H	2.97499700	3.86368100	1.13557700	C	2.55315400	-2.57512600	1.16347400
H	1.76918600	3.45066900	2.34653300	C	6.38837900	0.26009500	-0.39835800
H	4.29060800	1.84249400	1.70382200	C	-2.43577900	-2.45830300	0.80816900
H	4.02193000	2.79954200	3.15391500	C	-2.47621100	2.56640400	0.75401700
H	2.14544800	1.31684700	3.81933500	C	-6.66796200	0.00374600	-0.38258600
H	3.59917300	0.36105400	3.56662200	H	-1.59162500	-0.10973900	-3.15339200
H	1.65706000	-0.74126800	2.50431800	H	-1.41041500	0.76463300	3.29565900
H	2.82819500	-0.27733100	1.29452500	H	-1.31133400	-0.99446600	3.11744800
H	-0.03598200	-1.69604100	1.72747400	H	0.96706200	0.99939300	3.13739600
H	-1.44505300	0.52609100	2.57673700				

H	1.05199900	-0.75430400	3.39649500
H	4.67893300	2.27902700	0.23343200
H	5.00199600	-1.99548100	0.21831000
H	-5.03807800	-2.12135900	0.08986000
H	-5.07413000	2.16930500	0.02276900
H	1.09100000	2.37536000	1.12524900
H	2.43974100	2.78744800	2.20083600
H	2.44859900	3.29993900	0.51133300
H	2.84077600	-3.32364700	0.42138100
H	2.96064700	-2.89791100	2.13014800
H	1.46392800	-2.58436400	1.22833300
H	6.39365000	0.29481200	-1.49371900
H	6.88342600	1.17000700	-0.04788000
H	6.99877800	-0.59724500	-0.10205500
H	-1.63166500	-2.51368000	0.06206400
H	-1.95499000	-2.55887200	1.78772800
H	-3.08605100	-3.32443700	0.66760300
H	-3.14250000	3.42266200	0.62777900
H	-1.97373300	2.66552300	1.72272900
H	-1.68905200	2.63146800	-0.00865900
H	-7.33095600	0.01079100	0.49020400
H	-6.92519300	0.87793800	-0.98644800
H	-6.91021300	-0.89201000	-0.96062900
Cl	0.75565100	-2.29734100	-1.55457300
Cl	0.74294800	2.17112800	-1.70411400
H	-2.52535400	-0.07412100	-1.54751700

**Ethene**

C	-0.66987200	0.00000000	-0.00000300
C	0.66987200	0.00000000	0.00000300
H	-1.24278600	0.92633800	0.00001000
H	-1.24278600	-0.92633800	-0.00002300
H	1.24278600	-0.92633800	-0.00001000
H	1.24278600	0.92633800	0.00002300

**styrene**

C	-1.94515900	-0.53512500	-0.00000700
C	-2.96185700	0.33685300	0.00000700
H	-2.18130500	-1.60015800	-0.00002900
H	-2.80926600	1.41320200	0.00002100
H	-3.99177900	-0.00270300	0.00000300
C	-0.51530900	-0.22717400	-0.00000300

C	0.40994000	-1.28219500	0.00000400
C	-0.01740900	1.08637600	-0.00000400
C	1.78037500	-1.03981000	0.00000200
H	0.03977300	-2.30569700	0.00000500
C	1.34941600	1.33030300	-0.00000200
H	-0.70951600	1.92465300	-0.00000200
C	2.25630700	0.26870600	0.00000000
H	2.47632500	-1.87423500	0.00000700
H	1.71283600	2.35439300	0.00000200
H	3.32511600	0.46294000	0.00000100

**Cis-stilbene**

C	-3.91964900	-0.17739700	-0.00039000
C	-3.00735100	0.87061900	-0.00022900
C	-1.61928100	0.64135700	0.00017600
C	-1.17832100	-0.69540800	0.00047800
C	-2.09214600	-1.74319300	0.00030300
C	-3.46459500	-1.49382700	-0.00012100
C	-0.75054200	1.81807200	0.00027400
C	2.09945000	0.34006300	-1.20467900
C	1.60128200	0.85272400	0.00002400
C	0.59053500	1.93209800	0.00013600
C	2.09959300	0.33990400	1.20460200
H	1.71682300	0.72989100	2.14461500
C	3.05881100	-0.66984200	1.20448700
C	3.54037300	-1.17891400	-0.00022400
C	3.05864900	-0.66970900	-1.20480900
H	-1.30394800	2.75811900	0.00035100
H	-4.98561900	0.03332200	-0.00069900
H	-3.36566800	1.89835200	-0.00045300
H	-1.72780900	-2.76705900	0.00053300
H	-4.17082200	-2.31946900	-0.00021700
H	0.99068000	2.94719600	0.00020500
H	3.42959100	-1.06068600	2.14813800
H	4.28756600	-1.96766300	-0.00031800
H	3.42927300	-1.06047400	-2.14855400
H	-0.11752800	-0.92103000	0.00083000
H	1.71661600	0.73021000	-2.14459900

**PPh<sub>3</sub>**

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.84743560
C	2.46577279	0.00000000	1.42489706



C	-0.86028254	1.09942566	0.11166568
C	0.25785268	-0.52312345	-1.27598266
C	0.52977428	1.09611843	3.53947843
C	-1.23760889	-0.51802088	3.25727672
C	3.43958081	-0.51941619	2.29082855
C	2.80056742	1.09718989	0.62152178
C	-1.44072440	1.66321835	-1.02366524
H	-1.07601319	1.52059420	1.09086978
C	-0.30926282	0.04955287	-2.41050318
H	0.91514574	-1.38519806	-1.37684961
C	-0.16475013	1.66228042	4.60747491
H	1.48870108	1.51297740	3.24014362
C	-1.93758186	0.05654545	4.31384414
H	-1.65581100	-1.37759649	2.73614042
C	4.70522639	0.05406842	2.36861661
H	3.19692009	-1.37946563	2.91275146
C	4.07349374	1.66186823	0.68834699
H	2.06157395	1.51583196	-0.05793328
C	-1.16432220	1.14433476	-2.28654581
H	-2.10704721	2.51552333	-0.91916700
H	-0.09197267	-0.36521860	-3.39110654
C	-1.40035072	1.14857652	4.99479758
H	0.26070979	2.51231496	5.13444235
H	-2.89827945	-0.35419905	4.61239329
C	5.02713746	1.14602789	1.56323691
H	5.44406090	-0.35802094	3.05062684
H	4.31750374	2.51238549	0.05718190
H	-1.61612218	1.58705547	-3.16982755
H	-1.94045939	1.59322833	5.82601375
H	6.01773682	1.58925719	1.61458827
P	0.82194969	-0.82338168	1.42386742

**trans-stilbene**

C	-0.49848300	0.45477800	0.00005400
C	0.49848300	-0.45477800	0.00005200
H	-0.23880100	1.51415800	0.00009800
H	0.23880100	-1.51415800	0.00006800
C	-1.92904300	0.18770300	0.00001900
C	-2.81830400	1.27624800	0.00016900
C	-2.47931000	-1.10788500	-0.00018800
C	-4.19548900	1.08590500	0.00012800
H	-2.41073800	2.28542500	0.00032400
C	-3.85401200	-1.29830400	-0.00023900
H	-1.82252500	-1.97379400	-0.00033000

C	-4.72136500	-0.20389100	-0.00008100
H	-4.85941600	1.94585400	0.00024900
H	-4.25542400	-2.30826500	-0.00041100
H	-5.79656500	-0.35840500	-0.00012700
C	1.92904300	-0.18770300	0.00004300
C	2.81830400	-1.27624800	0.00019100
C	2.47931000	1.10788500	-0.00013600
C	4.19548900	-1.08590500	0.00017600
H	2.41073800	-2.28542500	0.00032500
C	3.85401200	1.29830400	-0.00016200
H	1.82252500	1.97379400	-0.00027600
C	4.72136500	0.20389100	-0.00000500
H	4.85941600	-1.94585400	0.00029500
H	4.25542400	2.30826500	-0.00031100
H	5.79656500	0.35840500	-0.00003100

**PCy<sub>3</sub>**

P	-0.23682600	-0.07006400	-1.10208200
C	0.76218900	-1.45988400	-0.34498800
H	0.06332700	-2.30811000	-0.44098600
C	1.16184800	-1.37274700	1.12912500
H	0.29632700	-1.11416700	1.75337300
H	1.89090500	-0.55857500	1.25703600
C	1.79645200	-2.67849500	1.60457800
H	2.08716000	-2.60056300	2.65909100
H	1.04650100	-3.48204500	1.54937900
C	2.99721200	-3.05190400	0.74281000
H	3.43272600	-3.99956100	1.08020900
H	3.78025000	-2.28929600	0.87071100
C	2.61457500	-3.13077600	-0.73111600
H	3.49125900	-3.37188300	-1.34383200
H	1.90066300	-3.95579100	-0.87460200
C	1.97514300	-1.83008100	-1.20880100
H	1.67504500	-1.90678500	-2.26067700
H	2.72498600	-1.02840000	-1.16270900
C	-1.80048000	-0.12442900	-0.07505200
H	-1.55868600	0.01669000	0.99218400
C	-2.51963300	-1.46954100	-0.21877600
H	-1.88740500	-2.28498400	0.15281600
H	-2.68814300	-1.67256500	-1.28803400
C	-3.85461000	-1.48612800	0.51912800
H	-4.35093800	-2.45322800	0.37573100
H	-3.66929400	-1.39195200	1.59958700
C	-4.75788100	-0.34543000	0.06767000

H	-5.01696100	-0.48760700	-0.99208100
H	-5.70369600	-0.35947300	0.62153000
C	-4.05681200	0.99682000	0.23417200
H	-3.87503800	1.18045700	1.30409300
H	-4.69819300	1.81516900	-0.11384600
C	-2.72687100	1.01854400	-0.51176800
H	-2.23177900	1.98860600	-0.37434500
H	-2.91344800	0.92415300	-1.59264400
C	0.52420300	1.54403000	-0.51596800
H	-0.00940200	2.28758100	-1.13361600
C	0.36341100	1.99564500	0.94103400
H	0.88266900	1.29826600	1.61175000
H	-0.69178100	1.97919000	1.24055200
C	0.93548600	3.40015000	1.13552900
H	0.34528700	4.11101200	0.53748600
H	0.82405700	3.71178100	2.18104500
C	2.39631700	3.47913100	0.70514200
H	2.78060400	4.49752400	0.83517700
H	3.00002800	2.83507900	1.36233900
C	2.56803000	3.01694400	-0.73676400
H	3.62500200	3.04172600	-1.02693500
H	2.04532300	3.71461800	-1.40760300
C	1.99780400	1.61711700	-0.92946100
H	2.12103200	1.28641200	-1.96900000
H	2.57571900	0.91388800	-0.31090200

**1a-RCB-0**

Ru	-1.59198400	0.00069500	-0.69352400
Cl	-1.64761000	-2.41868100	-0.69774500
Cl	-1.64556800	2.42022300	-0.69714900
C	-3.24137300	0.00151000	0.36873400
C	-3.76487100	0.00129500	-1.10221800
C	-2.71109400	0.00162500	-2.28944500
H	-3.44917100	-0.92548300	0.90642500
H	-4.33427400	0.92391700	-1.22551000
H	-4.33403700	-0.92145800	-1.22557000
H	-2.73531300	-0.92527000	-2.86475300
H	-2.73483300	0.92903400	-2.86395200
P	0.65356900	-0.00006400	0.00085800
C	1.71475800	1.44499700	-0.28939500
C	2.68261100	1.83650100	0.64368500
C	1.59821000	2.13496700	-1.50006200
C	3.52151800	2.91177800	0.36577500
H	2.77062500	1.31033300	1.59257400

C	2.44761000	3.20120700	-1.77808500
H	0.81863900	1.85748300	-2.20540300
C	3.40705400	3.59119000	-0.84627100
H	4.26328300	3.21997400	1.09729300
H	2.34673100	3.73876900	-2.71634900
H	4.06182800	4.43128200	-1.06032500
C	0.16011700	-0.00074600	1.74481300
C	-0.12921200	-1.21605600	2.38336000
C	-0.12761100	1.21407100	2.38499500
C	-0.67167700	-1.21075700	3.66367400
H	0.03973800	-2.15533600	1.86143900
C	-0.67003600	1.20775000	3.66531400
H	0.04257100	2.15383700	1.86439200
C	-0.93987400	-0.00175900	4.30530800
H	-0.89769300	-2.15275000	4.15501300
H	-0.89472700	2.14936100	4.15798900
H	-1.37060800	-0.00214400	5.30299900
C	1.71393100	-1.44555300	-0.29041800
C	1.59664300	-2.13497900	-1.50131500
C	2.68181500	-1.83799800	0.64224800
C	2.44531200	-3.20163200	-1.77998800
H	0.81701500	-1.85675000	-2.20629700
C	3.51999800	-2.91367000	0.36368000
H	2.77041300	-1.31228500	1.59133700
C	3.40478100	-3.59255200	-0.84859800
H	2.34383900	-3.73876300	-2.71843500
H	4.26177500	-3.22259900	1.09487700
H	4.05898100	-4.43296000	-1.06316200
H	-3.44864900	0.92881600	0.90607400

**1b-RCB-0**

Ru	-1.31401200	-0.59125300	-1.05426300
Cl	-0.37953200	-2.82896900	-1.27510000
Cl	-2.60204200	1.45244700	-0.85889400
P	0.55303300	0.23641700	0.25719300
C	-1.72607300	-0.66364800	-2.95389300
C	1.33449600	1.90721200	-0.09052000
C	2.03433000	-0.86313000	0.53823300
C	-0.16324900	0.41624600	1.97012300
C	0.34388200	2.93147000	-0.64748500
C	2.60437400	1.88948800	-0.94877900
C	2.68009300	-1.38453900	-0.75626800
C	1.77122500	-2.03957100	1.48795100

C	-1.22099000	-0.67318300	2.20929100	H	-1.63937000	2.77198400	4.02734300
C	-0.75254500	1.78493000	2.32524000	H	-0.34933400	1.65100200	4.43877300
C	0.96768600	4.31978500	-0.72539500	H	-2.53484000	0.69598300	5.10806300
C	3.22094000	3.28462000	-1.03408800	H	-3.14706000	0.88806100	3.47029900
C	2.23569500	4.31510100	-1.56624500	H	-3.78677800	-0.93479300	-0.24353800
C	3.97666200	-2.12855700	-0.45183300	H	-2.92731700	-2.57074300	-0.41653300
C	3.06024100	-2.80353400	1.77770600	H	-3.00569100	-2.35821200	-2.69785600
C	3.72528600	-3.29164700	0.49827800	H	-3.83785700	-0.71223000	-2.53478400
C	-1.68426400	-0.67554900	3.66083600	H	-1.97710100	0.29027200	-3.42222000
C	-1.21981600	1.79047100	3.77983000				
C	-2.23671200	0.68905600	4.05374900				
C	-2.98870200	-1.34935600	-2.28078200				
C	-3.01643300	-1.53156800	-0.73471700				
H	-1.14985800	-1.36310400	-3.56163400				
H	1.64157000	2.22938000	0.92047900				
H	2.75041300	-0.18581800	1.04143700				
H	0.69078500	0.23743300	2.64570500				
H	0.02731200	2.60505900	-1.64833200				
H	-0.57517500	2.95649300	-0.06064200				
H	3.34873000	1.19838200	-0.54168500				
H	2.35969900	1.53479000	-1.96092000				
H	0.23464800	5.02809600	-1.12619500				
H	1.20618600	4.66650600	0.29229900				
H	4.12313500	3.24689800	-1.65504000				
H	3.55215100	3.58663600	-0.02917700				
H	2.69502100	5.30986900	-1.58781000				
H	1.97814200	4.06906500	-2.60649800				
H	1.97328400	-2.06585500	-1.23949400				
H	2.86518900	-0.57809200	-1.47022400				
H	1.34046700	-1.69748100	2.43543400				
H	1.03866800	-2.71100900	1.02096600				
H	4.42524400	-2.48263500	-1.38689300				
H	4.70617600	-1.43703000	-0.00049200				
H	2.84476300	-3.64346700	2.44797800				
H	3.75674400	-2.14592700	2.32058400				
H	4.66000300	-3.81675200	0.72635200				
H	3.06570100	-4.01956300	0.00508000				
H	-2.08322400	-0.44796700	1.56184600				
H	-0.85603200	-1.66330300	1.91021100				
H	-0.01752200	2.58438400	2.17547900				
H	-1.59885400	1.99920200	1.65827100				
H	-2.43482000	-1.45872300	3.81429800				
H	-0.83216100	-0.93161600	4.30925300				
				<b>2-RCB-0</b>			
				Ru	-0.01404800	1.09579300	-0.04481800
				Cl	0.64287900	1.12783400	-2.38081500
				Cl	-0.67529200	1.30202500	2.27811300
				N	1.10010300	-1.68697500	0.13216800
				N	-1.07509600	-1.69875900	-0.15753300
				C	0.00871900	-0.91995900	-0.01102900
				C	-1.32667700	2.49251500	-0.44903800
				C	0.78418400	-3.11623400	-0.01558000
				C	-0.74568300	-3.12326900	0.00606100
				C	2.42917100	-1.15393300	0.15364400
				C	-2.40910100	-1.17727000	-0.11623300
				C	2.95121900	-0.72107800	1.38284100
				C	4.21783400	-0.13254500	1.38120600
				C	4.95890400	0.01887500	0.20789100
				C	4.42083000	-0.46635800	-0.98694000
				C	3.16211800	-1.06494200	-1.04177300
				C	-3.00859600	-0.78446900	-1.32261900
				C	-4.27924800	-0.20682400	-1.25923700
				C	-4.94658100	-0.02424200	-0.04721500
				C	-4.32720200	-0.46050100	1.12755300
				C	-3.06287600	-1.04795500	1.12123500
				C	2.18146100	-0.88408600	2.65508700
				C	6.29654500	0.69314400	0.22321200
				C	2.63949900	-1.61707600	-2.33147300
				C	-2.30810800	-0.96108700	-2.63269100
				C	-6.29834000	0.62034900	0.00127900
				C	-2.44569000	-1.53920300	2.39396400
				C	-0.03400700	3.32557000	-0.11865800
				C	1.28089400	2.53607700	0.23915300
				H	-1.62614300	2.55818100	-1.49654300
				H	1.23237300	-3.69284900	0.79975200
				H	1.19198900	-3.49044300	-0.96361500

H	-1.18746300	-3.71356500	-0.80282000
H	-1.15144800	-3.49068000	0.95796200
H	4.63477700	0.21396800	2.32569000
H	4.99288000	-0.37021800	-1.90882600
H	-4.75595400	0.11222800	-2.18513000
H	-4.83602600	-0.32937600	2.08168500
H	1.74204300	-1.88451300	2.73719400
H	2.82738000	-0.72483500	3.52179100
H	1.34797400	-0.17313600	2.72246500
H	6.71309900	0.74119600	1.23254600
H	7.01717800	0.17676700	-0.41791800
H	6.22359000	1.72161800	-0.14825900
H	2.91801900	-2.67292000	-2.44649300
H	1.55203200	-1.53654600	-2.40454000
H	3.05648300	-1.07520800	-3.18296300
H	-3.00425400	-0.83345400	-3.46518400
H	-1.49215900	-0.23721500	-2.75887900
H	-1.85138700	-1.95316700	-2.71823800
H	-6.27708900	1.54483400	0.58818700
H	-6.66209300	0.86993400	-0.99852000
H	-7.03874100	-0.03370300	0.47360800
H	-2.72775900	-2.58210500	2.58990600
H	-1.35457200	-1.47458600	2.37481200
H	-2.78087800	-0.94123300	3.24384900
H	-0.27589800	3.92894900	0.75743700
H	0.19661000	3.89277000	-1.02173300
H	2.05957800	2.62413600	-0.51987000
H	1.59531900	2.67645200	1.27505000
H	-2.12098500	2.61335000	0.28922900

**1a-RCB-1 $\alpha$**

Ru	-0.51815000	0.57844900	1.28823300
Cl	0.10808900	2.89087200	0.76820800
Cl	-0.87918900	-1.69320900	2.01895300
C	-2.35261400	1.24580500	0.84242800
C	-3.32552700	0.42497300	0.10761000
C	-3.82500600	0.94734400	-1.09754900
C	-4.75524000	0.24207800	-1.85378100
C	-5.20601500	-1.00204400	-1.41841800
C	-4.71493800	-1.53457500	-0.22433400
C	-3.78404600	-0.83399000	0.53062200
C	-2.31061700	1.20976000	2.42086500
C	-0.90413600	1.17847900	3.11743100

H	-2.31204500	2.27280800	0.47159200
H	-3.47014100	1.91971600	-1.43420800
H	-5.12859500	0.66555500	-2.78280900
H	-5.93670800	-1.55444200	-2.00353600
H	-5.06021100	-2.50588000	0.11951700
H	-3.38536100	-1.27205900	1.44102300
H	-2.92993300	0.39253400	2.79201400
H	-2.70208800	2.19788700	2.67581000
H	-0.52987400	2.16242600	3.40379100
H	-0.84690600	0.40604600	3.88622000
P	1.27305600	-0.08678800	-0.06775200
C	2.05620600	-1.71536400	0.15054000
C	2.40547700	-2.50283700	-0.95332700
C	2.39194800	-2.14360200	1.43868100
C	3.07888700	-3.70653100	-0.76709900
H	2.14049900	-2.18225300	-1.95904200
C	3.07250000	-3.34368900	1.61943700
H	2.09512200	-1.55016500	2.29950600
C	3.41544800	-4.12612400	0.51870100
H	3.33894100	-4.31654800	-1.62753100
H	3.32208100	-3.67404600	2.62355700
H	3.93889900	-5.06735100	0.66256200
C	0.15862800	-0.21593800	-1.49499500
C	-0.05154400	0.89153900	-2.33139700
C	-0.61679200	-1.37461400	-1.66114600
C	-0.99265400	0.81596400	-3.35247800
H	0.50865600	1.80894300	-2.16387100
C	-1.55598200	-1.43841100	-2.68494400
H	-0.49573000	-2.20984500	-0.97413300
C	-1.74028700	-0.34773000	-3.53261700
H	-1.15176100	1.67381200	-4.00018200
H	-2.16134300	-2.33257300	-2.80387300
H	-2.48381400	-0.39780100	-4.32389100
C	2.66058600	0.99360900	-0.53144900
C	3.20141900	1.87850100	0.40615500
C	3.25646300	0.86503400	-1.79182800
C	4.33004500	2.62659100	0.08249600
H	2.71719100	2.00249400	1.37090400
C	4.37946700	1.62139100	-2.11284600
H	2.83771300	0.17869300	-2.52555800
C	4.91782200	2.50081900	-1.17440600
H	4.74191800	3.31886800	0.81085100
H	4.83352600	1.52299200	-3.09480700
H	5.79443800	3.09133300	-1.42572900

**1b-RCB-1 $\alpha$** 

Ru	0.00000000	0.00000000	0.00000000	H	-3.46763248	-0.94268907	-4.17387916
Cl	0.00000000	0.00000000	2.44157020	H	-3.45919926	-2.66263708	-3.80205846
Cl	0.57527048	0.00000000	-2.37855722	H	-5.92492502	-2.41090238	-0.95219822
P	-0.95753643	-2.21569952	-0.06541458	H	-4.91376900	-3.53584454	-1.84600047
C	-0.84475074	1.77324926	0.19986525	H	-5.71789687	-1.73707853	-3.35694733
C	-1.86182626	2.11942423	-0.80637269	H	-5.02796757	-0.51145239	-2.29740212
C	-3.20215490	2.03101413	-0.38730107	H	-1.83207632	-1.55777938	2.90326782
C	-4.24711870	2.23261168	-1.28147986	H	-3.22394463	-1.89472616	1.90629900
C	-3.97308616	2.54534361	-2.61217063	H	0.42713107	-4.23344803	1.67640906
C	-2.64773237	2.66046076	-3.03403393	H	0.28256028	-2.81984832	2.72209270
C	-1.60117517	2.44769624	-2.14506826	H	-3.62052251	-2.76889488	4.16836541
C	-2.46442199	-2.38938089	-1.17850799	H	-3.49711726	-4.12711082	3.05692921
C	-1.45296058	-3.12732009	1.48842384	H	0.08927490	-4.94953902	4.00448735
C	0.31648739	-3.36177507	-0.79792467	H	-1.23807856	-5.47162681	2.97809594
C	-2.39726596	-1.44201740	-2.37900505	H	-2.14279379	-4.57946780	5.09592674
C	-3.82602439	-2.27031238	-0.48584648	H	-1.26910302	-3.06826624	4.86641193
C	-2.39647271	-2.36963645	2.43663158	H	1.94541733	-1.96012268	-0.83528556
C	-0.27198037	-3.67120762	2.30426806	H	1.76374553	-2.74950913	0.72722590
C	1.72347467	-2.92534763	-0.35471932	H	-0.70365829	-3.86940833	-2.65882873
C	0.28778127	-3.54806616	-2.31804276	H	0.50028491	-2.58766593	-2.80260069
C	-3.54957877	-1.66206475	-3.35091143	H	3.76515461	-3.62184772	-0.45731433
C	-4.96640803	-2.50053576	-1.47638879	H	2.57455624	-4.90002531	-0.25484953
C	-4.89755474	-1.54324224	-2.65629113	H	1.30573986	-4.70801631	-3.82587373
C	-2.92221694	-3.30789237	3.51799511	H	1.07673526	-5.55696972	-2.30373017
C	-0.76618939	-4.58316726	3.42530761	H	3.46425144	-4.93931224	-2.57659479
C	-1.77181746	-3.88658053	4.33191650	H	3.02319219	-3.24912824	-2.79279363
C	2.76976213	-3.95011310	-0.77655415	H	2.41211716	0.83523088	-0.61911714
C	1.33385815	-4.57865956	-2.73800298	H	2.17314458	0.91504138	1.21683898
C	2.73236016	-4.17847414	-2.28252027	H	0.89121955	2.76291893	0.85788328
C	0.68911574	2.09672737	0.01505776	H	0.86022128	2.54870936	-0.96281321
C	1.72534794	0.93277308	0.22316909				
H	-1.16593526	1.96748669	1.22732284				
H	-3.41030217	1.78323097	0.65265342	<b>2-RCB-1<math>\alpha</math></b>			
H	-5.27555186	2.14606175	-0.93985796	Ru	-0.31399200	-0.80219000	-0.28626300
H	-4.78637142	2.70087912	-3.31607873	Cl	-0.85785300	-0.10999800	-2.56145700
H	-2.42657259	2.90572565	-4.06922726	Cl	-0.07059900	-1.63242500	1.98345300
H	-0.57721930	2.49306633	-2.50124241	N	-1.98274800	1.45909400	0.80583400
H	-2.38122726	-3.42909005	-1.54072981	N	0.12810500	2.01889900	0.59323700
H	-2.00040552	-3.99729023	1.07564517	C	-0.76893600	1.04057700	0.40169600
H	0.09284529	-4.34259084	-0.34372709	C	1.22937700	-1.72438700	-1.15723900
H	-2.42060606	-0.40446198	-2.01108563	C	2.57150100	-1.89177300	-0.57415300
H	-1.44227418	-1.53461968	-2.89814071	C	3.65320000	-1.42413200	-1.34108000
H	-3.91308611	-2.99158067	0.33263118	C	4.96295000	-1.55976300	-0.89557000
H	-3.92806908	-1.26750974	-0.04443979	C	5.22084900	-2.15601000	0.33614500
				C	4.15689800	-2.62334900	1.10993400

C	2.84744000	-2.49789300	0.66256100	H	-3.43550900	1.71105400	-2.78309100
C	-1.95888600	2.88132000	1.18552200	H	1.69100600	3.28648600	-2.76342600
C	-0.46318200	3.16676600	1.29787300	H	0.47804200	2.06313900	-2.34063800
C	-3.19588800	0.77140700	0.46650700	H	0.45684200	3.63138800	-1.54225700
C	1.53637400	1.89217900	0.36210000	H	6.25228800	0.96746300	0.29358400
C	-3.77315300	-0.08557400	1.41748600	H	5.98308000	1.40834400	-1.40122300
C	-4.90621200	-0.80794000	1.03992900	H	6.21741900	2.66356200	-0.19150000
C	-5.47345300	-0.68128700	-0.23040100	H	2.05138500	1.86731800	3.44543000
C	-4.90831700	0.23208000	-1.12212900	H	0.79907100	0.81899100	2.74207000
C	-3.77745000	0.98275700	-0.79453200	H	2.37699700	0.16317100	3.12266000
C	2.03757500	2.31921700	-0.88163000	H	0.48686700	-3.57468600	-0.24118900
C	3.41113700	2.22526600	-1.09726500	H	0.09204600	-3.29226100	-2.00185500
C	4.28007800	1.73209300	-0.11885900	H	-1.99274900	-2.40480100	-1.53477000
C	3.74529300	1.32509900	1.10197900	H	-1.72600000	-2.94159500	0.21586100
C	2.37697500	1.40973900	1.37743900				
C	-3.20383500	-0.21277100	2.79404700				
C	-6.65728300	-1.50933500	-0.62749200	Ru	-0.75007500	-0.31659500	-0.35331700
C	-3.25963700	2.01444400	-1.74899700	Cl	-1.10536400	2.09011800	-0.33303600
C	1.12258400	2.85445600	-1.93649000	Cl	-0.36032900	-2.70095600	-0.37175600
C	5.75658600	1.68434900	-0.36674800	C	-2.17190500	-0.56267000	-1.67296700
C	1.86587500	1.04966100	2.73728000	C	-2.92046700	-0.91859700	-0.30590800
C	0.13903300	-2.86797600	-0.99615000	C	-2.15169100	-0.54173500	1.00921700
C	-1.32917300	-2.44155200	-0.66956800	H	-2.56421600	0.33993700	-2.14710900
H	1.28692400	-1.40126600	-2.20043200	H	-2.97988900	-2.01078800	-0.30449600
H	3.45146300	-0.95248700	-2.30126700	H	-2.50794500	0.37560700	1.48422100
H	5.78320600	-1.19771300	-1.51020200	H	-2.01420300	-1.39831000	1.67280600
H	6.24327100	-2.26027700	0.69101600	H	-2.09668700	-1.44338100	-2.31368500
H	4.34944200	-3.09194200	2.07164000	C	-4.29496600	-0.28016300	-0.31447300
H	2.02722800	-2.84484700	1.28386100	C	-5.40335100	-1.12956600	-0.30737500
H	-2.50150900	3.03823000	2.12243100	C	-4.48856000	1.10351700	-0.32622000
H	-2.44436600	3.47982500	0.40243500	C	-6.69447300	-0.60267200	-0.31172800
H	-0.15902000	4.10543800	0.82408900	H	-5.25470000	-2.20747400	-0.29806200
H	-0.11400900	3.17923500	2.33954600	C	-5.77924800	1.62386600	-0.33157400
H	-5.35947400	-1.48429800	1.76332700	H	-3.62442800	1.76451600	-0.33198200
H	-5.35645300	0.36671300	-2.10550400	C	-6.88628100	0.77578600	-0.32425900
H	3.81400200	2.54919800	-2.05628300	H	-7.54813400	-1.27516600	-0.30573500
H	4.40817400	0.92604700	1.86890000	H	-5.91925700	2.70150100	-0.34174700
H	-3.00636100	0.76818600	3.24023800	H	-7.89189800	1.18735400	-0.32867000
H	-3.89218900	-0.75058700	3.45036800	P	1.54884500	0.10150200	-0.09045900
H	-2.24763400	-0.74856500	2.78540500	C	2.34155100	1.69810600	-0.44625800
H	-7.28591600	-1.75487800	0.23286000	C	3.38954000	2.15207400	0.36366700
H	-7.27800800	-0.99923400	-1.36916300	C	1.96845400	2.43320900	-1.57577300
H	-6.34082600	-2.45909700	-1.07406500	C	4.05750400	3.33013000	0.04593100
H	-3.77271100	2.97307700	-1.59418000	H	3.67703500	1.59107800	1.25065200
H	-2.18412100	2.17725400	-1.64969800				

**1a-RCB-1 $\beta$**

C	2.64565400	3.60733900	-1.89335000
H	1.12908300	2.10167900	-2.18114600
C	3.68797400	4.05639900	-1.08504200
H	4.86508000	3.68117600	0.68219600
H	2.34715100	4.17916200	-2.76701100
H	4.20934700	4.97686100	-1.33309500
C	1.38060900	-0.02969800	1.71088800
C	1.43785900	-1.28507100	2.33421600
C	1.01131400	1.10474700	2.44968500
C	1.16201000	-1.39262500	3.69321400
H	1.66374300	-2.17139400	1.74582400
C	0.73520500	0.98522400	3.80708100
H	0.91535200	2.06676700	1.95152700
C	0.81346200	-0.26061900	4.42945000
H	1.20654600	-2.36534100	4.17443400
H	0.44715000	1.86417000	4.37613800
H	0.59058700	-0.35095200	5.48916900
C	2.75150500	-1.14283300	-0.64458100
C	2.51974000	-1.82174600	-1.84464100
C	3.92882200	-1.38392200	0.07332500
C	3.46006400	-2.72724300	-2.32606600
H	1.58835900	-1.66403300	-2.38296800
C	4.86134600	-2.29899700	-0.40656600
H	4.10974600	-0.86714000	1.01421700
C	4.62890100	-2.96770100	-1.60774300
H	3.26987200	-3.25794200	-3.25432900
H	5.76844700	-2.49096500	0.15966700
H	5.35783400	-3.68224900	-1.97942900

**1b-RCB-1 $\beta$**

Ru	-0.84429800	-0.39370200	-0.24423800
Cl	-1.56980200	1.84401400	0.28758200
Cl	-0.36175900	-2.76459800	-0.56455000
C	-2.01761000	-0.52328300	-1.80697000
C	-2.95776900	-1.06135300	-0.66893000
C	-2.36891900	-1.04969400	0.81020200
H	-2.34955100	0.42430400	-2.23613800
H	-3.01851300	-2.13540200	-0.87625700
H	-2.84677300	-0.30594200	1.45223000
H	-2.28193500	-2.05796200	1.21971400
H	-1.76773500	-1.30082800	-2.53070500
C	-4.32618400	-0.41540900	-0.62736800
C	-5.38813300	-1.22572400	-0.20750800

C	-4.58610400	0.91182800	-0.97530000
C	-6.68755900	-0.72930100	-0.15833600
H	-5.18995300	-2.25913400	0.07155000
C	-5.88577400	1.40971700	-0.91518000
H	-3.77216600	1.56684200	-1.26750400
C	-6.94070200	0.59403200	-0.51240100
H	-7.50053300	-1.37757300	0.15735800
H	-6.07173500	2.44546400	-1.18605600
H	-7.95283000	0.98719000	-0.47284400
P	1.49510300	0.15207200	0.08082600
C	2.77495800	-1.10705800	-0.41884200
C	1.66632100	0.25894200	1.93142300
C	2.28341800	1.74253000	-0.54832500
C	2.57662900	-1.60330800	-1.85979300
C	2.96238400	-2.30646300	0.51838800
C	0.74165900	-0.77150000	2.59897200
C	1.42574700	1.64230600	2.54133200
C	1.35962300	2.96210400	-0.53783100
C	2.97919200	1.65029400	-1.91315700
C	3.77664600	-2.42465700	-2.31465000
C	4.15427900	-3.14497600	0.05962900
C	4.00294800	-3.60983600	-1.38351500
C	0.96260700	-0.81429600	4.10625800
C	1.63843500	1.60133300	4.05342500
C	0.75077300	0.56135400	4.72503900
C	2.13462000	4.24193400	-0.83069700
C	3.74759500	2.93497700	-2.21908700
C	2.85332300	4.16449800	-2.16950200
H	3.71325100	-0.52308200	-0.37597300
H	2.71518200	-0.01886500	2.13272200
H	3.07839200	1.89807900	0.20463200
H	1.67478200	-2.22373000	-1.88353700
H	2.39668500	-0.77436200	-2.55148800
H	3.12761800	-1.98101100	1.55244800
H	2.04949600	-2.91440500	0.50949600
H	3.62543700	-2.76613100	-3.34495200
H	4.67757000	-1.79037000	-2.32688000
H	4.27904700	-4.00277900	0.73018300
H	5.07311200	-2.54519200	0.15154300
H	4.88249900	-4.18541800	-1.69387500
H	3.14159500	-4.28905500	-1.45427700
H	-0.29890000	-0.46345900	2.40355300
H	0.85448400	-1.76552300	2.15083300

H	2.09826100	2.38722000	2.10093900	C	-1.57002800	-3.04638800	2.52856700
H	0.39911700	1.96339200	2.31381400	C	2.40849300	0.25060100	2.69799500
H	0.29483400	-1.55446500	4.56043400	C	6.10756400	2.33437300	-0.00814400
H	1.98880100	-1.15726200	4.30895100	C	3.66477000	-1.68338300	-1.79707200
H	1.45680100	2.59558900	4.47627400	C	-0.89651500	2.39365500	-0.84679800
H	2.69292500	1.36476000	4.26186600	C	-1.71786900	1.03797100	-1.03612200
H	0.94063400	0.53406800	5.80388900	H	0.35519800	2.64427700	1.00281700
H	-0.30223600	0.85172700	4.60080700	H	1.10807400	-4.32670600	-0.39215700
H	0.57710200	2.81672000	-1.29394200	H	0.53712300	-4.35806800	1.28854600
H	0.81877000	3.05023600	0.40438600	H	2.40032100	-3.05446300	2.04716300
H	3.67686900	0.80951500	-1.95717700	H	3.15336600	-3.42688900	0.48510300
H	2.22478600	1.47895100	-2.69503200	H	-3.67418400	-2.68342100	-2.41449100
H	1.45043100	5.09695600	-0.80425500	H	-4.17497500	-3.12163200	1.82220100
H	2.87153400	4.41220100	-0.03016100	H	4.40224200	1.97552900	2.08213300
H	4.23512700	2.84292500	-3.19627800	H	5.47977200	0.32972100	-1.73019000
H	4.55642800	3.04638300	-1.48146200	H	-0.10036800	-3.18934100	-2.40721700
H	3.43784100	5.07289400	-2.35425800	H	-1.52482100	-2.80037300	-3.38221700
H	2.10816500	4.10433200	-2.97572200	H	-0.58729600	-1.52037500	-2.60553500

**2b-RCB-1 $\beta$**

Ru	-0.04561400	0.36791700	-0.26934400	H	-6.03815700	-3.74694300	0.07401200
Cl	-1.11733200	0.29042100	1.91382500	H	-6.04836800	-2.00172800	-0.13240600
Cl	1.01685200	0.48218300	-2.43717000	H	-1.26350300	-4.07905500	2.74207400
N	0.07684300	-2.58831400	0.22395600	H	-0.70095700	-2.39448000	2.65625600
N	2.02738800	-1.63357000	0.52745400	H	-2.30356300	-2.76404000	3.28689900
C	0.74755900	-1.42616300	0.18188400	H	2.86287200	0.85210600	3.48893100
C	0.43175400	2.26333200	-0.01886200	H	1.39717300	0.63581000	2.51993100
C	0.97183100	-3.72033500	0.51372900	H	2.27165000	-0.76634500	3.08101600
C	2.25444700	-3.02248800	0.95890500	H	5.88287900	2.99024400	-0.85599300
C	-1.33343100	-2.72796300	0.02801500	H	6.19227400	2.96171100	0.88252300
C	3.06731200	-0.65445400	0.42855400	H	7.09058900	1.89374400	-0.20343900
C	-1.86014200	-2.66598200	-1.27100600	H	3.93108100	-2.69422400	-1.46281500
C	-3.24885600	-2.73857900	-1.41319600	H	2.61764500	-1.69906200	-2.11843000
C	-4.09784300	-2.88854600	-0.31675900	H	4.27589400	-1.45720300	-2.67324300
C	-3.52768100	-2.99607300	0.95529400	H	-0.57614200	2.65392800	-1.85986400
C	-2.15094800	-2.92144700	1.15461200	H	-2.60018200	0.97216000	-0.39472700
C	3.25009700	0.27562100	1.46087200	H	-1.88090900	0.81094500	-2.09280800
C	4.24930300	1.24003400	1.29355400	H	1.30549900	2.59683900	-0.58172300
C	5.05463300	1.28109600	0.15562500	C	-1.83062500	3.44131400	-0.27769700
C	4.85985000	0.31290700	-0.83520400	C	-2.36105800	4.38248000	-1.16458600
C	3.87538700	-0.66474200	-0.72129100	C	-2.19140200	3.49594400	1.07157400
C	-0.97782800	-2.53715300	-2.47367900	C	-3.23426100	5.36958200	-0.71149700
C	-5.58506300	-2.92728000	-0.49197900	H	-2.08277000	4.34279400	-2.21589600
				C	-3.06826200	4.48006500	1.51907200



H	-1.79965500	2.75458100	1.76295500
C	-3.59215400	5.42062200	0.63314500
H	-3.63330200	6.09719900	-1.41307400
H	-3.34396600	4.50975200	2.56976600
H	-4.27442600	6.18778200	0.98891000

***1a-trans-RCB-2 $\alpha\alpha$***

Ru	0.07950400	0.86043200	0.34765300
Cl	-0.75322700	0.42232300	2.57791200
Cl	1.05118700	1.05973400	-1.91243200
C	1.15477700	2.31770600	1.18319500
C	2.45389000	2.77743900	0.67252800
C	3.59391500	2.42937600	1.41601800
C	4.86631900	2.79797800	0.99418300
C	5.02244800	3.53899800	-0.17584600
C	3.89794900	3.89947900	-0.91954600
C	2.62811900	3.51864000	-0.50495200
C	-0.19450500	3.02029400	0.75646600
C	-1.10490600	2.32922600	-0.32762600
H	1.15680100	2.16249700	2.26679300
H	3.46689000	1.85907100	2.33494000
H	5.73454000	2.51681700	1.58383900
H	6.01362100	3.83743300	-0.50620800
H	4.01321100	4.47270400	-1.83533000
H	1.76645900	3.77214400	-1.11647600
H	0.12927500	3.93445000	0.25272600
H	-0.77736400	3.22554500	1.65597800
H	-0.81539200	2.63047800	-1.33803600
C	-2.56311900	2.26492200	-0.16191000
C	-3.34235400	2.29349700	-1.33182500
C	-3.21791600	2.16073300	1.07627100
C	-4.72987600	2.22398100	-1.26948900
H	-2.83962200	2.36462700	-2.29472900
C	-4.60374900	2.09628500	1.13581900
H	-2.63186900	2.09809900	1.98844400
C	-5.36643100	2.12654200	-0.03368400
H	-5.31379200	2.24470100	-2.18602900
H	-5.09415000	2.01570200	2.10226300
H	-6.45065100	2.07456500	0.02037300
P	0.20758600	-1.44562800	-0.08021500
C	0.17957000	-2.60795600	1.32074400
C	-0.62065400	-3.75496600	1.31801100

C	1.05828500	-2.37935000	2.38497200
C	-0.54245600	-4.66074200	2.37358900
H	-1.31072500	-3.93779300	0.49665300
C	1.14032900	-3.29064600	3.43145700
H	1.66135100	-1.47379100	2.40252900
C	0.33868300	-4.43109100	3.42790400
H	-1.17200000	-5.54606400	2.37040300
H	1.81986500	-3.10287500	4.25773300
H	0.39654700	-5.13830700	4.25073600
C	-1.42073600	-1.49143900	-0.87476300
C	-1.53836500	-1.39029300	-2.26877600
C	-2.56984800	-1.45038000	-0.06822700
C	-2.80005200	-1.29653000	-2.84763600
H	-0.64334100	-1.35813500	-2.88552500
C	-3.82594700	-1.35825100	-0.65880300
H	-2.46937500	-1.46319700	1.01612000
C	-3.94149700	-1.28840400	-2.04625200
H	-2.89035000	-1.21869200	-3.92740200
H	-4.71235500	-1.31770600	-0.03240700
H	-4.92404600	-1.20272700	-2.50318900
C	1.43043700	-2.19402300	-1.19717000
C	2.71747000	-1.65345000	-1.27595000
C	1.12813300	-3.37758000	-1.87982400
C	3.69157800	-2.29278700	-2.03668800
H	2.94066900	-0.71903100	-0.76624000
C	2.10295600	-4.00580300	-2.64956200
H	0.12874300	-3.80455000	-1.81407400
C	3.38517000	-3.46422000	-2.72658300
H	4.68783200	-1.86506000	-2.10186300
H	1.86050000	-4.91798600	-3.18770200
H	4.14573000	-3.95558500	-3.32728900

***1a-cis-RCB-2 $\alpha\alpha$***

Ru	0.22989000	-0.73023700	0.67756300
Cl	-0.06138900	0.25957800	2.90701300
Cl	0.46166900	-1.50989000	-1.60829200
C	1.92200200	-1.46256400	1.46937500
C	3.19574400	-1.42442600	0.74024800
C	4.17961600	-0.55400300	1.24533700
C	5.40730100	-0.41214300	0.61034300
C	5.68423300	-1.15216500	-0.53857700
C	4.72207700	-2.02824000	-1.04360000

C	3.48886100	-2.16200700	-0.41748800
C	0.95223900	-2.70420500	1.39137200
C	-0.56836800	-2.35442700	1.53368200
H	2.02953000	-1.12127300	2.50272700
H	3.95881100	0.01770800	2.14556200
H	6.15094700	0.26903000	1.01581600
H	6.64419500	-1.04923400	-1.03746900
H	4.93132100	-2.60519800	-1.94017500
H	2.73391700	-2.81337300	-0.84649600
H	-0.83131300	-2.15495000	2.57559300
H	1.16674000	-3.20547100	2.34024400
H	1.16749600	-3.35087300	0.54005500
C	-1.62265200	-3.08083200	0.81318300
C	-2.93857500	-2.89122300	1.27463400
C	-1.42038300	-3.89770100	-0.30996300
C	-4.01747400	-3.48031700	0.62698000
H	-3.10048100	-2.25505900	2.14323300
C	-2.50016700	-4.49647100	-0.94813400
H	-0.41972200	-4.03750800	-0.70638800
C	-3.80136300	-4.28859700	-0.48864700
H	-5.02602800	-3.31316600	0.99576200
H	-2.32501000	-5.12433900	-1.81740400
H	-4.64044600	-4.75661700	-0.99635400
C	-2.04098400	1.18095200	-1.12442300
C	-0.80825300	2.79391200	0.88905500
C	0.85683400	1.79953200	-1.28431600
C	-2.67268400	2.32351900	-1.63736900
C	-2.62941300	-0.07597000	-1.30866400
C	0.00744400	3.92795000	0.85968700
C	-1.90739000	2.75495300	1.75740000
C	2.15266700	1.75760500	-0.74851400
C	0.67811800	2.03783100	-2.64864800
C	-3.86294600	2.20339000	-2.34629300
H	-2.23184300	3.30549300	-1.47509000
C	-3.83167400	-0.18732900	-2.00315900
H	-2.14472400	-0.97097900	-0.92354600
C	-0.27865200	5.01475400	1.68538800
H	0.86322100	3.96919300	0.19078600
C	-2.19178800	3.84228500	2.57261100
H	-2.53010400	1.86458300	1.80155200
C	3.25551100	1.95921600	-1.57035000
H	2.29598100	1.55203500	0.31333600
C	1.78632700	2.25006200	-3.46469100

H	-0.32179300	2.03254100	-3.07602800
C	-4.44443900	0.94774900	-2.52715700
H	-4.34172800	3.09121600	-2.75020400
H	-4.28203700	-1.16734300	-2.13224700
C	-1.37649300	4.97423300	2.53951100
H	0.35920700	5.89362000	1.65569000
H	-3.04429200	3.80295700	3.24451800
C	3.07251800	2.20718300	-2.92980100
H	4.25580900	1.90733900	-1.14967200
H	1.64365700	2.43200500	-4.52627000
H	-5.37985800	0.85817200	-3.07296300
H	-1.59733300	5.82205900	3.18211700
H	3.93364400	2.35686300	-3.57527900
P	-0.50162900	1.34675000	-0.16843200

*Ib-trans-RCB-2 $\alpha\alpha$*

Ru	-0.29561700	-0.91738000	-0.13944600
Cl	0.61988900	-1.63980200	2.03236300
Cl	-1.41204900	-0.32613900	-2.20839100
C	-1.79968000	-2.15685200	0.36397000
C	-3.20263200	-1.99362000	-0.04315800
C	-4.08763800	-1.49071700	0.92674400
C	-5.42891400	-1.27055400	0.63252300
C	-5.92109500	-1.57698100	-0.63418200
C	-5.06006300	-2.10067800	-1.59983800
C	-3.71675700	-2.29938400	-1.31223700
C	-0.79608100	-3.05321800	-0.45083900
C	0.45237800	-2.41506000	-1.18752600
H	-1.69731800	-2.35210500	1.43617300
H	-3.70539000	-1.26805600	1.92256900
H	-6.09140600	-0.87032600	1.39560200
H	-6.96974700	-1.41467100	-0.86777400
H	-5.43727000	-2.34353200	-2.58940500
H	-3.05334300	-2.66725600	-2.08866800
H	-1.38309000	-3.48251000	-1.26503400
H	-0.41673800	-3.79516100	0.25410200
H	0.23472900	-2.27610600	-2.25113800
C	1.83126500	-2.87154200	-0.94307900
C	2.80088200	-2.41881800	-1.85587200
C	2.24907400	-3.67311400	0.12861600
C	4.14484900	-2.73118000	-1.68948800
H	2.48273300	-1.79875400	-2.69304000
C	3.59106400	-3.99786300	0.28524900

H	1.52734500	-4.01493400	0.86326200
C	4.54587400	-3.52347200	-0.61484000
H	4.87833800	-2.36037400	-2.40041400
H	3.89559100	-4.61739500	1.12422400
H	5.59481200	-3.77362000	-0.48038100
P	0.41287500	1.37721200	0.19192600
C	0.73493900	2.62081400	-1.18745200
C	2.01190600	1.52787400	1.14459000
C	-0.88550900	2.18375100	1.25725200
C	-0.28531100	2.67570500	-2.32883100
C	2.13681700	2.55247200	-1.81402500
C	3.02251100	0.47949200	0.65153200
C	1.92942500	1.50950100	2.67480800
C	-1.44764800	1.15111300	2.24270200
C	-2.02953700	2.85477200	0.49093200
C	-0.07157400	3.92588300	-3.17566900
C	2.38420300	3.76366100	-2.71428000
C	1.32085100	3.92068900	-3.79120000
C	4.39955000	0.72344800	1.25484900
C	3.31399100	1.75385300	3.27204600
C	4.32752600	0.72795200	2.77727600
C	-2.46387800	1.76686600	3.19466600
C	-3.04272600	3.46896600	1.45466100
C	-3.59617000	2.44168900	2.43235100
H	0.67796900	3.57106300	-0.62159900
H	2.38464700	2.52951000	0.86662400
H	-0.35258800	2.96717500	1.82238300
H	-0.14934600	1.78858200	-2.95436400
H	-1.31402300	2.61366600	-1.97329100
H	2.92850400	2.51624500	-1.06120300
H	2.21655500	1.62545100	-2.40232500
H	-0.83853900	3.97832600	-3.95630600
H	-0.19915400	4.82648500	-2.55419500
H	3.38247400	3.68830600	-3.16073100
H	2.39776800	4.66682600	-2.08579200
H	1.49925500	4.83192800	-4.37361400
H	1.39276400	3.08112500	-4.49725800
H	2.66036600	-0.51115200	0.95198900
H	3.08010900	0.46385100	-0.44366400
H	1.22871700	2.27104200	3.03946200
H	1.55410900	0.53633900	3.00764600
H	5.10087700	-0.04154500	0.90175300
H	4.79126500	1.69151700	0.90351300

H	3.25053400	1.73669900	4.36606300
H	3.65782400	2.76350000	2.99800300
H	5.31466400	0.92540400	3.21084500
H	4.02528000	-0.27110300	3.12238100
H	-1.94135100	0.35907400	1.65388300
H	-0.64877500	0.64846200	2.79466900
H	-1.64498600	3.63561800	-0.17390600
H	-2.52662300	2.10704800	-0.14623400
H	-2.85028600	0.99523300	3.87077800
H	-1.95606100	2.50763000	3.83110100
H	-3.85179000	3.93783900	0.88348600
H	-2.55435000	4.27797400	2.01858600
H	-4.30563300	2.91145300	3.12290400
H	-4.15999900	1.68006700	1.87404600

*Ib-cis-RCB-2 $\alpha\alpha$*

Ru	-0.48698300	0.42905500	-0.84114000
Cl	-0.06129100	-0.93069500	-2.84173100
Cl	-1.27677300	1.65303500	1.11522100
C	0.03936700	1.94582000	-1.98685200
C	0.81960900	3.01670000	-1.34374000
C	2.20903800	2.98160400	-1.56303600
C	3.05695800	3.88944400	-0.93999100
C	2.53042800	4.86630000	-0.09564700
C	1.15205000	4.92457500	0.11358900
C	0.30360500	4.00914400	-0.49814800
C	-1.53763900	1.96118300	-2.05508700
C	-2.30312900	0.62914900	-1.71771800
H	0.47028500	1.61408000	-2.93662900
H	2.61494700	2.21516700	-2.22237900
H	4.12873100	3.83595600	-1.11445300
H	3.18841800	5.57954200	0.39344600
H	0.73446400	5.68369100	0.76933400
H	-0.76074900	4.04389400	-0.28841300
H	-2.33620100	-0.03448400	-2.58466700
H	-1.71988200	2.05378400	-3.12994000
H	-1.94213400	2.79625200	-1.48281400
C	-3.57205400	0.62717600	-0.97634300
C	-4.27797500	-0.58984700	-0.95773100
C	-4.12608800	1.72419000	-0.29941500
C	-5.46961200	-0.71983900	-0.25534400
H	-3.86051100	-1.44310000	-1.49128400
C	-5.32975600	1.60004000	0.38235900

H	-3.60538500	2.67602200	-0.28850400
C	-6.00169500	0.37789300	0.41919500
H	-5.98868900	-1.67484700	-0.24275700
H	-5.74242300	2.46194800	0.89949900
H	-6.93757000	0.28535200	0.96337900
P	0.90228000	-1.07904700	0.43745500
C	-0.27791600	-1.96289900	1.57847000
C	2.19740300	-0.30012700	1.56318800
C	1.83847800	-2.49220400	-0.34785500
C	-1.61317500	-2.14658800	0.83798100
C	-0.51769100	-1.30399900	2.94005500
C	1.78319600	1.08240100	2.07227600
C	3.62029700	-0.24248700	0.99553300
C	2.76669300	-2.10656800	-1.51117800
C	0.98039800	-3.68870600	-0.78141500
C	-2.60870600	-2.95196400	1.66190000
C	-1.51631900	-2.11828000	3.75909000
C	-2.83627500	-2.29455000	3.01719400
C	2.77902900	1.64200300	3.08068400
C	4.60302800	0.31088300	2.02509800
C	4.19023400	1.69003400	2.51610500
C	3.68581100	-3.27286300	-1.85708700
C	1.87276100	-4.86674600	-1.16991300
C	2.87135200	-4.49590600	-2.25937800
H	0.17353500	-2.95292700	1.76047600
H	2.22068900	-1.00133100	2.41599000
H	2.46801100	-2.83423400	0.49686400
H	-2.04003500	-1.14583900	0.66048100
H	-1.45930700	-2.59699600	-0.15113600
H	0.42241400	-1.20012900	3.49562100
H	-0.91382600	-0.29366500	2.78435900
H	-3.55218200	-3.04934500	1.11187300
H	-2.22242100	-3.97321500	1.80458900
H	-1.67995300	-1.63062700	4.72671900
H	-1.08995000	-3.10907800	3.97982900
H	-3.54019600	-2.88036600	3.61922400
H	-3.29892200	-1.30848300	2.85997300
H	1.70251400	1.76441600	1.21157700
H	0.78312200	1.05880800	2.50631100
H	3.95956800	-1.23320600	0.67881500
H	3.63348500	0.40254300	0.10416800
H	2.44915800	2.63851000	3.39611300
H	2.77094600	1.01349600	3.98512600

H	5.60932000	0.33184900	1.59079800
H	4.65149200	-0.37981100	2.88063000
H	4.89945700	2.06207300	3.26436800
H	4.21977600	2.39931600	1.67570000
H	2.14403200	-1.86262200	-2.37585300
H	3.34854100	-1.20741300	-1.29777200
H	0.29786900	-4.00690600	0.01437200
H	0.35962200	-3.38562500	-1.63479500
H	4.36717200	-2.98278100	-2.66507200
H	4.32024000	-3.51980200	-0.99057500
H	1.24999200	-5.71100400	-1.48750200
H	2.42146300	-5.20730500	-0.27822600
H	3.52631600	-5.34577300	-2.48347500
H	2.32467500	-4.26807900	-3.18542300

*2-trans-RCB-2 $\alpha$*

Ru	-0.02183900	-0.46185500	-0.21412800
Cl	-0.08228900	-0.84742700	2.21325400
Cl	0.18103800	0.06965800	-2.57654000
N	1.25225900	2.25194500	0.21459200
N	-0.84877500	2.21372800	0.83132200
C	0.15217800	1.48377800	0.30667300
C	-1.42726400	-1.89213100	-0.21496600
C	-2.67932900	-1.87637800	-0.98985800
C	-3.86391100	-2.15108000	-0.28434200
C	-5.09314600	-2.19225900	-0.93170600
C	-5.16587400	-1.94593500	-2.30111200
C	-3.99870900	-1.66370700	-3.01367900
C	-2.76702000	-1.63093200	-2.36975600
C	1.05004200	3.55081900	0.87806800
C	-0.46485000	3.62523900	0.98271100
C	2.55733800	1.83627100	-0.20324200
C	-2.20871900	1.78110600	0.91734500
C	2.99068300	2.23452000	-1.48072900
C	4.26985200	1.85708100	-1.88539400
C	5.12360100	1.13321000	-1.04660900
C	4.67749700	0.80930500	0.23256700
C	3.39454500	1.13868900	0.68029300
C	-2.75048800	1.54771800	2.19618200
C	-4.06417100	1.09546800	2.27577700
C	-4.84663500	0.89196900	1.13269200
C	-4.29164300	1.18238800	-0.10939200
C	-2.97652900	1.64099000	-0.24902500

C	2.09787900	3.02842900	-2.38103900
C	6.47208200	0.68297600	-1.51895800
C	2.95956000	0.72710800	2.04917100
C	-1.94633700	1.79922200	3.43264800
C	-6.24684500	0.37303800	1.25013400
C	-2.46866900	1.98509600	-1.61534000
C	-0.15318500	-2.61392900	-0.81508000
C	1.25671800	-1.94895600	-0.65289100
H	-1.60591300	-2.21622000	0.81403000
H	-3.80517800	-2.33146400	0.78791400
H	-5.99465100	-2.41567200	-0.36691800
H	-6.12462800	-1.97513500	-2.81253400
H	-4.04892000	-1.46739100	-4.08157600
H	-1.86540200	-1.38599400	-2.92557800
H	1.49155300	4.35738000	0.28569600
H	1.54164900	3.53867800	1.86156500
H	-0.81835800	4.01969000	1.93957600
H	-0.91775500	4.21805100	0.17440200
H	4.60938700	2.13981000	-2.88086800
H	5.33578400	0.26234400	0.90652600
H	-4.48690200	0.88747100	3.25802000
H	-4.88939900	1.03525300	-1.00880800
H	1.72010800	3.93339600	-1.88992600
H	2.62835300	3.33635700	-3.28504200
H	1.22529600	2.43597300	-2.67883600
H	6.90173400	1.37262200	-2.25057600
H	7.17771200	0.58066300	-0.68959800
H	6.40741000	-0.29810300	-2.00657800
H	3.79516600	0.77732600	2.75328200
H	2.13352200	1.32921200	2.43711800
H	2.59004100	-0.30515400	2.04888300
H	-2.38411400	1.28771500	4.29299900
H	-0.91860400	1.44277500	3.31677200
H	-1.91432400	2.86969400	3.67515300
H	-6.70898800	0.24487300	0.26764800
H	-6.26830100	-0.59861700	1.75748300
H	-6.88086200	1.04685400	1.83650000
H	-3.14780700	2.69364300	-2.10183000
H	-1.46447000	2.41502400	-1.61225100
H	-2.41335500	1.09692800	-2.25334500
H	-0.32448700	-2.78765600	-1.87911900
H	-0.10297400	-3.54416400	-0.24427000
H	1.68365600	-1.73178700	-1.63624900

C	2.25873000	-2.49960900	0.27156600
C	3.60745400	-2.26577500	-0.04092400
C	1.96102400	-3.23445200	1.43019500
C	4.62705700	-2.72397800	0.78605900
H	3.84495500	-1.70050100	-0.94076800
C	2.97937100	-3.70168900	2.25069600
H	0.92513200	-3.41156100	1.70375200
C	4.31598500	-3.44305700	1.93824500
H	5.66402700	-2.52113100	0.52734000
H	2.73033900	-4.26395300	3.14640100
H	5.10773100	-3.80657000	2.58784200

*2-cis-RCB-2 $\alpha$*

Ru	0.03618100	0.40061700	-0.42182000
Cl	0.78704600	-0.65535500	-2.52676600
Cl	-0.61850600	1.23920400	1.75362700
C	1.26028300	1.90038300	-0.99538700
C	2.16595300	2.60221200	-0.07361100
C	3.54480400	2.43036200	-0.28461300
C	4.48035200	3.04047200	0.54345700
C	4.05560400	3.84820900	1.59617300
C	2.68893400	4.03924800	1.80961700
C	1.75306300	3.42299100	0.98871500
C	-0.17173200	2.45416500	-1.28550000
C	-1.25957400	1.36668500	-1.62189200
H	1.76667500	1.60964500	-1.91967900
H	3.87190200	1.79536100	-1.10660500
H	5.54188400	2.88360900	0.36449100
H	4.78238100	4.32920400	2.24543700
H	2.35034200	4.66737500	2.62907900
H	0.69483500	3.55025200	1.19206200
H	-1.12674400	1.00420200	-2.64635000
H	-0.04560400	2.95546300	-2.24966500
H	-0.51940600	3.15238400	-0.52230600
N	1.31971600	-2.18586200	0.50096500
N	-0.85863000	-2.21159200	0.71257500
C	0.19402400	-1.47742500	0.31163600
C	1.05514100	-3.45925100	1.19145200
C	-0.46181900	-3.57064300	1.11147600
C	2.65630700	-1.79243800	0.17963800
C	-2.22233100	-1.78408000	0.77671100
C	3.31855000	-0.85671200	0.98896800
C	4.63661900	-0.53209500	0.66201700

C	5.28858400	-1.09514100	-0.43521400
C	4.60335800	-2.04190400	-1.19929800
C	3.29169500	-2.41630400	-0.90655900
C	-2.99974900	-1.76224900	-0.39028000
C	-4.33700600	-1.37295800	-0.27390800
C	-4.89919400	-1.01090600	0.94892700
C	-4.09286700	-1.05734500	2.09036200
C	-2.75851900	-1.45199600	2.03358700
C	2.64929000	-0.21630600	2.16370100
C	6.67447200	-0.65977000	-0.80165500
C	2.59556600	-3.45602100	-1.72827500
C	-2.43106200	-2.14291200	-1.72099500
C	-6.33491800	-0.59370100	1.04427900
C	-1.93324300	-1.52943100	3.28036900
H	1.42721300	-3.40141500	2.22365200
H	1.57664600	-4.27801400	0.68770700
H	-0.79966400	-4.29231300	0.35521200
H	-0.92800300	-3.83467600	2.06535600
H	5.16025800	0.19582200	1.28016000
H	5.09846700	-2.49834200	-2.05542700
H	-4.95310100	-1.35054200	-1.17111400
H	-4.51235200	-0.77026400	3.05398500
H	2.07032100	-0.93459900	2.75497400
H	3.38468500	0.25741300	2.81901400
H	1.93598300	0.56248900	1.86570400
H	7.25163600	-0.36423900	0.07922900
H	7.22615800	-1.44680100	-1.32283300
H	6.64798100	0.20856800	-1.47205000
H	2.74248200	-4.46161800	-1.31182800
H	1.52148000	-3.26074200	-1.79490000
H	2.98854100	-3.47102100	-2.74764500
H	-3.22899300	-2.33930300	-2.44180100
H	-1.78708100	-1.35770200	-2.13645400
H	-1.79522600	-3.03276300	-1.66024000
H	-6.92819000	-1.32058800	1.61056900
H	-6.43669500	0.36816900	1.55812900
H	-6.78758100	-0.49103200	0.05433400
H	-1.97388400	-2.53233500	3.72618100
H	-0.88593800	-1.28232800	3.08722100
H	-2.30099300	-0.82758300	4.03221800
C	-2.67760700	1.64360200	-1.34084600
C	-3.60918200	1.25471800	-2.31952100
C	-3.15393900	2.28971400	-0.18822200

C	-4.96739400	1.50908200	-2.16275300
H	-3.24838000	0.75320300	-3.21643400
C	-4.51129100	2.54124100	-0.03294800
H	-2.45663300	2.56597900	0.59733400
C	-5.42360000	2.15692800	-1.01706400
H	-5.66827700	1.20268300	-2.93547000
H	-4.86281700	3.03732200	0.86853900
H	-6.48448900	2.35616700	-0.88640800

*Ia-trans-RCB-2 $\alpha\beta$*

Ru	0.51473700	-0.40071900	0.32636600
Cl	0.57708100	-1.84074000	-1.64788900
Cl	0.22371200	0.65916500	2.48317300
C	1.73695000	-1.69329700	1.19071400
C	2.71105000	-0.53802000	0.77687500
C	2.15938200	0.42795200	-0.38378400
H	1.91925400	-2.63510500	0.67116600
H	2.44010200	0.02938500	-1.36449900
C	2.29882600	1.88947500	-0.29373300
C	2.22514900	2.60128500	-1.50486700
C	2.42611500	2.61566200	0.90099900
C	2.25856800	3.99103200	-1.52258700
H	2.13036100	2.04371700	-2.43517700
C	2.47116300	4.00436200	0.87915500
H	2.44572100	2.09326500	1.85239100
C	2.38130600	4.69911500	-0.32820800
H	2.19184800	4.52091600	-2.46891900
H	2.56669800	4.54928700	1.81446800
H	2.40948900	5.78533400	-0.33683400
H	1.60969600	-1.76634000	2.27213900
H	2.89094500	0.07792000	1.66182100
C	4.01345500	-1.10780000	0.24112600
C	5.20545900	-0.63351200	0.79127300
C	4.05519500	-2.05413300	-0.78655100
C	6.43120000	-1.11145500	0.32926400
H	5.17254500	0.11132200	1.58407300
C	5.28157300	-2.52542200	-1.24525600
H	3.12537400	-2.40454800	-1.23110400
C	6.47274800	-2.05940000	-0.68911100
H	7.35242700	-0.73754800	0.76782100
H	5.30510300	-3.26090000	-2.04492800
H	7.42710800	-2.43218100	-1.05007500
P	-1.80402600	-0.21305500	-0.04489300

C	-2.51042200	-0.54329200	-1.68880100	H	-1.54529500	1.18949500	1.95734700
C	-3.70461900	-1.24901600	-1.85911400	H	-2.40672300	-0.57538100	2.69658800
C	-1.87751600	0.02605500	-2.80005900	C	-2.41552200	1.26961800	0.01921100
C	-4.25629100	-1.38849600	-3.13155700	C	-2.73300200	2.61403400	0.27712500
H	-4.20297600	-1.69522400	-1.00130700	C	-2.79206200	0.72093900	-1.21900600
C	-2.43515800	-0.10915800	-4.06546600	C	-3.41136200	3.38636100	-0.66032300
H	-0.93344600	0.55292800	-2.67091800	H	-2.43778100	3.04876400	1.23072700
C	-3.62398800	-0.81891300	-4.23339700	C	-3.48054600	1.48938800	-2.14792300
H	-5.18156600	-1.94382400	-3.25822000	H	-2.52900700	-0.30705200	-1.44928300
H	-1.93366000	0.32772700	-4.92422000	C	-3.79382400	2.82327500	-1.87542300
H	-4.05415700	-0.93122200	-5.22465100	H	-3.64436600	4.42483300	-0.43942200
C	-2.49760200	-1.43972500	1.08956100	H	-3.77374300	1.04489300	-3.09554900
C	-2.99842200	-1.08080700	2.34600800	H	-4.33277500	3.41851900	-2.60824500
C	-2.39992800	-2.79345600	0.73258000	H	-1.45463500	-2.95166800	1.25332300
C	-3.43605500	-2.07007900	3.22169800	C	-3.58440100	-1.27391500	1.02957900
H	-3.02473500	-0.03514200	2.64086800	C	-4.69951700	-0.50611500	1.38919000
C	-2.84026400	-3.77424700	1.61476200	C	-3.74856000	-2.29808400	0.09494200
H	-1.96940200	-3.06817000	-0.22957000	C	-5.94777600	-0.74816500	0.82710800
C	-3.36294500	-3.41317800	2.85641300	H	-4.57758900	0.30281500	2.10834900
H	-3.82513800	-1.78986300	4.19638600	C	-4.99809200	-2.53526100	-0.47609700
H	-2.76806500	-4.82125000	1.33487800	H	-2.89280500	-2.88664100	-0.22084000
H	-3.70378200	-4.18114500	3.54531900	C	-6.09999800	-1.76356900	-0.11581000
C	-2.47488300	1.43071200	0.35435700	H	-6.79881500	-0.13890700	1.11888700
C	-1.61776500	2.53463500	0.41269900	H	-5.10603100	-3.32852800	-1.21091200
C	-3.85610500	1.61470600	0.49507600	H	-7.07125300	-1.95160500	-0.56513200
C	-2.13857800	3.81019500	0.61487000	P	1.93611200	-0.15101600	-0.03820200
H	-0.54199600	2.39490700	0.32268900	C	2.66623000	-0.99646300	-1.47664900
C	-4.36961300	2.88856200	0.71560900	C	3.27882800	-0.27564000	-2.50791500
H	-4.52849200	0.76038400	0.43456500	C	2.68692400	-2.39462700	-1.50323800
C	-3.51130400	3.98677300	0.77265800	C	3.90322800	-0.94902500	-3.55449500
H	-1.46433200	4.66087100	0.65939200	H	3.25947600	0.81236100	-2.50104200
H	-5.44054600	3.02482300	0.83714200	C	3.31970800	-3.06305000	-2.54650300
H	-3.91598900	4.98121500	0.93952600	H	2.18265200	-2.95667500	-0.72107200

***1a-cis-RCB-2 $\alpha$  $\beta$***

Ru	-0.20148300	-0.68945100	0.77118700	H	4.37058900	-0.38359600	-4.35584200
Cl	0.52465800	0.17528400	2.94480200	H	3.32457700	-4.14901200	-2.56492900
Cl	-0.60957000	-1.92798700	-1.26724000	H	4.41339500	-2.86563100	-4.39102800
C	-1.21435200	-2.04086600	1.80327600	C	1.25287700	1.42621100	-0.62518800
C	-2.26789100	-0.91304000	1.66414700	C	1.29974200	2.56848500	0.19033300
C	-1.70852700	0.54606800	1.08789900	C	0.52616700	1.45647300	-1.82562900
H	-0.88063700	-2.19539200	2.82918100	C	0.67195700	3.73774200	-0.22198200
				H	1.80934900	2.52679300	1.15038300
				C	-0.10005500	2.63254400	-2.22786300

H	0.43542800	0.55141400	-2.42388100
C	-0.02148600	3.77304000	-1.43302000
H	0.71058300	4.61967300	0.41126400
H	-0.67479100	2.64623400	-3.14949100
H	-0.52753400	4.68383400	-1.74248900
C	3.37961900	0.22791100	1.00129000
C	3.64769000	-0.51770400	2.15288000
C	4.28386000	1.21273500	0.58435800
C	4.80993900	-0.27390800	2.88045300
H	2.93081400	-1.26041800	2.49110300
C	5.43766800	1.45897400	1.32063200
H	4.08136400	1.79619300	-0.31185800
C	5.70227100	0.71352200	2.46859500
H	5.01073500	-0.85032500	3.77886900
H	6.12993800	2.23120000	0.99698600
H	6.60323200	0.90578700	3.04467200

*1b-trans-RCB-2 $\alpha\beta$*

Ru	0.41883400	-0.37571400	0.55418400
Cl	0.51212400	-2.19276000	-1.09317500
Cl	0.40914500	1.34573000	2.24010900
C	1.34089300	-1.54398600	1.84115800
C	2.54352600	-0.73264700	1.24913800
C	2.27273100	0.00468600	-0.13818300
H	1.37357200	-2.61096400	1.61181300
H	2.48965300	-0.67237600	-0.96854600
C	2.81170100	1.34972400	-0.39321900
C	3.06857700	1.66822600	-1.74003700
C	3.07972100	2.32440500	0.58162200
C	3.55875200	2.91610900	-2.10543200
H	2.86975800	0.91474500	-2.50107100
C	3.58679100	3.56568000	0.21606000
H	2.86268800	2.11803700	1.62475200
C	3.82310600	3.87127300	-1.12519000
H	3.74141100	3.14023000	-3.15324900
H	3.78990200	4.30610100	0.98483900
H	4.21172000	4.84722800	-1.40343600
H	1.17080900	-1.29974200	2.89165400
H	2.78673500	0.04766400	1.97494300
C	3.74999200	-1.61984800	0.99102900
C	4.99250200	-1.13855100	1.41107800
C	3.67484300	-2.85620000	0.34365900
C	6.14589500	-1.89431800	1.21192300

H	5.05391600	-0.16794500	1.89966000
C	4.83120000	-3.60456400	0.14188400
H	2.71539100	-3.21707600	-0.01867300
C	6.06817400	-3.13162000	0.57811700
H	7.10388300	-1.51170000	1.55319200
H	4.76238700	-4.56533700	-0.36129600
H	6.96598400	-3.72288900	0.42048000
P	-1.89396300	-0.01330500	-0.09399800
C	-2.81394900	-1.25165700	-1.14907800
C	-1.74868800	1.47753000	-1.20120700
C	-3.25830300	0.46453100	1.12203500
C	-2.78752900	-2.67853000	-0.57987000
C	-2.47977400	-1.28684600	-2.64503600
C	-0.47111300	1.34949400	-2.04286800
C	-1.75763500	2.82568700	-0.47486900
C	-2.81784900	1.29201400	2.33203100
C	-4.14112300	-0.69316900	1.60967400
C	-3.80220900	-3.55735500	-1.30208700
C	-3.48154500	-2.17921500	-3.37647300
C	-3.51739000	-3.58857600	-2.79891700
C	-0.32627900	2.49581800	-3.03393900
C	-1.60218600	3.97657200	-1.46700900
C	-0.33977500	3.83448600	-2.30803200
C	-4.02327000	1.82446500	3.10125900
C	-5.34281900	-0.17247000	2.39509300
C	-4.92757100	0.69504000	3.57274100
H	-3.85046600	-0.87304700	-1.07686500
H	-2.63074200	1.43990000	-1.86355100
H	-3.89082800	1.10333200	0.47716700
H	-1.78109300	-3.08230400	-0.72143300
H	-2.96864300	-2.68804800	0.49908100
H	-2.50668700	-0.28219600	-3.08238000
H	-1.46251400	-1.67308400	-2.78000500
H	-3.78344200	-4.57016500	-0.88373200
H	-4.81943100	-3.16958400	-1.12996500
H	-3.23846200	-2.20612600	-4.44479400
H	-4.48489400	-1.73202500	-3.29943200
H	-4.26244700	-4.19800100	-3.32332800
H	-2.54362200	-4.07060900	-2.96536900
H	0.38330800	1.39081000	-1.35006900
H	-0.40712000	0.37566000	-2.54109800
H	-2.68737300	2.95406100	0.09151900
H	-0.93381800	2.84845100	0.25388500



H	0.60001500	2.37306500	-3.60779900
H	-1.15243100	2.45570200	-3.76050400
H	-1.60111100	4.92847100	-0.92416500
H	-2.47870100	4.00110100	-2.13217700
H	-0.25552600	4.66401800	-3.01933100
H	0.54287700	3.89162700	-1.65336800
H	-2.21004300	0.65727200	2.98930500
H	-2.15737000	2.11049900	2.04427500
H	-4.51286800	-1.30277100	0.78264200
H	-3.54238600	-1.35681000	2.25060400
H	-3.67703300	2.42703500	3.94805900
H	-4.59724500	2.50482500	2.45269800
H	-5.95421900	-1.01917300	2.72751500
H	-5.97795500	0.41732600	1.71703400
H	-5.80861200	1.08878600	4.09233600
H	-4.38411300	0.07938200	4.30384100

*Ib-cis-RCB-2 $\alpha\beta$*

Ru	0.31320300	-0.42082600	-0.72093700
Cl	-0.33055700	0.74773300	-2.79128000
Cl	0.99512100	-1.72045900	1.18256900
C	1.08793700	-1.76776700	-1.92078900
C	2.27829500	-0.76062500	-1.79635900
C	1.97965000	0.64320300	-1.01737300
H	0.67406300	-1.80578800	-2.92884100
H	1.79737500	1.40391500	-1.77972800
H	2.32623800	-0.34215700	-2.80836900
C	2.81919600	1.19439200	0.06248400
C	2.98296600	2.59324600	0.03984100
C	3.42154200	0.47779600	1.11112200
C	3.70763700	3.25600600	1.02431500
H	2.51867700	3.16046200	-0.76599700
C	4.16121600	1.13971100	2.08277000
H	3.29140500	-0.59562400	1.17347500
C	4.30535400	2.52788200	2.05052900
H	3.80850700	4.33753600	0.98583300
H	4.62370100	0.56499700	2.88054700
H	4.87693000	3.03719600	2.82180700
H	1.27969300	-2.73915800	-1.46232600
C	3.60657400	-1.34953700	-1.38996900
C	4.75368700	-0.64789600	-1.78285800
C	3.76095800	-2.52885900	-0.65824200
C	6.02362500	-1.10497800	-1.44963100

H	4.64206200	0.27695700	-2.34708600
C	5.03340700	-2.98094600	-0.31294400
H	2.88894600	-3.07938300	-0.32085700
C	6.16762500	-2.27381300	-0.70431800
H	6.89900300	-0.54423900	-1.76552300
H	5.13439100	-3.89354800	0.26838500
H	7.15701500	-2.63181300	-0.43280900
P	-1.91125800	0.00025500	0.19069300
C	-1.58342200	1.43787100	1.33290400
C	-2.87895100	-1.20669900	1.27627100
C	-3.28110300	0.62505100	-0.91571700
C	-0.54599000	2.37113300	0.69303900
C	-1.12194100	1.04991900	2.74127300
C	-2.03513900	-2.12749500	2.16064800
C	-3.93741700	-2.05070400	0.55202600
C	-3.51484000	-0.25844000	-2.15069000
C	-3.20984000	2.09812400	-1.33448900
C	-0.30717600	3.61592200	1.53598000
C	-0.86436700	2.29360700	3.58945100
C	0.14528300	3.23057100	2.93827000
C	-2.90703300	-2.86339700	3.17274900
C	-4.80590800	-2.81237000	1.55160000
C	-3.98095400	-3.68946300	2.47996200
C	-4.80720400	0.13949300	-2.85439600
C	-4.49146100	2.49865800	-2.06264700
C	-4.76581700	1.60582600	-3.26633900
H	-2.54854800	1.96597900	1.42161300
H	-3.42384500	-0.50117700	1.93099700
H	-4.16287800	0.53502600	-0.25473000
H	0.40216400	1.81575200	0.63826500
H	-0.80580400	2.62521400	-0.34079100
H	-1.87094200	0.42184000	3.23711000
H	-0.20192600	0.44993400	2.66673700
H	0.43850900	4.25487200	1.04800700
H	-1.23591400	4.20498000	1.59041800
H	-0.52506500	1.99115700	4.58654500
H	-1.81374400	2.83103000	3.73649700
H	0.29770700	4.12191100	3.55737800
H	1.12033100	2.72530300	2.86956700
H	-1.52068200	-2.85442000	1.51987400
H	-1.23454600	-1.58569200	2.66421200
H	-4.59331500	-1.43924600	-0.07244000
H	-3.43404900	-2.76366800	-0.11720800

H	-2.27626100	-3.49634000	3.80645400	C	2.99379900	1.32132100	-2.43749300
H	-3.38465300	-2.13273800	3.84427700	C	6.81426000	-1.35656300	-0.57997900
H	-5.54952800	-3.40674700	1.00830400	C	3.87109000	1.24375900	2.55454500
H	-5.37339500	-2.08395400	2.15031700	C	-1.36794000	1.38307200	2.63299200
H	-4.62586900	-4.18886900	3.21201400	C	-5.51288800	2.78880000	0.16797500
H	-3.50011800	-4.48584300	1.89397600	C	-0.99302100	3.92099600	-1.73134400
H	-2.66908600	-0.12383100	-2.83182600	H	2.68131200	3.98637000	-0.32925800
H	-3.53012500	-1.32108800	-1.88995100	H	3.13314200	3.63540900	1.35326800
H	-3.07362400	2.75003000	-0.46400500	H	0.86308700	3.84584300	2.12127000
H	-2.34274300	2.24457800	-1.98877700	H	0.58985300	4.73559000	0.60899100
H	-4.96883200	-0.50315800	-3.72723000	H	5.15080200	-0.28250900	-2.44592900
H	-5.66414000	-0.02865500	-2.18220000	H	5.89887200	-0.35536200	1.77494400
H	-4.42781100	3.54945400	-2.36754600	H	-3.99462100	1.65667500	2.11842600
H	-5.33952400	2.43152300	-1.36343200	H	-3.69874600	3.79855000	-1.58456800
H	-5.70183500	1.89927400	-3.75552100	H	2.50241800	2.28159900	-2.25428300
H	-3.96587500	1.74455300	-4.00736600	H	3.65251800	1.43341200	-3.30293800

**2-trans-RCB-2 $\alpha$  $\beta$**

Ru	0.27331400	-0.19494700	-0.28551100	H	7.10994100	-1.38831100	-1.63163200
Cl	1.26863700	-0.89150900	1.85255200	H	7.68504800	-1.04997300	0.00733100
Cl	-0.44240500	0.52538900	-2.47552800	H	6.57424500	-2.38197300	-0.27726800
C	1.01352700	-1.84819000	-1.07736600	H	4.32309000	2.21850500	2.78171200
C	-0.46870600	-2.26869100	-0.84259500	H	2.79059600	1.32205700	2.70206900
C	-1.24574600	-1.38410700	0.25598500	H	4.25240400	0.53337400	3.29136400
H	1.74051100	-2.39823700	-0.47647200	H	-1.99074600	1.49985900	3.52431600
H	-1.04333500	-1.79440900	1.25166800	H	-1.24140400	0.30757200	2.45939900
N	2.27623500	2.01082600	0.29953700	H	-0.36496800	1.75815800	2.85466300
N	0.19378200	2.65617800	0.51028300	H	-5.88122800	3.81706000	0.25716600
C	0.99425000	1.62344500	0.19771300	H	-5.86570100	2.40732400	-0.79610600
C	2.37915800	3.45236600	0.58303300	H	-5.98623400	2.19436200	0.95393400
C	0.96423600	3.79754400	1.02767900	H	-0.42400900	4.78121000	-1.35667700
C	3.42540100	1.19467800	0.06202200	H	-0.27585900	3.19660600	-2.13305600
C	-1.23497100	2.65236100	0.43683900	H	-1.61229700	4.27427300	-2.55876200
C	3.76570600	0.83649700	-1.25034700	C	-2.68168000	-1.12813000	0.06591500
C	4.87725500	0.00738200	-1.43210800	C	-3.51358600	-1.29685500	1.18682000
C	5.64804300	-0.44211800	-0.36147900	C	-3.27208100	-0.75523700	-1.15276400
C	5.30238700	-0.02242800	0.92662800	C	-4.88776900	-1.10250400	1.09749900
C	4.20250400	0.79799900	1.16466800	H	-3.06547400	-1.59578600	2.13325900
C	-1.99463500	2.06088600	1.45488500	C	-4.64532300	-0.56558400	-1.24000400
C	-3.38876000	2.11537100	1.33835900	H	-2.64243000	-0.58650300	-2.02161900
C	-4.01886800	2.73297600	0.26144700	C	-5.45966000	-0.73723100	-0.11913400
C	-3.22270100	3.31813200	-0.73073700	H	-5.51210200	-1.24267200	1.97644600
C	-1.83362600	3.29608500	-0.66320700	H	-5.08421700	-0.27141500	-2.19039200
				H	-6.53317500	-0.58227100	-0.19441900

H	1.25939400	-1.76111500	-2.13835700
H	-1.01400700	-2.15746200	-1.78454900
C	-0.56134300	-3.69580800	-0.33731400
C	-1.41537800	-4.57526000	-1.00497100
C	0.15548000	-4.14403400	0.77667000
C	-1.53712400	-5.89742300	-0.57918800
H	-1.98526600	-4.22210900	-1.86229600
C	0.02658100	-5.46307900	1.20028900
H	0.79958300	-3.45052300	1.31474400
C	-0.81507200	-6.34559900	0.52336900
H	-2.20033300	-6.57371200	-1.11199100
H	0.58825000	-5.80235100	2.06656600
H	-0.90935800	-7.37558200	0.85635300

**2-cis-RCB-2 $\alpha\beta$**

Ru	0.39156200	0.42642500	-0.13415900
Cl	1.54502400	0.53753600	-2.29435800
Cl	-0.39156600	0.35642500	2.15787300
C	0.80425100	2.35776600	-0.01295700
C	-0.57932800	2.40469300	-0.70374900
C	-1.17724500	0.93588200	-1.22336800
H	1.62281500	2.69975000	-0.64689300
H	-0.94612200	0.87662700	-2.29216900
H	-0.35389500	2.80223100	-1.69863000
N	2.70088600	-1.47771200	0.38441700
N	0.75862800	-2.48960400	0.36422600
C	1.37894500	-1.30596000	0.21917100
C	3.01026400	-2.84377000	0.83866200
C	1.72285500	-3.59102100	0.51945500
C	3.71183800	-0.47510500	0.24412300
C	-0.65145000	-2.71365900	0.28079800
C	3.88659100	0.49786900	1.23554100
C	4.86923600	1.47305800	1.02439200
C	5.67089500	1.48294500	-0.11401500
C	5.48769400	0.47143000	-1.06371300
C	4.51739500	-0.51332200	-0.90949700
C	-1.28449400	-2.70419400	-0.97184100
C	-2.65990400	-2.95243600	-1.00699000
C	-3.39564200	-3.21575600	0.14673300
C	-2.72394100	-3.23066200	1.37295600
C	-1.35459100	-2.99312700	1.46651500
C	3.07073200	0.52691700	2.49018000
C	6.70411600	2.54694800	-0.32633300

C	4.31012000	-1.55975200	-1.95893400
C	-0.52943100	-2.46014700	-2.24200900
C	-4.86611300	-3.49392200	0.08025100
C	-0.65775700	-3.05288800	2.79008000
H	3.23558400	-2.82769700	1.91441000
H	3.88498100	-3.23535000	0.31336800
H	1.78268100	-4.16669300	-0.41517800
H	1.40316400	-4.26627400	1.31809800
H	5.01197600	2.24124300	1.78349200
H	6.10163000	0.46409400	-1.96314900
H	-3.16795300	-2.93839200	-1.97032900
H	-3.28392800	-3.42779800	2.28651100
H	2.59021300	-0.43031100	2.70750300
H	3.69128100	0.80660900	3.34639600
H	2.25454100	1.25518200	2.42981900
H	6.79302400	3.20186900	0.54392100
H	7.69089800	2.11653800	-0.52560800
H	6.45484200	3.17434900	-1.18889100
H	4.62123700	-2.55631600	-1.62067800
H	3.25397700	-1.61344300	-2.24398200
H	4.88766300	-1.32870900	-2.85662000
H	-1.10985200	-2.79770700	-3.10445900
H	-0.28944100	-1.40081700	-2.39662300
H	0.43386200	-2.98154500	-2.25561200
H	-5.08747600	-4.53829100	0.32816300
H	-5.42079000	-2.87306100	0.79184700
H	-5.26713800	-3.29516600	-0.91717600
H	-0.23426600	-4.04888400	2.97604400
H	0.15142400	-2.31968700	2.85237500
H	-1.35467800	-2.84375300	3.60487600
C	-2.57916000	0.55735000	-0.97527800
C	-3.34553600	0.22514100	-2.10565000
C	-3.19810900	0.51911400	0.28449400
C	-4.69013600	-0.11320600	-1.99078200
H	-2.87070800	0.24431700	-3.08601500
C	-4.54159200	0.18655400	0.39666200
H	-2.61360400	0.73383700	1.17282000
C	-5.29489200	-0.12541700	-0.73604600
H	-5.26446800	-0.36306900	-2.87921800
H	-5.00389600	0.16318000	1.38075400
H	-6.34558000	-0.38851800	-0.63884900
H	0.81707400	2.74746300	1.00719800
C	-1.65194600	3.21658300	-0.02793300

C	-2.65265700	3.76261400	-0.84121300
C	-1.71566500	3.43312900	1.34995500
C	-3.69441000	4.50436500	-0.29536100
H	-2.61703100	3.58763300	-1.91575800
C	-2.76337600	4.17066400	1.89878600
H	-0.96888900	2.99449600	2.00467300
C	-3.75486100	4.70834400	1.08223400
H	-4.46136400	4.91716200	-0.94526200
H	-2.80261900	4.32135600	2.97436400
H	-4.56944500	5.28259800	1.51534300

**1a-trans,trans-RCB-3**

Cl	-0.14597200	-0.07827300	2.57354600
Cl	-0.14000900	-0.55095400	-2.28160500
C	-1.79134600	-1.48357800	0.38638100
C	-2.01229700	-2.69570900	-0.41799400
C	-1.64783800	-3.92107200	0.16724500
C	-1.81558100	-5.12127000	-0.51344600
C	-2.37182800	-5.12443800	-1.79153500
C	-2.74938600	-3.91759500	-2.37970400
C	-2.56630900	-2.71593300	-1.70657500
C	-2.50164300	-0.12830300	-0.00481200
C	-1.66045400	1.17698100	0.32325900
H	-1.89622300	-1.67782700	1.45847800
H	-1.22742400	-3.91564800	1.17184800
H	-1.52183100	-6.05541800	-0.04206000
H	-2.51439400	-6.06072100	-2.32423000
H	-3.18375200	-3.91127100	-3.37574500
H	-2.84229900	-1.78725700	-2.19661200
H	-1.78310400	1.45185900	1.37416500
H	-2.72780500	-0.13430400	-1.07323900
C	-1.74575900	2.34903600	-0.55882400
C	-1.65292000	3.61521800	0.04470200
C	-1.91314000	2.28620300	-1.95275600
C	-1.72443300	4.77867300	-0.71389000
H	-1.51891100	3.67239700	1.12331900
C	-1.98969800	3.44928800	-2.70732500
H	-1.94896900	1.31985500	-2.44727700
C	-1.89504900	4.70034400	-2.09425700
H	-1.64733800	5.74705700	-0.22581700
H	-2.11961800	3.38036100	-3.78403000
H	-1.95419600	5.60693800	-2.69074900
C	-3.79432900	-0.04051000	0.79057400
C	-4.99506700	-0.00567800	0.08077600

C	-3.81491600	-0.00204200	2.18789300
C	-6.21022900	0.06750600	0.76056600
H	-4.97705500	-0.03581700	-1.00696000
C	-5.03055100	0.07083300	2.86088500
H	-2.87668200	-0.02992500	2.74090300
C	-6.23116600	0.10591700	2.15157500
H	-7.13893500	0.09420700	0.19706700
H	-5.03855700	0.10015500	3.94708800
H	-7.17753900	0.16340600	2.68210100
C	2.03561200	1.71713100	0.03631100
C	3.04978200	-0.50009800	1.69128300
C	3.11378200	-0.72802100	-1.14771200
C	1.97703700	2.53524200	1.17488900
C	1.90151200	2.28458600	-1.24088600
C	4.19294000	0.23566600	2.02212500
C	2.71024700	-1.62992000	2.44182600
C	2.82339300	-1.96737500	-1.72665700
C	4.25584300	-0.02507500	-1.54966200
C	1.83683000	3.91111000	1.02976100
H	2.02566800	2.08686200	2.16456800
C	1.75281200	3.66135800	-1.37348300
H	1.89283800	1.64319900	-2.11973900
C	4.98120700	-0.14898400	3.10322500
H	4.46326200	1.11579400	1.44189100
C	3.50782000	-2.01734200	3.51394900
H	1.80378000	-2.18081100	2.20246200
C	3.67083700	-2.49639300	-2.69643300
H	1.92093500	-2.50215800	-1.43873700
C	5.09482000	-0.55430800	-2.52537100
H	4.48467100	0.94326900	-1.10871000
C	1.72776200	4.47413300	-0.24189500
H	1.79885200	4.54294200	1.91270900
H	1.63863300	4.09682600	-2.36205800
C	4.64034200	-1.27653600	3.84784700
H	5.86133100	0.43264900	3.36235000
H	3.23473700	-2.89058400	4.09899300
C	4.80411100	-1.79133700	-3.09729600
H	3.43573100	-3.45543400	-3.14900400
H	5.97427000	0.00114500	-2.83882700
H	1.60363700	5.54845300	-0.35050900
H	5.25543300	-1.57515800	4.69216300
H	5.45874500	-2.20387200	-3.86006900
P	2.08069600	-0.08800400	0.20924900

Ru -0.24734500 -0.23364800 0.10625400

H -4.64886500 0.98223100 -1.79962300

C -5.14414700 0.42988700 1.99195200

H -3.00753200 0.58518900 2.15044500

C -6.25166600 0.43711000 1.14731500

H -6.92508600 0.64849000 -0.88986800

H -5.27323000 0.26388900 3.05818600

H -7.24867400 0.28102200 1.54976700

C 2.64390100 0.84635600 0.81118900

C 2.32255800 -2.05163900 1.18449900

C 2.93270900 -1.04729900 -1.40668400

C 2.66170000 1.00958200 2.20308400

C 3.03155900 1.90685100 -0.02260300

C 3.57022300 -2.15445100 1.81035500

C 1.38630900 -3.07959300 1.33257300

C 2.32061500 -1.71590500 -2.47209600

C 4.30558000 -0.78206200 -1.45331600

C 3.10767200 2.20814400 2.75285900

H 2.31002300 0.20694800 2.84723200

C 3.47570700 3.09973100 0.53712800

H 2.96474100 1.79804200 -1.10289600

C 3.87188800 -3.26945600 2.58686600

H 4.30378200 -1.35820800 1.69756000

C 1.69657300 -4.19821100 2.10048300

H 0.40638600 -2.98756700 0.86852400

C 3.07539000 -2.11530600 -3.57015700

H 1.24799900 -1.89731400 -2.45042300

C 5.05531800 -1.17471800 -2.55907600

H 4.78970200 -0.25865300 -0.63133400

C 3.51968100 3.24939700 1.92290600

H 3.12402600 2.32957300 3.83236100

H 3.76836500 3.92102900 -0.11110900

C 2.93585200 -4.29248100 2.73060200

H 4.83838700 -3.33916800 3.07831900

H 0.96209300 -4.98964700 2.21792700

C 4.44158300 -1.84318400 -3.61643400

H 2.59171500 -2.62659000 -4.39727700

H 6.11908800 -0.95649700 -2.59306400

H 3.86131400 4.18616300 2.35578900

H 3.17245600 -5.16207800 3.33736400

H 5.02735400 -2.14676800 -4.47954700

P 1.94610100 -0.65881100 0.07256800

*1a-trans, cis-RCB-3*

Ru -0.29566800 0.07950400 -0.17807600

Cl 0.37698500 0.93983500 -2.35799000

Cl -0.58401900 -0.55999700 2.17467000

C -1.85727600 -0.54804400 -1.15647700

C -2.71286000 -1.71554400 -0.88973200

C -3.31583100 -2.32203300 -2.00618500

C -4.16461400 -3.41350400 -1.86018800

C -4.43018600 -3.91806000 -0.58884200

C -3.82840600 -3.33478100 0.52713600

C -2.97223500 -2.25038900 0.38261000

C -2.32122300 1.01831500 -0.51904600

C -1.30887800 1.76969300 0.32779600

H -1.77694200 -0.36054000 -2.23404300

H -3.12064300 -1.91251100 -2.99583700

H -4.62362500 -3.86438400 -2.73588100

H -5.09876400 -4.76632800 -0.46766200

H -4.02589100 -3.73087500 1.51975100

H -2.48886800 -1.81187000 1.25053100

H -1.51708200 1.69904600 1.39713800

C -0.76892900 3.09219300 -0.01903700

C -0.11618700 3.78623600 1.01440300

C -0.86673200 3.70597300 -1.27683500

C 0.43578600 5.04325000 0.79805300

H -0.03659700 3.31358600 1.99266800

C -0.32021200 4.96466600 -1.49031500

H -1.35487100 3.18878500 -2.09632300

C 0.33643300 5.63768800 -0.45820200

H 0.94408500 5.55701800 1.60997800

H -0.40556800 5.42549000 -2.47056700

H 0.76123200 6.62256500 -0.63321800

H -2.39186200 1.52452200 -1.48584200

C -3.67462100 0.83720400 0.11421000

C -4.79060400 0.83821900 -0.72933800

C -3.86375000 0.62962600 1.48295200

C -6.07054600 0.64356200 -0.21869800

**1a-cis, cis-RCB-3**

Ru	0.22128200	0.03891500	-0.42776900
Cl	-0.65594600	-0.10447700	-2.75323600
Cl	0.74937000	0.15000400	1.89422600
C	1.52012100	-1.28559800	-1.16799700
C	1.98336100	-2.47400600	-0.43477400
C	1.81234000	-3.70344700	-1.09997900
C	2.19992900	-4.90309400	-0.51509100
C	2.78083200	-4.89812200	0.75109600
C	2.95578500	-3.68810500	1.42503500
C	2.55452600	-2.48974500	0.84972300
C	2.32921900	0.11619100	-1.20856100
C	1.39276600	1.42455400	-1.21849400
H	1.24595300	-1.55192300	-2.19146700
H	1.37230100	-3.70252700	-2.09646000
H	2.05644400	-5.83833100	-1.04975000
H	3.09389300	-5.83075900	1.21288000
H	3.40122700	-3.67831700	2.41613700
H	2.66209200	-1.56363100	1.40305000
H	1.12066600	1.62281500	-2.26093700
C	1.87322200	2.66895300	-0.55787200
C	2.97287800	3.32294000	-1.13410400
C	1.25837600	3.24635600	0.55750600
C	3.47105600	4.49911500	-0.58722300
H	3.45486900	2.88380000	-2.00607400
C	1.74985200	4.43434300	1.09687500
H	0.40644800	2.74893500	1.01566100
C	2.86074700	5.05857600	0.53463900
H	4.33636500	4.97911400	-1.03655000
H	1.26259200	4.86793400	1.96620000
H	3.24579600	5.97949300	0.96389000
H	2.54862600	0.07761600	-2.28123100
C	3.62693400	0.12335800	-0.44928300
C	4.68857100	-0.57109700	-1.04479900
C	3.84388900	0.74155200	0.78648100
C	5.93104400	-0.65879200	-0.42665400
H	4.52946800	-1.06268300	-2.00405300
C	5.08796100	0.65094300	1.40738100
H	3.03677900	1.26805500	1.28177900
C	6.13392000	-0.04776000	0.80917200
H	6.73665600	-1.20597900	-0.90836400
H	5.23474000	1.13176300	2.37078400
H	7.10049400	-0.11505200	1.30116500

C	-2.64506400	0.58548900	1.70423600
C	-3.17051400	0.94413700	-1.08492900
C	-2.67723500	-1.74928600	0.01414000
C	-3.29855900	1.81267800	1.86420700
C	-2.32504900	-0.17384300	2.83959600
C	-4.44849200	0.51213800	-1.44302900
C	-2.69535300	2.17386800	-1.55504800
C	-1.98071000	-2.67940900	-0.76859000
C	-3.78553400	-2.17312200	0.76240900
C	-3.63958200	2.26533900	3.13777800
H	-3.55458500	2.41450300	0.99616100
C	-2.67571600	0.27750900	4.10578500
H	-1.79780200	-1.11760700	2.72768400
C	-5.24655800	1.30655800	-2.26491000
H	-4.81781100	-0.44938100	-1.09354200
C	-3.49988300	2.96967400	-2.36220700
H	-1.68335700	2.49211100	-1.30637300
C	-2.38291000	-4.01236800	-0.79310700
H	-1.13720900	-2.35140300	-1.37165400
C	-4.18897500	-3.50410100	0.72331500
H	-4.32767100	-1.46177800	1.38133800
C	-3.33177300	1.49921800	4.25816400
H	-4.15164700	3.21704900	3.24932300
H	-2.42499000	-0.32104400	4.97667800
C	-4.77613000	2.53542300	-2.72035700
H	-6.23546300	0.95964100	-2.55180600
H	-3.12320900	3.92077300	-2.72706100
C	-3.48494000	-4.42672700	-0.04957400
H	-1.82768500	-4.72669800	-1.39494600
H	-5.05085400	-3.82111800	1.30370800
H	-3.60101600	1.85204900	5.25006400
H	-5.39937200	3.15176000	-3.36209400
H	-3.79484800	-5.46785200	-0.06856100
P	-2.12590900	-0.01128600	0.05824500

**1b-trans ,trans-RCB-3**

Ru	-0.42979000	-0.07465600	0.06933300
Cl	-0.40287900	-0.07089400	2.56100600
Cl	-0.34982800	-0.00400900	-2.33827400
C	-1.65962700	-1.63710900	0.28759500
C	-1.50696000	-2.81926100	-0.57418000
C	-0.89738700	-3.94515000	0.00804300

C	-0.66640500	-5.09960400	-0.72998300	H	5.83639400	-0.71209000	3.17398300
C	-1.05830100	-5.15970800	-2.06648300	H	4.31287600	-0.24208000	3.91780500
C	-1.68222100	-4.05733800	-2.65153000	C	4.37275700	-2.30766100	3.30293700
C	-1.90122500	-2.89762500	-1.91860500	H	4.72054000	-2.66560300	4.27862000
C	-2.65058600	-0.46522900	-0.08406800	H	4.89521900	-2.91391000	2.54761700
C	-2.12536200	0.97516200	0.32221100	C	2.86826500	-2.51815700	3.15961200
H	-1.76247300	-1.90599100	1.34377900	H	2.61805200	-3.58032700	3.26250300
H	-0.60153300	-3.89678500	1.05470800	H	2.34208400	-1.99532200	3.97099900
H	-0.18746100	-5.95469400	-0.26060600	C	2.35111700	-1.98658800	1.82672000
H	-0.88379500	-6.06078300	-2.64809700	H	1.26253800	-2.10048400	1.76581400
H	-1.99425600	-4.09859800	-3.69141600	H	2.78912000	-2.56873400	1.00411900
H	-2.35812100	-2.03981700	-2.40198900	C	2.14362800	2.14621000	0.46318100
H	-2.30709700	1.16051500	1.38473800	H	3.23240900	2.31586900	0.42226800
H	-2.83997900	-0.48156200	-1.15927800	C	1.63262700	2.68359100	1.80178100
C	-2.43193700	2.15329700	-0.50116600	H	2.10043200	2.15531300	2.64077500
C	-2.30495300	3.40803300	0.12191900	H	0.55650000	2.47832100	1.88680200
C	-2.81428700	2.11822000	-1.85109900	C	1.89342400	4.18259200	1.90609200
C	-2.51804500	4.58640100	-0.58378600	H	1.52499300	4.55653800	2.86795000
H	-2.02177900	3.44157900	1.17320400	H	2.97900900	4.36502700	1.89973100
C	-3.04471900	3.29592800	-2.55060200	C	1.24736400	4.93951900	0.75245700
H	-2.90443100	1.16684200	-2.36477400	H	0.15544700	4.82876500	0.81882400
C	-2.88860400	4.53436900	-1.92653000	H	1.45648900	6.01273400	0.82879100
H	-2.40116600	5.54499800	-0.08449400	C	1.71645600	4.39939000	-0.59304600
H	-3.33966500	3.24837900	-3.59512900	H	2.79013600	4.60976800	-0.71639100
H	-3.06197600	5.45191400	-2.48219100	H	1.20274300	4.91137600	-1.41481200
C	-3.95307800	-0.69233900	0.66623200	C	1.48699700	2.89694800	-0.70478500
C	-5.11433600	-0.86088300	-0.08918900	H	1.85256700	2.52426000	-1.66938100
C	-4.02385800	-0.73336800	2.06169800	H	0.40434900	2.68934300	-0.70035600
C	-6.33940700	-1.06964600	0.54222400	C	2.80374100	-0.06080900	-1.33106300
H	-5.05734800	-0.82960600	-1.17563700	H	2.12394500	0.37325300	-2.07723800
C	-5.24978500	-0.94120600	2.68672800	C	4.17637300	0.58903500	-1.53326700
H	-3.11701600	-0.59983000	2.65051500	H	4.90525000	0.19083200	-0.81628300
C	-6.41044800	-1.10953200	1.93153000	H	4.12711700	1.67119800	-1.36250800
H	-7.23663300	-1.20006300	-0.05682300	C	4.67190000	0.32523600	-2.95409100
H	-5.29750400	-0.97068000	3.77184800	H	3.99581800	0.82415300	-3.66378100
H	-7.36474000	-1.27029800	2.42515500	H	5.65960600	0.77963400	-3.09419900
P	1.91044000	0.32334200	0.24726700	C	4.71438400	-1.16610000	-3.26548500
C	2.72222000	-0.50525200	1.68176600	H	5.05511900	-1.33193700	-4.29383500
H	2.25528700	0.00837000	2.53458300	H	5.45746100	-1.64894400	-2.61266300
C	4.23891400	-0.31857400	1.76915500	C	3.35313400	-1.81315400	-3.04148000
H	4.52157100	0.73423300	1.63582900	H	3.39787100	-2.88985500	-3.24047700
H	4.72471500	-0.87965400	0.95725900	H	2.62289800	-1.39489200	-3.74844400
C	4.75018500	-0.84371000	3.10772200	C	2.85177100	-1.56497000	-1.62243800

H 1.85661800 -2.01095500 -1.48540900  
H 3.52965300 -2.05735700 -0.90849500

*1b-trans,cis-RCB-3*

Ru 0.40834300 0.23633400 0.12907400  
Cl -0.25779000 1.12614800 2.31707100  
Cl 0.84984400 -0.38037600 -2.19423700  
C 1.83344700 -0.58571600 1.19594400  
C 2.37190100 -1.92917600 0.92036100  
C 2.38438400 -2.81760300 2.01066000  
C 2.81152800 -4.13334600 1.86479900  
C 3.25056100 -4.58512100 0.62234000  
C 3.24619500 -3.71418600 -0.46897800  
C 2.80291200 -2.40569700 -0.32960400  
C 2.53447600 0.82751300 0.62682100  
C 1.64435000 1.80349900 -0.17704000  
H 1.69093900 -0.43474400 2.27090900  
H 2.04916100 -2.45921900 2.98246200  
H 2.80738800 -4.80139500 2.72174400  
H 3.59188500 -5.61002500 0.50267500  
H 3.58203700 -4.06111800 -1.44259600  
H 2.76520600 -1.75484500 -1.19560100  
H 1.87839000 1.79630000 -1.24463700  
C 1.33294200 3.16563000 0.28438300  
C 0.76981400 4.03203200 -0.66946500  
C 1.53668600 3.65458900 1.58248300  
C 0.39263900 5.32749600 -0.33405300  
H 0.61998600 3.66340800 -1.68428400  
C 1.17665700 4.95460500 1.91410800  
H 1.95460600 3.00688700 2.34690000  
C 0.59638000 5.79471100 0.96299900  
H -0.05191400 5.97413900 -1.08662300  
H 1.34149200 5.31342900 2.92631400  
H 0.31109500 6.80826600 1.23092200  
H 2.66887100 1.30631700 1.60151900  
C 3.87642600 0.51593000 0.00923300  
C 4.91533100 0.17961900 0.88546800  
C 4.13517200 0.52913100 -1.36340200  
C 6.18374400 -0.13172700 0.40762500

H 4.71851100 0.15408000 1.95647900  
C 5.40314700 0.20680700 -1.84276500  
H 3.33956900 0.75343500 -2.06744300  
C 6.43185000 -0.12159500 -0.96354000  
H 6.97575000 -0.38661600 1.10666600  
H 5.58417800 0.21414800 -2.91431400  
H 7.41962800 -0.36815200 -1.34320200  
P -1.89477400 -0.31948700 -0.23994600  
C -1.98924800 -1.82685900 -1.30363500  
H -1.57329100 -1.45685800 -2.25430000  
C -3.38413200 -2.39580700 -1.56450200  
H -4.08474000 -1.61074600 -1.87907500  
H -3.78466000 -2.81981500 -0.63175200  
C -3.30712800 -3.49637600 -2.62152900  
H -4.30440900 -3.91299900 -2.80439500  
H -2.97614400 -3.05264600 -3.57174500  
C -2.33252000 -4.59608400 -2.21165200  
H -2.26554000 -5.35695300 -2.99760900  
H -2.72641700 -5.10743400 -1.32034700  
C -0.95241500 -4.02994300 -1.89169400  
H -0.27636000 -4.82382300 -1.55376200  
H -0.50270200 -3.60494100 -2.80071200  
C -1.03605200 -2.93648000 -0.83354500  
H -0.03881000 -2.52395200 -0.63691500  
H -1.39683600 -3.37106200 0.10856700  
C -2.72983500 1.07083900 -1.13460200  
H -3.78103300 0.75985400 -1.25911300  
C -2.15079900 1.34764300 -2.52340600  
H -2.16903900 0.44537600 -3.14620200  
H -1.08933500 1.61543400 -2.42604700  
C -2.90722500 2.48499000 -3.20101100  
H -2.48699200 2.66810200 -4.19624000  
H -3.95475200 2.18562500 -3.35774600  
C -2.86502800 3.75221700 -2.35626800  
H -1.82247300 4.09410800 -2.27561600  
H -3.42015200 4.56155700 -2.84418100  
C -3.41211300 3.49661000 -0.95738100  
H -4.48589800 3.26324100 -1.02493700  
H -3.32856200 4.39772100 -0.33902400  
C -2.68934000 2.34191700 -0.27308600  
H -3.11821600 2.16113600 0.71997300  
H -1.63803600 2.61427800 -0.09116200  
C -2.88480400 -0.53391100 1.30436200



H	-2.58614200	0.34992700	1.88518300
C	-4.41177900	-0.50734600	1.17190900
H	-4.76915800	-1.38522800	0.61701400
H	-4.74396600	0.37490200	0.61108800
C	-5.04287700	-0.49871900	2.56326600
H	-4.76069700	0.43362300	3.07392500
H	-6.13565700	-0.48775600	2.47782400
C	-4.58082600	-1.68798400	3.39808300
H	-5.03077900	-1.64985700	4.39666000
H	-4.94346000	-2.61655400	2.93146600
C	-3.06005500	-1.73911300	3.49610200
H	-2.73990000	-2.61789200	4.06724400
H	-2.69301200	-0.85902700	4.04242700
C	-2.42458800	-1.75184500	2.11133000
H	-1.32837300	-1.75953500	2.18956400
H	-2.72026100	-2.67344400	1.58711600

*1b-cis,cis-RCB-3*

Ru	0.33702300	-0.06533100	-0.44411000
Cl	-0.38302900	0.14087500	-2.82078500
Cl	0.77360500	-0.32975100	1.91435100
C	1.38810800	-1.59032400	-1.18287600
C	1.56938300	-2.87533800	-0.48625400
C	1.04107200	-3.99778300	-1.15323900
C	1.11109100	-5.26973300	-0.59756000
C	1.72745100	-5.45194400	0.63864800
C	2.26003900	-4.35099400	1.31096600
C	2.17534700	-3.07648900	0.76527600
C	2.44849400	-0.37416300	-1.17562400
C	1.79805800	1.11018400	-1.12150600
H	1.08086900	-1.76540200	-2.21710400
H	0.57035500	-3.85475000	-2.12457400
H	0.69125900	-6.11749900	-1.13230800
H	1.79301100	-6.44418000	1.07695800
H	2.73704100	-4.48411300	2.27809700
H	2.55573700	-2.22876600	1.32003400
H	1.61012800	1.38902100	-2.16134700
C	2.41508600	2.27015400	-0.43209000
C	3.00089600	3.23823100	-1.26905500
C	2.37351700	2.53658400	0.94597900
C	3.54951400	4.40739600	-0.75374200
H	3.02030200	3.06003600	-2.34251400

C	2.90901300	3.71285500	1.45991300
H	1.88799400	1.82878400	1.61149000
C	3.50283200	4.65153100	0.61707100
H	4.00136300	5.13253300	-1.42504400
H	2.85254100	3.90031600	2.52925000
H	3.91508700	5.57075300	1.02423200
H	2.64637700	-0.38611800	-2.25255500
C	3.74234100	-0.63423400	-0.45645200
C	4.72250700	-1.32699300	-1.17902500
C	4.03075800	-0.25461600	0.85694700
C	5.95482200	-1.63385400	-0.61083900
H	4.50871300	-1.63690900	-2.20114100
C	5.26502300	-0.55920200	1.42637900
H	3.27494400	0.24018900	1.45321400
C	6.23213700	-1.24782300	0.69870100
H	6.69664900	-2.17475200	-1.19217600
H	5.46553500	-0.25855700	2.45134700
H	7.19298200	-1.48375000	1.14796700
P	-1.99041100	0.33177200	0.04672400
C	-3.16213000	-0.29889300	-1.23305000
H	-2.88347700	0.29784300	-2.11459400
C	-4.64583800	-0.06861300	-0.93671100
H	-4.83705000	0.96789500	-0.62798900
H	-4.95601000	-0.70924000	-0.09805000
C	-5.48103100	-0.42110300	-2.16523100
H	-6.54504700	-0.26053200	-1.95576800
H	-5.21730400	0.26452600	-2.98356300
C	-5.23078700	-1.85858200	-2.60841000
H	-5.81012300	-2.08607900	-3.51051900
H	-5.59693100	-2.54136100	-1.82677900
C	-3.74649800	-2.11977400	-2.84372900
H	-3.58125500	-3.16749300	-3.11982000
H	-3.39200000	-1.51556600	-3.69101200
C	-2.91605700	-1.76534100	-1.61491400
H	-1.85029700	-1.93005800	-1.81100200
H	-3.20008300	-2.42280500	-0.78195600
C	-2.17377300	2.17541300	0.10129100
H	-3.23080500	2.38024900	0.34155200
C	-1.84243900	2.85201400	-1.23249300
H	-2.47004500	2.45664600	-2.03994600
H	-0.81005400	2.60200700	-1.51477500
C	-1.98848400	4.36577500	-1.12420500
H	-1.75000300	4.82790200	-2.08863300

H	-3.03770600	4.62064700	-0.91004600
C	-1.09715400	4.92660800	-0.02272000
H	-0.04311500	4.74346300	-0.27975800
H	-1.21377900	6.01356000	0.05387800
C	-1.40587100	4.26185000	1.31250300
H	-2.42708800	4.52738300	1.62666000
H	-0.73423400	4.63363300	2.09528500
C	-1.28988200	2.74512100	1.22000700
H	-1.52510400	2.28491100	2.18750300
H	-0.24422800	2.47335800	1.00782300
C	-2.50665000	-0.22917200	1.73401200
H	-1.64980300	0.09358300	2.34199100
C	-3.76190600	0.41028100	2.33888700
H	-4.66099400	0.08876500	1.79781100
H	-3.72598100	1.50371100	2.26197000
C	-3.88641200	0.00120500	3.80521000
H	-3.02921400	0.40821900	4.36149000
H	-4.78445900	0.45073800	4.24494500
C	-3.91342400	-1.51548600	3.96053900
H	-3.98082200	-1.78972500	5.01942600
H	-4.82341300	-1.90792300	3.48180000
C	-2.69159200	-2.16208100	3.31740500
H	-2.74302600	-3.25329100	3.40276200
H	-1.78272900	-1.84964500	3.85076200
C	-2.55950800	-1.75568700	1.85380300
H	-1.66100500	-2.20662500	1.40972600
H	-3.42467400	-2.13853200	1.29147800

**2-trans,trans-RCB-3**

Ru	0.01927500	-0.02123200	-0.07123200
Cl	0.76481100	0.03924900	-2.43748300
Cl	-0.61315800	-0.27256300	2.24283400
C	1.17157800	1.62525500	0.10958600
C	2.06638800	1.85168200	1.25447700
C	3.44656300	1.75259200	1.00909500
C	4.37226700	1.93726000	2.02943100
C	3.93701400	2.24016900	3.31801500
C	2.56946100	2.35613500	3.57341900
C	1.64273000	2.16068800	2.55740800
C	-0.27667100	2.23359600	0.09738000
C	-1.33598500	1.34680200	-0.68093700
H	1.67666000	1.81312300	-0.84199500
H	3.78163700	1.51046400	0.00132800

H	5.43551100	1.84888100	1.81710900
H	4.65698200	2.39061700	4.11790300
H	2.22265600	2.59531800	4.57511600
H	0.58282100	2.22331600	2.78180900
H	-1.22300400	1.49970800	-1.75881300
H	-0.63027600	2.37391600	1.12228000
N	1.42176000	-2.67657700	-0.45849600
N	-0.75536800	-2.87587100	-0.31190400
C	0.26920200	-2.00407500	-0.29765400
C	1.20261500	-4.13223000	-0.45390100
C	-0.30552500	-4.23867400	-0.63427800
C	2.74849800	-2.14266300	-0.50309900
C	-2.12669900	-2.57753700	-0.02929900
C	3.36867100	-1.72075200	0.68434000
C	4.69040600	-1.27785800	0.60649700
C	5.38581800	-1.22548700	-0.60134200
C	4.73993600	-1.67082000	-1.75638300
C	3.42950400	-2.14988100	-1.73166400
C	-2.94058300	-2.01793100	-1.02446600
C	-4.28044600	-1.77514300	-0.70583800
C	-4.81059100	-2.07484100	0.54713100
C	-3.96710200	-2.64221600	1.50758400
C	-2.62693100	-2.91043300	1.24192100
C	2.65683400	-1.73089700	1.99935200
C	6.77562700	-0.66924900	-0.65695300
C	2.78784400	-2.67097500	-2.97976900
C	-2.40669300	-1.68862500	-2.38278500
C	-6.25248600	-1.81213100	0.85794000
C	-1.74970500	-3.53509300	2.28154700
H	1.55002200	-4.55325700	0.50019800
H	1.77029300	-4.60270300	-1.26135300
H	-0.59470000	-4.49001800	-1.66410000
H	-0.77398000	-4.96310400	0.03763000
H	5.18017700	-0.94724800	1.52147600
H	5.26871200	-1.64604200	-2.70831300
H	-4.92469600	-1.33233500	-1.46361200
H	-4.36115100	-2.87421500	2.49629500
H	2.07487900	-2.64607400	2.15412600
H	3.36651400	-1.62902000	2.82433400
H	1.93996300	-0.90534400	2.08760500
H	7.34575400	-0.91222700	0.24460800
H	7.33009800	-1.04246400	-1.52202800
H	6.75619400	0.42502900	-0.73514600

H	2.91951900	-3.75722200	-3.07418300	C	2.91629100	0.93809000	-0.06998200
H	1.71770200	-2.44675300	-3.00356200	C	4.10093400	0.78550600	0.67128600
H	3.23920900	-2.21704700	-3.86520500	C	5.34878900	0.90963800	0.07119200
H	-3.22266900	-1.49679000	-3.08424600	C	5.43742900	1.18660500	-1.29153100
H	-1.75385800	-0.80664500	-2.36956000	C	4.26975100	1.33124800	-2.04316400
H	-1.78763800	-2.49637600	-2.78907900	C	3.02186800	1.20635500	-1.44382900
H	-6.80192900	-2.74510600	1.02753500	C	-1.95082500	-3.80823400	-0.56479900
H	-6.36194000	-1.21074100	1.76681300	C	-0.48657900	-4.21370500	-0.49106100
H	-6.74700900	-1.27761600	0.04252000	C	-3.04960000	-1.56108800	-0.84483300
H	-1.61224000	-4.61048700	2.10722100	C	1.55553600	-2.87475900	0.20107600
H	-0.76149600	-3.06583500	2.30204100	C	-3.45953100	-1.33751500	-2.17295800
H	-2.18801500	-3.42416200	3.27580600	C	-4.63425800	-0.62036800	-2.38471000
C	-2.75218200	1.42816400	-0.28992900	C	-5.41991900	-0.16281200	-1.32081700
C	-3.70020500	1.50037800	-1.32550600	C	-5.01206300	-0.45887800	-0.02344300
C	-3.21130800	1.47649700	1.03638900	C	-3.82479500	-1.14736600	0.24779200
C	-5.05916800	1.61126100	-1.05049300	C	2.02093400	-3.24729700	1.47700100
H	-3.35245000	1.47534100	-2.35708600	C	3.38278700	-3.12294000	1.73571700
C	-4.56873300	1.58653500	1.30894000	C	4.28274900	-2.66891800	0.76406800
H	-2.49988700	1.39909300	1.85288500	C	3.79183900	-2.36397400	-0.50135100
C	-5.49905700	1.65347400	0.27041500	C	2.43168500	-2.46622400	-0.81635200
H	-5.77345900	1.66903200	-1.86817100	C	-2.65904100	-1.86344300	-3.32170600
H	-4.90550100	1.61464400	2.34223500	C	-6.65142900	0.65271900	-1.56961100
H	-6.56048100	1.73481700	0.49170500	C	-3.42038100	-1.38599300	1.66696400
C	-0.20938700	3.57893700	-0.60409900	C	1.08805200	-3.78920100	2.51389000
C	-0.54553800	4.71858200	0.12722000	C	5.73743500	-2.51637600	1.08719800
C	0.17972800	3.70652100	-1.94156200	C	1.98367300	-2.17175500	-2.21456500
C	-0.49476900	5.97749400	-0.46969600	C	0.58537500	2.09885900	0.72993500
H	-0.84782800	4.61795100	1.16800500	C	-0.89270300	1.80517200	0.36385500
C	0.22667000	4.96504100	-2.53301900	H	1.86169100	0.56704800	1.73052600
H	0.44665100	2.81725300	-2.51177500	H	4.02834600	0.56559100	1.73564800
C	-0.10938400	6.10391400	-1.80115800	H	6.25095400	0.79134000	0.66636000
H	-0.75851500	6.85742900	0.11049000	H	6.40951300	1.28874000	-1.76693100
H	0.52991900	5.05538400	-3.57270600	H	4.33183000	1.54525100	-3.10713500
H	-0.06932100	7.08437500	-2.26764300	H	2.11639900	1.30778500	-2.03504400
<i>2-trans,cis-RCB-3</i>				H	-2.47473500	-4.20510100	-1.43905700
Ru	-0.04370800	-0.00583900	0.10367500	H	-2.51589100	-4.09575600	0.33362600
Cl	-0.16887300	-0.58270700	2.48395000	H	-0.29096200	-5.01531200	0.22677700
Cl	-0.21326200	0.45543900	-2.28336200	H	-0.07957800	-4.51667100	-1.46697400
N	-1.86568900	-2.33946400	-0.63798200	H	-4.94906700	-0.42131300	-3.40818200
N	0.15122500	-2.96334200	-0.05671800	H	-5.61892100	-0.12582500	0.81760200
C	-0.65784000	-1.90265800	-0.24153100	H	3.75244100	-3.38451500	2.72664800
C	1.65612400	0.83037100	0.68851600	H	4.47948000	-2.01481900	-1.27152200
				H	-2.58020600	-2.95747000	-3.29529200

H	-3.11756900	-1.59042700	-4.27493700	Ru	0.07595300	-0.12904400	-0.31540300
H	-1.64015900	-1.46316300	-3.30321900	Cl	0.65742800	-1.00510000	-2.55882200
H	-7.20328600	0.30424100	-2.44748600	Cl	-0.46679500	0.38147300	1.99303400
H	-7.32859100	0.63404200	-0.71110600	C	1.46480000	1.22270500	-0.78773300
H	-6.39372000	1.70308000	-1.75465500	C	2.45712500	1.84321100	0.10936900
H	-4.29455700	-1.60220700	2.28799400	C	3.77391300	1.90063400	-0.38341100
H	-2.69695000	-2.19772700	1.78045300	C	4.80008500	2.47891100	0.35482200
H	-2.93184800	-0.49784000	2.08659400	C	4.53126200	3.01250100	1.61319800
H	1.53452800	-3.72869000	3.50906400	C	3.23280600	2.95410500	2.12213600
H	0.14740400	-3.23200900	2.53400000	C	2.20645800	2.37464700	1.38531300
H	0.85863800	-4.84652400	2.32615700	C	0.07931500	1.97473500	-1.18751200
H	6.31041100	-2.18996000	0.21536500	C	-1.18821400	1.00617100	-1.36888600
H	5.89074200	-1.77521400	1.88038300	H	1.95173400	0.91283900	-1.71520600
H	6.17217600	-3.45516400	1.44666900	H	3.98207200	1.47691500	-1.36491800
H	2.55170100	-2.77859100	-2.92813900	H	5.80781400	2.51211800	-0.05218000
H	0.91900200	-2.35271200	-2.37624400	H	5.32704000	3.46898700	2.19603300
H	2.15576700	-1.12171300	-2.47214800	H	3.01716600	3.36078300	3.10671000
H	-1.14776100	2.16894600	-0.63338000	H	1.21057700	2.30849600	1.80783600
C	-1.99275200	2.07393500	1.30557700	H	-1.15980100	0.67257800	-2.40987500
C	-3.26532700	2.24873300	0.73622800	N	1.19725000	-2.87382100	0.24420600
C	-1.86970000	2.17922700	2.70051200	N	-0.98368400	-2.83884000	0.44340900
C	-4.37973400	2.50563400	1.52636000	C	0.10411800	-2.09566500	0.17787200
H	-3.37091400	2.15898800	-0.34456500	C	0.86617700	-4.22766700	0.71506200
C	-2.98229800	2.44515500	3.48897500	C	-0.64279000	-4.27005800	0.52345900
H	-0.90480500	2.02223300	3.17231400	C	2.54475400	-2.42153400	0.08451200
C	-4.24265200	2.60527800	2.90894800	C	-2.33639600	-2.37255500	0.50244200
H	-5.35464500	2.62614600	1.05930400	C	3.14377700	-1.64198100	1.08576600
H	-2.86764500	2.52092900	4.56679100	C	4.44057200	-1.17024800	0.85823800
H	-5.10831500	2.81167200	3.53258100	C	5.14195700	-1.46743900	-0.30672700
H	0.58320200	2.27030800	1.81043900	C	4.53478000	-2.30197600	-1.25152000
C	1.18489300	3.28489900	0.01020800	C	3.24541300	-2.79905100	-1.07659100
C	2.18369100	3.99940500	0.68273100	C	-3.05957300	-2.11890100	-0.67134700
C	0.83884100	3.67406400	-1.28568000	C	-4.38413300	-1.68345700	-0.53823400
C	2.82833600	5.07190000	0.07593900	C	-4.99096800	-1.52129900	0.70287200
H	2.46983800	3.69382900	1.68829000	C	-4.24223700	-1.80650200	1.85083000
C	1.48577900	4.74821300	-1.89402900	C	-2.92095900	-2.23700000	1.77715600
H	0.09166600	3.11751100	-1.84381300	C	2.46340600	-1.30398700	2.37531600
C	2.48145300	5.45006500	-1.21986600	C	6.50235000	-0.89184300	-0.55558300
H	3.60447000	5.60911400	0.61430400	C	2.64351500	-3.72563300	-2.08670500
H	1.20880200	5.03190600	-2.90591500	C	-2.48079900	-2.30188600	-2.03869000
H	2.98492100	6.28473800	-1.69981900	C	-6.41492300	-1.06951000	0.81358900
				C	-2.13861700	-2.54030300	3.01602100
				H	1.16402700	-4.33323100	1.76845800

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H	1.40103600	-4.97961600	0.12820500
H	-0.93688600	-4.76720000	-0.41203400
H	-1.17726800	-4.74945900	1.34797700
H	4.90224400	-0.53627000	1.61485400
H	5.07648600	-2.56448700	-2.15949900
H	-4.95049700	-1.45994600	-1.44187200
H	-4.69874400	-1.68358400	2.83227800
H	1.57730300	-1.91506200	2.56525800
H	3.15690900	-1.42892900	3.21274600
H	2.12265300	-0.26271000	2.38885000
H	6.93689000	-0.47631200	0.35753100
H	7.19505700	-1.63880600	-0.95501100
H	6.45537300	-0.07971000	-1.29152600
H	2.83061400	-4.77477000	-1.82116000
H	1.56419400	-3.57892800	-2.17748900
H	3.08016600	-3.56135600	-3.07443800
H	-3.19469200	-2.81289700	-2.69222400
H	-2.24874800	-1.33807600	-2.50669000
H	-1.54105500	-2.85822600	-2.03911300
H	-7.07050300	-1.88872700	1.13067500
H	-6.52546500	-0.27067500	1.55459700
H	-6.79004900	-0.69277900	-0.14151000
H	-1.85706300	-3.59904300	3.07588000
H	-1.21623100	-1.95110700	3.04493600
H	-2.71927400	-2.30647700	3.91110500
C	-2.58256300	1.38462200	-1.03330100
C	-3.43113000	1.60949200	-2.13387400
C	-3.14298900	1.46578200	0.25039500
C	-4.76967300	1.94609300	-1.96391600
H	-3.02133300	1.51990700	-3.13856100
C	-4.48064200	1.80544200	0.41974000
H	-2.53851300	1.21403200	1.11514200
C	-5.29976400	2.05309400	-0.67974800
H	-5.39684800	2.12267000	-2.83387100
H	-4.89120700	1.85253100	1.42598300
H	-6.34730400	2.30762300	-0.53706500
H	0.32038900	2.11467200	-2.24584200
C	-0.09600100	3.32878100	-0.56102200
C	0.47316200	4.40797100	-1.25025000
C	-0.73677800	3.58168100	0.65394900
C	0.40725900	5.70189400	-0.74436200
H	0.98456500	4.22423900	-2.19454000
C	-0.80886500	4.87798500	1.15938800

H	-1.14370600	2.75955100	1.22981800
C	-0.23815500	5.94244100	0.46676600
H	0.86145400	6.52041600	-1.29625500
H	-1.30924800	5.05083600	2.10867700
H	-0.29398500	6.95099700	0.86735500

## MPWB1K

### 1a-PC

Ru	0.14942700	-0.12133400	0.04713900
Cl	0.19105000	0.12933100	-2.32558600
Cl	0.34977500	-1.17826000	2.17897900
P	-2.20223900	-0.55408200	0.02018600
P	2.50015600	-0.11831000	-0.03865800
C	0.07537900	1.53969600	0.79850700
H	0.61541000	1.64939600	1.74630100
C	-1.93159400	5.12561200	-0.21709300
C	-1.42467000	4.93870100	1.06041000
C	-0.75925900	3.76846600	1.36685800
C	-0.61610800	2.75494500	0.41275500
C	-1.12865000	2.96056400	-0.87061800
C	-1.77241700	4.14182500	-1.18132600
H	-2.44485300	6.04319000	-0.46273500
H	-1.54058500	5.70775200	1.80853200
H	-0.34649800	3.62156900	2.35495000
H	-0.99666200	2.18969600	-1.61384200
H	-2.16167700	4.29056800	-2.17669400
C	3.35847700	1.23709200	-0.88932800
C	4.75154700	1.27382500	-0.89994300
C	2.64409300	2.27333600	-1.47246800
C	5.41739200	2.32262300	-1.50467900
H	5.31321400	0.48253100	-0.42354100
C	3.31473700	3.32889300	-2.07092800
H	1.56646800	2.24693200	-1.46607700
C	4.69714100	3.35259400	-2.09209000
H	6.49649000	2.34165900	-1.51092600
H	2.75043500	4.13099800	-2.52107600
H	5.21700700	4.17467800	-2.56041200
C	3.39575400	-0.15363500	1.54658500
C	3.89568500	-1.32016100	2.10517700
C	3.53557400	1.04490400	2.23982500
C	4.52940500	-1.28892700	3.33605700

H	3.79893100	-2.25838600	1.58364100
C	4.16603300	1.07370700	3.46976600
H	3.16715400	1.96482500	1.80743000
C	4.66451200	-0.09523200	4.02171200
H	4.91572300	-2.20352300	3.75920700
H	4.27217900	2.01062300	3.99510100
H	5.15766100	-0.07341400	4.98149400
C	2.94141300	-1.65119200	-0.90496400
C	2.37298000	-2.83329300	-0.43294400
C	3.71403800	-1.67852700	-2.05751600
C	2.60264300	-4.02794300	-1.09046700
H	1.75129200	-2.81086300	0.45302100
C	3.93610400	-2.87689200	-2.71512300
H	4.12670200	-0.76544000	-2.45619700
C	3.38679400	-4.05186100	-2.23203700
H	2.15900500	-4.93796700	-0.71590500
H	4.53360900	-2.88851400	-3.61383400
H	3.55931400	-4.98262400	-2.75055700
C	-2.46395500	-2.24425700	-0.60996300
C	-1.64822300	-3.24156700	-0.08155000
C	-3.43053600	-2.58217300	-1.54829800
C	-1.79645400	-4.55399500	-0.49133500
H	-0.91376500	-2.98815400	0.67065900
C	-3.57187300	-3.89772500	-1.95944700
H	-4.08005700	-1.82419600	-1.95715800
C	-2.75488600	-4.88422700	-1.43527800
H	-1.16095500	-5.31913100	-0.07189600
H	-4.32461300	-4.14965600	-2.69086000
H	-2.86663600	-5.90777000	-1.75920500
C	-3.05814400	-0.58461400	1.62600800
C	-4.21333100	-1.34245900	1.78690700
C	-2.60565600	0.19831000	2.67853900
C	-4.90900400	-1.31153000	2.98187500
H	-4.56737400	-1.96193000	0.97597700
C	-3.30660200	0.23363600	3.87236400
H	-1.68947300	0.75728300	2.57356100
C	-4.45720300	-0.52002400	4.02573100
H	-5.80150800	-1.90710800	3.09851800
H	-2.94211400	0.83924200	4.68777300
H	-4.99737900	-0.49785600	4.96008800
C	-3.29037400	0.50392400	-0.98478600
C	-4.22540600	1.33900300	-0.38385300
C	-3.13595800	0.54637800	-2.37010200

C	-4.99674400	2.19618400	-1.15123300
H	-4.35337100	1.32805600	0.68692800
C	-3.91109100	1.40212400	-3.13206800
H	-2.39818100	-0.07922400	-2.84731100
C	-4.84255400	2.22997600	-2.52529000
H	-5.71769600	2.83845300	-0.66897600
H	-3.78257700	1.42204200	-4.20362400
H	-5.44624400	2.89615600	-3.12317700

### 1b-PC

Ru	-0.03074500	0.01737700	0.07133600
Cl	-0.10203200	-0.26456400	-2.31820400
Cl	0.00165400	0.80038400	2.35742300
P	2.32632900	0.45033300	0.02186100
P	-2.40788100	0.27838400	0.00395300
C	-0.02263300	-1.68321600	0.73496000
H	-0.23012300	-1.71533900	1.80950900
C	3.21365900	0.17648100	1.61448000
H	2.67960800	0.87471900	2.26471100
C	4.69030200	0.55271600	1.60873500
H	4.84287000	1.53587900	1.16298300
H	5.25122200	-0.15832500	0.99943700
C	5.24183100	0.53078300	3.02611600
H	6.30160500	0.78399700	3.01731200
H	4.73859800	1.30146300	3.61454200
C	5.02246900	-0.82030600	3.68096600
H	5.40068800	-0.80981100	4.70245200
H	5.59811600	-1.57673100	3.14158800
C	3.55345000	-1.20143300	3.66123600
H	3.40945600	-2.18370900	4.10993000
H	2.98440600	-0.49183400	4.26550200
C	2.99995100	-1.19155600	2.24658500
H	1.93648100	-1.41241000	2.26612000
H	3.48872900	-1.97223200	1.66512100
C	2.57348500	2.25974500	-0.28177300
H	3.62499200	2.38503300	-0.55393000
C	2.30677600	3.14704500	0.92693600
H	2.93942900	2.86142400	1.76504900
H	1.27758800	3.01463000	1.26267100
C	2.56210300	4.60412500	0.57965700
H	2.36706700	5.22865900	1.45044100
H	3.61793700	4.73654200	0.32945900
C	1.70805800	5.04720600	-0.59130400

H	0.65752400	4.98766900	-0.29767500	H	-2.43370400	0.40570200	2.33079700
H	1.90508300	6.08957300	-0.83904300	C	-3.44466200	-1.42419700	1.97089000
C	1.94367300	4.16164800	-1.80112700	H	-4.24980000	-1.80998700	1.34219300
H	2.97027400	4.29579800	-2.15128600	H	-2.55525000	-2.00995600	1.73862300
H	1.29344400	4.45585700	-2.62487700	C	-3.83904900	-1.60211700	3.42632300
C	1.71727500	2.69848300	-1.46534700	H	-3.02079600	-1.26060600	4.06319100
H	1.89631400	2.06419600	-2.33327200	H	-3.99368500	-2.65822300	3.64510700
H	0.66118300	2.55062100	-1.21693500	C	-5.09223400	-0.80609000	3.73871600
C	3.22817900	-0.35901600	-1.37653700	H	-5.36283700	-0.91473000	4.78820300
H	2.44687100	-0.43486600	-2.13810000	H	-5.92564300	-1.20788600	3.15695800
C	4.40163800	0.39487700	-1.99150500	C	-4.89924600	0.65842000	3.39425500
H	5.19781000	0.52310100	-1.25468400	H	-5.81232400	1.21990900	3.58968400
H	4.09828400	1.39071600	-2.30875500	H	-4.12706000	1.07797100	4.04239900
C	4.93872800	-0.35847100	-3.20011200	C	-4.47619000	0.85332100	1.94546200
H	4.16761000	-0.37147100	-3.97337900	H	-4.30577900	1.91400600	1.77515600
H	5.79144000	0.17603300	-3.61756100	H	-5.28894000	0.54989500	1.28307300
C	5.32118200	-1.78624800	-2.85937600	C	-2.81645100	2.02671300	-0.44659000
H	5.67109200	-2.30608000	-3.75031800	H	-3.87967100	2.15845500	-0.22930900
H	6.15497200	-1.77801300	-2.15304700	C	-2.60878900	2.35058600	-1.92054700
C	4.15041800	-2.52180700	-2.23518600	H	-3.20978100	1.69497100	-2.54744700
H	4.43500000	-3.53759400	-1.96284900	H	-1.56849500	2.17053200	-2.19628700
H	3.34008600	-2.60455500	-2.96325100	C	-2.98024800	3.79511700	-2.20831500
C	3.64782100	-1.77766700	-1.01129600	H	-2.82012100	4.01184100	-3.26367400
H	2.82125600	-2.31317800	-0.54846400	H	-4.04676200	3.93899200	-2.01696300
H	4.45208100	-1.73860800	-0.27435300	C	-2.18047200	4.74730200	-1.34269400
C	-3.29707700	-0.69090300	-1.28406300	H	-1.12289700	4.64270900	-1.59704000
H	-2.85727300	-0.28427800	-2.19824400	H	-2.45316000	5.78091400	-1.55222000
C	-2.96767300	-2.17607000	-1.31236700	C	-2.37685000	4.43338300	0.12929100
H	-3.34923400	-2.67827600	-0.42393900	H	-3.41930300	4.61856400	0.40050700
H	-1.88947400	-2.29921700	-1.31859200	H	-1.77212000	5.09681900	0.74732900
C	-3.57602400	-2.81772200	-2.54842800	C	-2.02721300	2.98831700	0.43482800
H	-3.10438000	-2.38733700	-3.43456000	H	-0.95838100	2.83422000	0.26477900
H	-3.35145000	-3.88358400	-2.56025300	H	-2.17864500	2.76304000	1.49022000
C	-5.07627700	-2.59089300	-2.61338000	C	0.69425300	-5.66262500	-0.55992700
H	-5.49051100	-3.03701500	-3.51676700	C	0.38708400	-5.38096800	0.76061400
H	-5.55335200	-3.09479500	-1.76887000	C	0.15402100	-4.07355500	1.14336900
C	-5.40551300	-1.11094500	-2.55793100	C	0.22286500	-3.02418300	0.22084400
H	-5.00721000	-0.61941700	-3.44854900	C	0.53465000	-3.32804000	-1.10759600
H	-6.48429600	-0.95811200	-2.57069600	C	0.76594900	-4.63399700	-1.48976300
C	-4.80203600	-0.46165200	-1.32346800	H	0.87891200	-6.68125100	-0.86624400
H	-5.25993700	-0.89755000	-0.43327400	H	0.33114200	-6.17574900	1.48842100
H	-5.03873100	0.60263400	-1.30928900	H	-0.08240800	-3.84820600	2.17367500
C	-3.21398300	0.04870000	1.65410900	H	0.58793900	-2.52413800	-1.82526300

H 1.00568500 -4.85405200 -2.51902700

**pseudo-E 2b-PC**

Ru 0.02886900 -0.27446200 0.13446000  
C -0.13343300 -2.34075800 0.27474200  
N 0.89908200 -3.19203000 0.32069500  
N -1.23814100 -3.04246200 0.57421000  
C 0.52757200 -4.51110900 0.81499800  
H 0.88229400 -4.63277400 1.83805700  
H 0.97489400 -5.28760400 0.20037400  
C -0.98161200 -4.46788700 0.72822700  
H -1.47184700 -4.85178200 1.61792600  
H -1.36908500 -5.00725500 -0.13796200  
Cl 0.66657500 -0.40864300 -2.17749100  
Cl -0.01643300 -0.40752000 2.54857500  
C -2.59144000 -2.64550900 0.41788600  
C -3.38828100 -2.46361200 1.54405800  
C -3.12566000 -2.57821400 -0.87012000  
C -4.72782000 -2.15088300 1.35140100  
C -4.46931200 -2.27834300 -1.01341400  
C -5.28560100 -2.05437600 0.08648700  
H -5.35284100 -1.99320200 2.21968600  
H -4.88506700 -2.20700300 -2.00931200  
C 2.24508900 -2.99399700 -0.09278100  
C 3.23167500 -2.67594700 0.83639000  
C 2.56803400 -3.31612800 -1.41303000  
C 4.54761700 -2.61709800 0.39674100  
C 3.89274600 -3.23582800 -1.80651900  
C 4.89698700 -2.87951200 -0.91736000  
H 5.32131400 -2.36656200 1.10971000  
H 4.14771300 -3.47006800 -2.83068800  
C -2.25160700 -2.80468700 -2.05743500  
H -1.80502800 -3.79895600 -2.03923400  
H -2.81828100 -2.70674200 -2.97858800  
H -1.43013200 -2.08935200 -2.07877800  
C -2.83552700 -2.63006100 2.92125200  
H -3.48366400 -2.15823100 3.65420800  
H -2.76667100 -3.68632900 3.18473900  
H -1.84405300 -2.19513700 3.00381100  
C 2.91062100 -2.44108000 2.27558400  
H 2.00152000 -1.86039000 2.40193000  
H 2.77372700 -3.38679500 2.80099800

H 3.72574500 -1.91473000 2.76601200  
C 1.51294200 -3.77114600 -2.36648800  
H 0.79598800 -2.97541400 -2.54858700  
H 1.95430900 -4.05999200 -3.31564500  
H 0.96743400 -4.62986000 -1.97469900  
C -6.72901200 -1.70981900 -0.09691500  
H -7.21080200 -2.39046400 -0.79522500  
H -7.26953800 -1.75285300 0.84447900  
H -6.83458600 -0.70379500 -0.49983100  
C 6.31760100 -2.76800700 -1.37146400  
H 7.00991600 -2.91816400 -0.54751600  
H 6.54471500 -3.49651600 -2.14542800  
H 6.51256600 -1.77937500 -1.78631800  
C -1.74191700 0.15685900 0.20684100  
H -2.15772100 0.11337400 1.21789900  
C -2.74847700 0.61168400 -0.74248200  
C -2.62360100 0.52392000 -2.13000700  
C -3.94125000 1.10999300 -0.21075700  
C -3.65969800 0.92101300 -2.95152500  
H -1.71167000 0.12497600 -2.54510400  
C -4.96912300 1.53041600 -1.03333400  
H -4.05221500 1.15782000 0.86329300  
C -4.83163700 1.42860900 -2.40788500  
H -3.55438500 0.83824300 -4.02271800  
H -5.87780700 1.92564300 -0.60494700  
H -5.63513000 1.74443800 -3.05645500  
H 0.90286200 4.82515000 3.75392800  
C 0.72099500 3.79992900 4.08840400  
C -0.74914400 3.64138700 4.42875700  
C 1.14653500 2.82798900 2.99813600  
H 1.33559900 3.64729600 4.97491800  
C -1.60749700 3.82503700 3.19164900  
H -0.91579200 2.64077500 4.83247800  
H -1.03942900 4.35021400 5.20368100  
C 0.28436300 3.02373400 1.75698700  
H 1.04204300 1.80788300 3.35903600  
H 2.19839900 2.98942900 2.76551600  
C -1.19266000 2.85691600 2.09677200  
H -1.50595500 4.85182700 2.83009700  
H -2.66035600 3.68152600 3.43322400  
P 0.73037500 2.06123300 0.22396600  
H 0.42308800 4.06367600 1.45344100  
H -1.35563600 1.83496600 2.43185900



H	-1.81335600	3.01061300	1.21255100	Cl	-0.15068700	-0.34935100	2.56125400
C	2.57602800	2.08111000	0.19515100	C	0.62245700	-2.35553900	0.27390700
C	0.14528800	3.32735500	-1.01066200	P	-1.17245300	1.71213500	0.15298100
C	3.20625100	2.01593500	-1.19142300	N	-0.25373200	-3.36894500	0.26293100
C	3.08108800	0.88934400	1.00641700	N	1.83496100	-2.88212600	0.48157400
H	2.89336400	3.01222600	0.67696800	C	1.81696300	-4.32954800	0.65359900
C	-0.01212000	2.84621500	-2.44534400	H	2.11285200	-4.59023600	1.66811700
C	0.91280000	4.65029400	-0.99802100	H	2.51806500	-4.79730400	-0.03396600
H	-0.86586500	3.53508800	-0.64065500	C	0.37087800	-4.67934600	0.35946800
C	4.72183100	2.07172100	-1.07755500	H	0.24975600	-5.21383200	-0.58280200
H	2.89943800	1.08962300	-1.67788800	H	-0.09460400	-5.26754300	1.14634100
H	2.86132500	2.82770500	-1.82342800	C	3.09837800	-2.23946200	0.43947600
C	4.59192500	0.92488100	1.14256000	C	3.70859200	-2.06147800	-0.80087700
H	2.80168100	-0.02390000	0.46497000	C	4.98043300	-1.51446700	-0.83613500
H	2.59975300	0.82495600	1.97977600	H	5.44961100	-1.34293000	-1.79533600
C	-0.73613400	3.88906400	-3.27964400	C	5.65393700	-1.16579000	0.32508500
H	0.96489400	2.63653400	-2.88082800	C	5.01955400	-1.36268600	1.54260400
H	-0.54774300	1.90708800	-2.46493200	H	5.52694900	-1.08490700	2.45640800
C	0.17886800	5.69753500	-1.82068200	C	3.74370400	-1.90235000	1.62605600
H	1.90230600	4.50213200	-1.42947900	C	2.97737200	-2.41203700	-2.05265100
H	1.07226200	5.02803700	0.00904500	H	3.59412000	-2.22482800	-2.92645900
C	5.25759300	0.94036300	-0.22030900	H	2.06318200	-1.82520400	-2.14296500
H	5.01297300	3.02978700	-0.63843200	H	2.68482100	-3.46245700	-2.06323100
H	5.16721000	2.03581400	-2.07121400	C	7.03502800	-0.59619500	0.25967700
H	4.87875700	1.81762600	1.70446500	H	7.25852400	0.00320400	1.13832000
H	4.93179600	0.06801800	1.72349400	H	7.15572700	0.03070400	-0.62015200
C	-0.02320700	5.22753200	-3.24892700	H	7.78096800	-1.38820000	0.20430600
H	-1.75136900	4.00987300	-2.89250300	C	3.07411900	-2.09610000	2.94647200
H	-0.83516600	3.53448600	-4.30505600	H	2.08599800	-1.63968800	2.95626900
H	-0.79301900	5.89657400	-1.36283000	H	3.66675200	-1.65707000	3.74372900
H	0.73190400	6.63630400	-1.80181700	H	2.94761700	-3.15324300	3.17752300
H	5.05119600	-0.00787800	-0.71932600	C	-1.62556600	-3.31152600	-0.10242500
H	6.33981600	1.01908500	-0.11738800	C	-1.97895200	-3.45171800	-1.44249000
H	0.95205000	5.12536000	-3.73093200	C	-3.33019500	-3.47178000	-1.76536900
H	-0.57755800	5.97201100	-3.81947000	H	-3.61195800	-3.55551600	-2.80591300

**pseudo-Z 2b-PC**

Ru	0.05685100	-0.36584500	0.15597400	H	-4.68077900	-3.33525800	1.31016100
C	1.70615800	0.38563200	0.36471700	C	-2.59363400	-3.28632800	0.90620500
H	2.03792200	0.39507800	1.40766300	C	-0.96886000	-3.66949300	-2.52262400
C	2.70667200	1.01931000	-0.48533000	H	0.02410900	-3.34833200	-2.23130700
Cl	-0.25373600	-0.52052800	-2.22577100	H	-1.23332700	-3.10295600	-3.40989500
				H	-0.93809600	-4.72632200	-2.79157000

C	-5.76386700	-3.51198200	-1.16343200
H	-6.35047100	-2.74536400	-0.66205600
H	-6.17800600	-4.47637400	-0.87316800
H	-5.90600800	-3.39896600	-2.23435600
C	-2.20420700	-3.26450600	2.34746000
H	-3.08760100	-3.23999600	2.97907600
H	-1.58204300	-2.40552000	2.58338600
H	-1.63436500	-4.15582000	2.60917900
C	2.67744800	1.03116300	-1.88221500
H	1.84334900	0.57290300	-2.38807300
C	3.69669100	1.62714400	-2.59661800
H	3.66520800	1.62235300	-3.67579100
C	4.75310400	2.24207600	-1.93742000
H	5.54258300	2.71344700	-2.50376900
C	4.78664500	2.25946000	-0.55355700
H	5.60168400	2.74046000	-0.03424200
C	3.77710400	1.64259000	0.16224300
H	3.81167500	1.62865900	1.24228200
C	-1.01978600	2.70368500	-1.40755200
H	-0.85439300	1.91807800	-2.14913400
C	-2.22743700	3.51750100	-1.86297200
H	-3.11644500	2.89384700	-1.92929400
H	-2.44612600	4.30869900	-1.14311000
C	-1.96412000	4.13195100	-3.23035300
H	-1.86266500	3.32674200	-3.96119000
H	-2.82407700	4.72673400	-3.53747700
C	-0.70245000	4.97416100	-3.24507300
H	-0.52613100	5.37333300	-4.24334400
H	-0.83355400	5.83314200	-2.58223100
C	0.48838900	4.16072800	-2.77438900
H	1.39065100	4.77129900	-2.75690400
H	0.67161100	3.34461600	-3.47659400
C	0.22589400	3.58194900	-1.39593200
H	0.08489700	4.40691700	-0.69487600
H	1.08828900	3.01692000	-1.05171000
C	-0.91877600	2.80711800	1.61965300
H	-1.26344500	2.16257100	2.43141000
C	0.53215400	3.12367400	1.96289800
H	1.08566500	2.19244600	2.04409400
H	1.00247100	3.72101100	1.18241800
C	0.60884600	3.87309000	3.28459200
H	0.25547500	3.21520000	4.08155000
H	1.64741800	4.11117400	3.51274900

C	-0.23267500	5.13463600	3.26514200
H	-0.17182400	5.64862000	4.22379600
H	0.16399600	5.82278200	2.51433000
C	-1.67540500	4.80881100	2.92975900
H	-2.27679600	5.71681900	2.89290900
H	-2.09570100	4.18383400	3.72110800
C	-1.77345400	4.06832800	1.60601300
H	-1.43707700	4.73140300	0.80736000
H	-2.81600300	3.82946100	1.39689000
C	-2.98506800	1.36076300	0.23816200
H	-3.47366400	2.31533100	0.02724000
C	-3.41195300	0.37094400	-0.83965300
H	-3.00114400	0.63977000	-1.81235300
H	-3.00012700	-0.61652500	-0.61060900
C	-4.92839200	0.29708100	-0.90110200
H	-5.31560900	1.26506500	-1.23167700
H	-5.23372600	-0.43193800	-1.65185400
C	-5.53286100	-0.05248600	0.44784000
H	-6.62112800	-0.01460900	0.39571400
H	-5.26200500	-1.07700600	0.69855900
C	-5.02472700	0.85484800	1.55262300
H	-5.41475200	0.52768200	2.51600600
H	-5.39745100	1.87024600	1.39426100
C	-3.50492300	0.89184600	1.58962800
H	-3.10269000	-0.09855600	1.81369700
H	-3.18053600	1.54975200	2.39294500

**1a-Inact-C PPh<sub>3</sub>Cl<sub>2</sub>Ru=CHPh**

Ru	-0.87841700	-0.54378400	-0.91893500
Cl	-0.74704500	0.87329500	-2.72449600
Cl	-0.80857400	-2.75024700	-0.27152000
P	0.98810800	0.06516500	0.09637500
C	-1.93002900	0.29704000	0.28746100
H	-1.54753000	1.00540000	1.02438500
C	-3.37638900	0.16697700	0.26392300
C	-4.16419800	1.16802700	0.83812300
C	-5.54227900	1.09665400	0.78542600
C	-6.15618000	0.01542400	0.17209500
C	-5.38744100	-0.99596300	-0.38328300
C	-4.00933000	-0.92473000	-0.33817600
H	-7.23318400	-0.04406700	0.13615600
H	-6.13956300	1.88018300	1.22573300

H	-3.68253300	2.00843500	1.31647000	C	2.12124100	0.46421800	-0.11038900
H	-3.41340100	-1.73510600	-0.73404100	H	1.77770200	1.49446300	-0.15580800
H	-5.86473700	-1.84687600	-0.84393300	C	-1.11356400	0.98176200	1.60506200
C	1.06053000	1.79005500	0.67019500	H	-1.08382200	0.16424000	2.33119100
C	1.81763200	2.13853000	1.78489700	C	0.04140600	1.89991900	1.98381000
C	0.37902400	2.77996900	-0.03101900	H	0.14321900	2.70959200	1.25896800
C	1.89811300	3.46077100	2.18600500	H	0.96651500	1.32940200	1.97985600
H	2.34062400	1.37943600	2.34527100	C	-0.17778400	2.48554600	3.36923100
C	0.46407400	4.10090800	0.37491500	H	-0.14217500	1.67495700	4.09996500
H	-0.20950000	2.51403700	-0.89629500	H	0.64080200	3.16089000	3.61385400
C	1.22203400	4.44318400	1.48200200	C	-1.51066000	3.19994600	3.47990900
H	2.48636600	3.72088000	3.05256100	H	-1.64921900	3.59061400	4.48691700
H	-0.06664000	4.86154100	-0.17672900	H	-1.52042200	4.06063800	2.80637400
H	1.28328200	5.47334100	1.79838000	C	-2.64919000	2.26668400	3.11501600
C	1.44259500	-0.89774600	1.56786300	H	-2.69129200	1.44879400	3.83765900
C	2.76668200	-1.21829100	1.84314700	H	-3.60549000	2.78519900	3.17106600
C	0.44835600	-1.26180800	2.46783300	C	-2.45765800	1.69127800	1.72146300
C	3.09135600	-1.88770900	3.01173800	H	-2.50515500	2.50502800	0.99594000
H	3.54502300	-0.94881400	1.14510000	H	-3.27482400	1.00933600	1.48546200
C	0.77630100	-1.92328100	3.63636500	C	-1.34467100	1.08476700	-1.45440400
H	-0.58512400	-1.05030500	2.23855100	H	-0.88359500	0.50637200	-2.25937000
C	2.09797900	-2.23657800	3.90995200	C	-0.67876100	2.45848700	-1.44168700
H	4.12103900	-2.13803200	3.21596700	H	-1.09584600	3.06423200	-0.63475300
H	-0.00279800	-2.20911000	4.32579200	H	0.38676600	2.36163900	-1.25093100
H	2.35147000	-2.76129900	4.81840200	C	-0.89327600	3.18316000	-2.76012200
C	2.38085800	-0.15371200	-1.03822400	H	-0.40639600	2.62058300	-3.55882100
C	2.60473100	-1.43523900	-1.53535800	H	-0.41248600	4.15993300	-2.72404700
C	3.18106400	0.90095200	-1.45203700	C	-2.37016700	3.32562000	-3.06989200
C	3.63292400	-1.65596300	-2.43215800	H	-2.51295300	3.82644800	-4.02621900
H	1.97293200	-2.25406700	-1.21688000	H	-2.83950300	3.95696700	-2.31138100
C	4.20810400	0.67312500	-2.35346000	C	-3.03994300	1.96611600	-3.08046500
H	3.00263500	1.89705700	-1.07724300	H	-4.10682600	2.06460300	-3.27682600
C	4.43501400	-0.60162400	-2.84152100	H	-2.62482100	1.36919400	-3.89514500
H	3.80458100	-2.64969300	-2.81587500	C	-2.83280200	1.22016400	-1.77176700
H	4.82812400	1.49520700	-2.67620300	H	-3.29785300	0.24162100	-1.86044500
H	5.23405600	-0.77478200	-3.54602400	H	-3.34750100	1.74803700	-0.96730200

**1b-Inact-C PCy<sub>3</sub>Cl<sub>2</sub>Ru=CHPh**

Ru	1.05863700	-0.98905400	-0.18192700	C	-2.42638600	-1.95240500	1.40253300
Cl	1.06740400	-1.70203100	2.02360900	H	-2.56527400	-1.26569500	2.23607600
Cl	0.94835300	-1.41649900	-2.45298900	H	-1.51727700	-2.51562200	1.60945800
P	-0.91014200	0.05131000	0.02764100	C	-3.62048700	-2.89299300	1.32929500
				H	-3.70514800	-3.44505900	2.26421100

H -4.53574100 -2.30340200 1.23081100  
C -3.51812000 -3.84851900 0.15573100  
H -2.65605000 -4.50332400 0.29852400  
H -4.39668800 -4.49087800 0.11398500  
C -3.35321100 -3.08766300 -1.14618600  
H -4.25490100 -2.50092900 -1.34110500  
H -3.23953900 -3.77569800 -1.98231200  
C -2.15432200 -2.15995000 -1.07794800  
H -1.24839100 -2.75628700 -0.94755400  
H -2.01849500 -1.63014000 -2.02036300  
C 6.33825200 0.04518700 -0.11795500  
C 5.75308400 1.24490400 -0.49168400  
C 4.37883800 1.37842700 -0.46531800  
C 3.56525800 0.31160700 -0.07590600  
C 4.17141300 -0.88791700 0.31249500  
C 5.54524900 -1.01763300 0.28760600  
H 7.41233900 -0.05906700 -0.13316800  
H 6.36972500 2.07523400 -0.79956700  
H 3.92009100 2.31195500 -0.75712400  
H 3.56194100 -1.70430600 0.67500200  
H 6.00124200 -1.94569500 0.59550100

**2b-Inact-C NHC-Cl<sub>2</sub>Ru=CHPh**

Ru 0.25385800 0.81831300 0.12332100  
C 0.48445900 -1.10729000 0.04703200  
N 1.72398700 -1.62557100 0.02842900  
N -0.37616000 -2.13441600 0.07514300  
C 1.74806600 -3.06941400 0.15380600  
H 2.13094200 -3.35340600 1.13419500  
H 2.39040700 -3.50925500 -0.60474000  
C 0.28371000 -3.42823100 -0.02635700  
H -0.08763700 -4.10518900 0.73850300  
H 0.07825400 -3.87294700 -1.00021600  
Cl 0.80618600 1.39955000 -2.05578700  
Cl 0.53226600 1.00465500 2.41651200  
C -1.78512100 -2.09019100 -0.04124200  
C -2.55395400 -2.17073200 1.11503400  
C -2.35884100 -1.98009600 -1.30463800  
C -3.93423400 -2.15480200 0.98197200  
C -3.74259400 -1.96966800 -1.39097700  
C -4.54496800 -2.06448300 -0.26169300  
H -4.54631200 -2.20549800 1.87176100

H -4.20483500 -1.87311100 -2.36354500  
C 2.92759600 -0.87180500 -0.00940000  
C 3.56969000 -0.51981000 1.17623000  
C 3.49076400 -0.59164000 -1.25742400  
C 4.72930100 0.23914700 1.08506100  
C 4.65111100 0.16020400 -1.29584000  
C 5.26922200 0.60796700 -0.13528300  
H 5.22323500 0.54131700 1.99810300  
H 5.08279900 0.40520900 -2.25601500  
C -1.50363000 -1.78540500 -2.51380600  
H -0.70844600 -2.52597600 -2.57512100  
H -2.09554800 -1.85005100 -3.42151600  
H -1.02490500 -0.80604300 -2.48639500  
C -1.89386700 -2.19779500 2.45462100  
H -2.63204300 -2.24025000 3.24948200  
H -1.23623800 -3.05923100 2.56090500  
H -1.28181800 -1.30773400 2.59629000  
C 3.10910600 -1.01072800 2.51085900  
H 2.05191500 -1.24848100 2.52225100  
H 3.67685600 -1.89968800 2.78885300  
H 3.27343500 -0.25794900 3.27555900  
C 2.88824200 -1.14187800 -2.50946800  
H 1.81351400 -0.99105900 -2.53480600  
H 3.31057000 -0.65565800 -3.38317400  
H 3.09158300 -2.21061700 -2.59139000  
C -6.03560300 -2.09162400 -0.38492700  
H -6.39139300 -3.11204300 -0.52111700  
H -6.51462100 -1.69578800 0.50641300  
H -6.37326800 -1.51202500 -1.23979000  
C 6.48689800 1.47310600 -0.20645400  
H 7.09486800 1.37771800 0.68890500  
H 7.10224700 1.22138900 -1.06626900  
H 6.20508200 2.52074200 -0.30248600  
C -1.54380600 0.99044800 0.02793400  
H -2.24901400 0.16686700 0.05262600  
C -2.16031900 2.30295000 0.00385600  
C -1.41067900 3.46900000 -0.18396200  
C -3.53915900 2.41715900 0.19896300  
C -2.02014000 4.70588900 -0.16260600  
H -0.34880600 3.40349800 -0.37882700  
C -4.14825200 3.65684900 0.22099700  
H -4.12381800 1.51898900 0.33790600  
C -3.38893700 4.80248600 0.04155600

H -1.43157600 5.59740800 -0.31280000  
H -5.21370800 3.73243500 0.37507500  
H -3.86427400 5.77143300 0.05486600

**PPH<sub>3</sub>**

C -0.89397800 -1.36175900 -0.42771800  
C 1.66522700 -0.11540800 -0.38856100  
C -0.70472300 1.46267700 -0.43686400  
C -0.41911400 -2.14933700 0.61419200  
C -2.16392100 -1.62167400 -0.93779700  
C 2.01555000 0.61982000 0.73752200  
C 2.60641700 -0.97832600 -0.94437300  
C -0.52231400 2.68510900 -1.07649200  
C -1.44568000 1.42745800 0.73967700  
C -1.20055800 -3.16879200 1.13629000  
H 0.56449300 -1.96849600 1.02078700  
C -2.94956600 -2.62684500 -0.40639700  
H -2.53945500 -1.02814800 -1.75952700  
C 3.27535500 0.48810200 1.29897600  
H 1.30319700 1.30107800 1.17737000  
C 3.85904700 -1.12175600 -0.37525700  
H 2.35390200 -1.53988200 -1.83275400  
C -1.04955400 3.84883800 -0.54469300  
H 0.03362600 2.72245200 -2.00246800  
C -1.98255400 2.59005100 1.26715300  
H -1.60733400 0.48594500 1.24338100  
C -2.46675000 -3.40745200 0.63225200  
H -0.81644800 -3.77452000 1.94316600  
H -3.93396400 -2.80957300 -0.80964600  
C 4.19743000 -0.38482400 0.74784100  
H 3.53507900 1.06966000 2.17059900  
H 4.57496300 -1.79849200 -0.81632400  
C -1.78353700 3.80274400 0.62853600  
H -0.89767800 4.78892500 -1.05276900  
H -2.55777500 2.54717600 2.17970200  
H -3.07292900 -4.20065200 1.04235400  
H 5.17831400 -0.48545800 1.18673500  
H -2.20490200 4.70707200 1.04035600  
P 0.04345500 -0.00874700 -1.22553800

**PCy<sub>3</sub>**

P -0.23490400 -0.07238900 -1.03581900  
C 0.76340600 -1.46126300 -0.30371800  
H 0.05732800 -2.29524300 -0.37144400  
C 1.21769800 -1.37339200 1.14545000  
H 0.38923800 -1.09508600 1.79694500  
H 1.97032300 -0.58858000 1.23881000  
C 1.83361600 -2.68778300 1.59990500  
H 2.16012600 -2.61213000 2.63676100  
H 1.07254300 -3.47111600 1.56743000  
C 2.99509400 -3.08039600 0.70541400  
H 3.41599300 -4.03307700 1.02465400  
H 3.78992900 -2.33751300 0.80784700  
C 2.56474700 -3.15137600 -0.74865300  
H 3.41381600 -3.40063500 -1.38433600  
H 1.83732800 -3.95801400 -0.86802300  
C 1.93494100 -1.84543300 -1.20415000  
H 1.59672900 -1.92456500 -2.23629700  
H 2.69280300 -1.06098200 -1.18489900  
C -1.79876200 -0.13754300 -0.03288000  
H -1.57327500 -0.05691800 1.03514500  
C -2.53277100 -1.45254000 -0.27176400  
H -1.92883200 -2.29585600 0.05741700  
H -2.68639200 -1.57894200 -1.34669100  
C -3.87506400 -1.49417300 0.43779300  
H -4.37528700 -2.43885400 0.22696000  
H -3.71196300 -1.46114000 1.51758800  
C -4.75127300 -0.32569000 0.03047600  
H -4.98695800 -0.40681600 -1.03318400  
H -5.70005300 -0.35471100 0.56479700  
C -4.03810100 0.98829700 0.28389700  
H -3.88035700 1.11044900 1.35816200  
H -4.65538600 1.82653300 -0.03768400  
C -2.69705700 1.03150500 -0.42920500  
H -2.20075600 1.98032100 -0.22805400  
H -2.86219000 0.99209800 -1.50914500  
C 0.51824200 1.53881800 -0.47892700  
H -0.05251800 2.26620000 -1.06768500  
C 0.42383300 1.98234200 0.97645000  
H 0.99772500 1.30960200 1.61277100  
H -0.60604700 1.93966700 1.32822000  
C 0.96372800 3.39711800 1.13555000  
H 0.33065100 4.08534500 0.57010400

H	0.90266300	3.70442900	2.17920100
C	2.39191800	3.50973900	0.63312000
H	2.74949600	4.53367300	0.73456400
H	3.04015800	2.88908700	1.25663000
C	2.49979100	3.04703400	-0.80772200
H	3.53445000	3.09374200	-1.14593400
H	1.92851200	3.72191900	-1.44908300
C	1.96043700	1.63696000	-0.96189800
H	2.03588200	1.30846000	-1.99877500
H	2.58133900	0.96114500	-0.37031700

**TPSS**

**1a-PC**

Ru	0.14902400	-0.06981700	0.03492500
Cl	0.15655200	0.20973100	-2.34367600
Cl	0.32270000	-1.19001400	2.15733600
P	-2.23796300	-0.52749500	0.02206200
P	2.53563000	-0.13346900	-0.05769600
C	0.14495700	1.65614700	0.73117900
H	0.83434300	1.81655700	1.58028200
C	-1.95397200	5.28567900	-0.16269200
C	-1.27742200	5.12886200	1.05983100
C	-0.59651800	3.93907300	1.32954700
C	-0.60321400	2.86493500	0.39697500
C	-1.28712100	3.04371700	-0.83200500
C	-1.94566800	4.24590300	-1.10739000
H	-2.47646100	6.21638000	-0.37982600
H	-1.27387300	5.93610200	1.79086300
H	-0.05417600	3.82062900	2.26815500
H	-1.26269500	2.24124700	-1.56539600
H	-2.45898100	4.37074700	-2.05940900
C	3.45836400	1.21276100	-0.92593700
C	4.87087800	1.23040800	-0.90018100
C	2.76978500	2.25663600	-1.57070300
C	5.57789800	2.26624400	-1.52362500
H	5.41488700	0.44078600	-0.38324400
C	3.48229700	3.29729000	-2.18707000
H	1.68321300	2.24472600	-1.59977200
C	4.88361000	3.30300700	-2.16835300
H	6.66671500	2.26766400	-1.49882600
H	2.93744100	4.10041500	-2.68083000
H	5.43396500	4.11118000	-2.64814400

C	3.46389400	-0.19173200	1.54467600
C	3.98360000	-1.37944000	2.09007800
C	3.61627200	1.01326900	2.26306300
C	4.64495400	-1.36245100	3.32713700
H	3.88201600	-2.31862400	1.55156500
C	4.27337800	1.02670000	3.49984900
H	3.23904200	1.94733000	1.84799000
C	4.78949000	-0.16261300	4.03677100
H	5.04476500	-2.29035800	3.73353900
H	4.38557300	1.96581600	4.03990000
H	5.30156900	-0.15219500	4.99768900
C	2.96602800	-1.69648600	-0.94019400
C	2.39468400	-2.89947900	-0.46834400
C	3.75007400	-1.72062800	-2.10940100
C	2.63413200	-4.10650500	-1.13879800
H	1.75958200	-2.88416300	0.41799200
C	3.97929900	-2.93088100	-2.77999300
H	4.16908000	-0.79816400	-2.50467300
C	3.42830600	-4.12569400	-2.29502300
H	2.19039400	-5.02733900	-0.76306700
H	4.58366700	-2.93570300	-3.68593500
H	3.60657000	-5.06264100	-2.82054200
C	-2.51254600	-2.29896700	-0.47443500
C	-1.76799000	-3.29019600	0.20160400
C	-3.43781400	-2.69525600	-1.46022300
C	-1.94549900	-4.64495800	-0.10858300
H	-1.06331300	-2.99683100	0.97945200
C	-3.60665700	-4.05355000	-1.77058900
H	-4.03347000	-1.95223200	-1.98521300
C	-2.86098800	-5.03200300	-1.09878700
H	-1.36738500	-5.39699400	0.42697900
H	-4.32568600	-4.34200500	-2.53619500
H	-2.99423500	-6.08516700	-1.34191700
C	-3.09615600	-0.44465700	1.66074400
C	-4.24986100	-1.21530100	1.91299200
C	-2.61856600	0.42293700	2.65979200
C	-4.91769500	-1.10967000	3.14062400
H	-4.62269500	-1.90016500	1.15286000
C	-3.29209500	0.53198700	3.88481900
H	-1.71084600	0.99479300	2.48428200
C	-4.44165500	-0.23299900	4.12810100
H	-5.80520100	-1.71338200	3.32525800
H	-2.90842100	1.20309900	4.65173000

H	-4.95888800	-0.15415500	5.08330500
C	-3.38592900	0.42060500	-1.07925000
C	-4.42206600	1.21481900	-0.54542500
C	-3.20438400	0.39050200	-2.48122100
C	-5.26605400	1.94849300	-1.39195200
H	-4.57288000	1.26298600	0.53056800
C	-4.05292700	1.12397900	-3.32185200
H	-2.39172200	-0.19063900	-2.90952900
C	-5.08779000	1.90313700	-2.78177600
H	-6.06200200	2.55400900	-0.96052800
H	-3.90044300	1.08554100	-4.39960100
H	-5.74665000	2.47025900	-3.43803200

**1b-PC**

Ru	-0.02720700	-0.01319700	0.07667800
Cl	-0.07336000	-0.28475500	-2.33733500
Cl	-0.02036500	0.82699700	2.36991300
P	2.36165000	0.45474300	0.02797000
P	-2.43958700	0.28873400	-0.00618800
C	-0.01662200	-1.73763300	0.77027600
H	-0.21755700	-1.76828600	1.85762300
C	3.27598200	0.14609300	1.65011300
H	2.74624800	0.84364200	2.31904300
C	4.77937100	0.51430400	1.64114800
H	4.93903200	1.51951900	1.22682000
H	5.32982600	-0.19021700	0.99881600
C	5.36026500	0.44620200	3.07187300
H	6.43302900	0.68864500	3.04666200
H	4.87291800	1.21475400	3.69339400
C	5.13545300	-0.93822000	3.70773100
H	5.52081700	-0.94911800	4.73766800
H	5.70940900	-1.69265000	3.14451600
C	3.64186600	-1.31635800	3.68881300
H	3.49761700	-2.32420900	4.10498300
H	3.07939800	-0.62036500	4.33101000
C	3.06067500	-1.25735700	2.26004500
H	1.98734600	-1.47631900	2.28749300
H	3.54312300	-2.02737100	1.64173300
C	2.63755900	2.30643000	-0.24904300
H	3.70920600	2.40708100	-0.48796100
C	2.35378500	3.20174000	0.97985600
H	2.95229600	2.88052300	1.84239200
H	1.30128200	3.10183200	1.27928600

C	2.68486200	4.67583800	0.65832300
H	2.45938000	5.30090600	1.53454000
H	3.76758800	4.77086600	0.47096400
C	1.91184700	5.18337100	-0.57304800
H	0.83556300	5.19912400	-0.33918700
H	2.20097300	6.21863800	-0.80585100
C	2.15223900	4.27423000	-1.79318500
H	3.20784800	4.35133600	-2.10264400
H	1.54694200	4.60921300	-2.64825600
C	1.82800300	2.80053300	-1.47261600
H	2.01088500	2.16727600	-2.35081900
H	0.75320000	2.70243300	-1.25082900
C	3.29838000	-0.33630200	-1.41611100
H	2.52292300	-0.33976100	-2.20020000
C	4.53471000	0.40846200	-1.97917400
H	5.33643800	0.44366700	-1.22601800
H	4.28668700	1.44597900	-2.23764200
C	5.06051300	-0.30339000	-3.24730900
H	4.29134800	-0.24131300	-4.03371100
H	5.94693200	0.22780200	-3.62439100
C	5.39276200	-1.78326400	-2.98108500
H	5.72358600	-2.27128000	-3.90938600
H	6.23399800	-1.84566700	-2.27098700
C	4.17570800	-2.51917500	-2.39071600
H	4.43385400	-3.56189200	-2.15454300
H	3.36732600	-2.54903600	-3.13824800
C	3.66109600	-1.81147700	-1.11985400
H	2.79279900	-2.34644900	-0.71627400
H	4.45082800	-1.84562300	-0.35345100
C	-3.35801500	-0.68758900	-1.33344800
H	-2.88497900	-0.29657300	-2.24908500
C	-3.06365400	-2.20477700	-1.32653800
H	-3.49199200	-2.67593000	-0.43042600
H	-1.98159800	-2.36457800	-1.29771000
C	-3.66219000	-2.87411600	-2.58224000
H	-3.15256000	-2.47710400	-3.47469200
H	-3.46129800	-3.95503400	-2.55428800
C	-5.17680600	-2.61395400	-2.69836600
H	-5.57364900	-3.06306000	-3.62053600
H	-5.69547300	-3.10340600	-1.85725900
C	-5.48109200	-1.10448400	-2.66852200
H	-5.05647800	-0.62914400	-3.56758500
H	-6.56701000	-0.93063500	-2.69839200

C	-4.88178400	-0.43170500	-1.41347300
H	-5.36970600	-0.84803600	-0.51875900
H	-5.10688500	0.64385900	-1.43045500
C	-3.27301600	0.06273500	1.67736100
H	-2.50630100	0.49690500	2.34075800
C	-3.42132600	-1.42645800	2.07104700
H	-4.20303400	-1.89642700	1.45421100
H	-2.48674800	-1.96948800	1.87937300
C	-3.81662700	-1.55674500	3.55716200
H	-3.00670800	-1.14709300	4.18073800
H	-3.92221000	-2.61935900	3.82159400
C	-5.12586200	-0.80018300	3.84992800
H	-5.37567500	-0.86572900	4.91887100
H	-5.95218200	-1.28012000	3.29958900
C	-5.01736600	0.67426600	3.41839400
H	-5.97316900	1.19345700	3.58298600
H	-4.26521300	1.18034200	4.04422700
C	-4.60514900	0.81060000	1.93425700
H	-4.51225300	1.87668900	1.69089300
H	-5.40479200	0.40212200	1.29823200
C	-2.86548200	2.07513100	-0.46507900
H	-3.95413000	2.15711300	-0.30817900
C	-2.58280800	2.43297000	-1.94350400
H	-3.10738900	1.74435400	-2.61805800
H	-1.51029700	2.31771300	-2.15635400
C	-3.03376900	3.87827900	-2.24884100
H	-2.80112200	4.12067900	-3.29601100
H	-4.12952800	3.94414300	-2.14392800
C	-2.37253400	4.89724400	-1.30306100
H	-1.28758800	4.91190700	-1.49287600
H	-2.74515900	5.91054400	-1.51264400
C	-2.62316500	4.52884000	0.17122900
H	-3.69900000	4.62649800	0.39316700
H	-2.09852300	5.22977200	0.83688900
C	-2.17023800	3.08598900	0.47838800
H	-1.08011200	3.00665300	0.34900700
H	-2.36211100	2.84018000	1.53102000
C	0.59228900	-5.77731700	-0.57465100
C	0.36595200	-5.48464500	0.77956700
C	0.17208900	-4.15872900	1.18137600
C	0.20602900	-3.09120300	0.24361100
C	0.43907200	-3.40852700	-1.11851600
C	0.62462600	-4.73496500	-1.51806700

H	0.74102800	-6.80811200	-0.89344800
H	0.33860400	-6.28593900	1.51667200
H	-0.00743200	-3.93004400	2.23230900
H	0.45652800	-2.59823500	-1.84527300
H	0.79676400	-4.96027700	-2.56980600

***pseudo E 2b-PC***

Ru	-0.02986900	-0.30297400	0.09286200
C	-0.31648100	-2.35862000	0.21685600
N	0.67738600	-3.29962100	0.24710100
N	-1.48323900	-3.00544000	0.52572900
C	0.20937000	-4.62956500	0.71937300
H	0.59429800	-4.81873100	1.73063100
H	0.57730400	-5.41649000	0.05046700
C	-1.31402800	-4.47294200	0.69315500
H	-1.79435200	-4.80635900	1.61955700
H	-1.78285500	-4.99891900	-0.15137900
Cl	0.45151000	-0.40806800	-2.28118000
Cl	0.05622200	-0.43980100	2.53237600
C	-2.83881100	-2.53541000	0.39230300
C	-3.60569800	-2.30254100	1.55614100
C	-3.42018600	-2.48595800	-0.89784900
C	-4.96448300	-1.97416300	1.39684700
C	-4.78183300	-2.16288100	-1.00075000
C	-5.57079700	-1.89901600	0.13265600
H	-5.56274400	-1.78165300	2.28893800
H	-5.23442800	-2.11409500	-1.99216400
C	2.06939700	-3.19124200	-0.12456500
C	3.05816800	-3.02338000	0.87231700
C	2.42274300	-3.47166600	-1.46841500
C	4.40918600	-3.06184000	0.47789900
C	3.78468600	-3.49681600	-1.80776100
C	4.79467200	-3.28829300	-0.85234200
H	5.17749900	-2.92885900	1.24133500
H	4.06062000	-3.70669700	-2.84222800
C	-2.60069100	-2.77498200	-2.13545500
H	-2.19939600	-3.79877100	-2.12280100
H	-3.21647900	-2.66864900	-3.03596300
H	-1.74245200	-2.09388000	-2.21565600
C	-3.00011400	-2.41342400	2.93845400
H	-3.68391200	-1.99918900	3.68914800
H	-2.81575300	-3.46446100	3.20968400



H	-2.04098200	-1.88286100	2.99711800
C	2.70625900	-2.86804700	2.33620600
H	1.83023900	-2.22570000	2.48475600
H	2.48954100	-3.84836800	2.78868400
H	3.55176600	-2.43973300	2.88809900
C	1.37406800	-3.77857500	-2.51381200
H	0.75366700	-2.89482300	-2.70917700
H	1.85099300	-4.08665200	-3.45167400
H	0.70902000	-4.59150400	-2.18826000
C	-7.03268700	-1.52697300	-0.01264200
H	-7.53340300	-2.16180900	-0.75541100
H	-7.56631300	-1.62727800	0.94034200
H	-7.13750400	-0.48523400	-0.34902900
C	6.25691900	-3.31538000	-1.25110200
H	6.90240000	-3.50793300	-0.38544100
H	6.44920700	-4.09081400	-2.00371000
H	6.56396100	-2.35335800	-1.68683100
C	-1.78689900	0.28046000	0.23121300
H	-2.17430000	0.27031700	1.26575400
C	-2.78270300	0.85272500	-0.68808300
C	-2.72153300	0.79044700	-2.10176100
C	-3.90319100	1.49632900	-0.09749900
C	-3.73291300	1.35507800	-2.88458400
H	-1.87484000	0.28910900	-2.56623200
C	-4.90283600	2.08074400	-0.88283400
H	-3.97482000	1.53306400	0.98947100
C	-4.82190900	2.00938100	-2.28253900
H	-3.67099300	1.29059500	-3.97039900
H	-5.74463600	2.58238900	-0.40681600
H	-5.60102000	2.45609600	-2.89916400
H	1.38795100	4.77730000	3.83821200
C	1.15366400	3.75181200	4.17170500
C	-0.32954800	3.68078400	4.57997900
C	1.48471700	2.75618200	3.03663100
H	1.79947100	3.54543100	5.03795400
C	-1.24131900	3.91791500	3.36154100
H	-0.54166500	2.68551700	5.00115000
H	-0.54384500	4.41774000	5.36811300
C	0.57067900	3.01089000	1.81595900
H	1.34393700	1.72743000	3.39197100
H	2.54041100	2.87543200	2.75624200
C	-0.91922100	2.92667000	2.22265200
H	-1.10622400	4.95173500	3.00082200

H	-2.29862600	3.81776400	3.64892400
P	0.90950100	2.00751300	0.22665400
H	0.76297400	4.04823200	1.49486700
H	-1.12970700	1.90120100	2.55273500
H	-1.56909400	3.13397500	1.35929900
C	2.79240800	1.93742800	0.11615800
C	0.37537500	3.38941400	-0.97958700
C	3.33302800	1.77876100	-1.32662400
C	3.35245000	0.78225400	0.98348100
H	3.15444500	2.89851300	0.52257900
C	0.08202700	2.96557900	-2.43455800
C	1.28833300	4.64564900	-0.97899500
H	-0.59181900	3.68599800	-0.53487200
C	4.87677900	1.81656600	-1.33043300
H	2.97563100	0.82479600	-1.73998500
H	2.94927600	2.56889700	-1.98229500
C	4.89470500	0.81571200	1.00543700
H	3.02012400	-0.17224300	0.54388600
H	2.95358600	0.80984400	2.00320300
C	-0.58996600	4.11933100	-3.20933100
H	1.01493400	2.67957900	-2.94055400
H	-0.55387000	2.07819700	-2.44401900
C	0.61557900	5.80520100	-1.74778700
H	2.24390600	4.40556500	-1.46745400
H	1.52986800	4.97824100	0.03979800
C	5.47497300	0.72922100	-0.41867900
H	5.21550700	2.80898000	-0.98835800
H	5.24391800	1.69382200	-2.36005900
H	5.22938300	1.75049500	1.48573700
H	5.27415300	-0.01145900	1.62289300
C	0.27035800	5.39637200	-3.19203100
H	-1.57187400	4.33402200	-2.75636800
H	-0.78160900	3.80264700	-4.24511900
H	-0.30679100	6.09932400	-1.22055900
H	1.27869700	6.68313600	-1.74394500
H	5.23441400	-0.25973200	-0.83727300
H	6.57179300	0.81280700	-0.39251900
H	1.20453800	5.21151400	-3.74748400
H	-0.24804200	6.21878200	-3.70671100

**pseudo Z 2b-PC**

Ru	0.08510600	-0.34010400	0.08596200
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C	1.78253300	0.38694800	0.28435700	C	-0.98474600	-3.80329700	-2.52829500
H	2.13879700	0.36482000	1.32982700	H	-0.45025900	-2.85999500	-2.69811400
C	2.77020400	1.05717000	-0.57625000	H	-1.43033600	-4.12869800	-3.47565900
Cl	-0.24095300	-0.38775400	-2.31884200	H	-0.24647100	-4.55791100	-2.22134500
Cl	-0.10107700	-0.40136600	2.51886500	C	-5.88837300	-3.83856300	-1.25869900
C	0.57481500	-2.35081000	0.23130100	H	-6.28252200	-2.89252900	-1.65801100
P	-1.16985200	1.79226600	0.15663900	H	-6.51196800	-4.12213400	-0.40216600
N	-0.33398000	-3.37547100	0.25137500	H	-6.01025500	-4.59888200	-2.04088000
N	1.78843300	-2.89601000	0.55571100	C	-2.38868500	-3.20390400	2.34997700
C	1.74434100	-4.37467900	0.71040600	H	-3.26654800	-2.86409400	2.91282600
H	2.24698400	-4.67381300	1.63682600	H	-1.57006300	-2.49505000	2.52133300
H	2.26131200	-4.85066800	-0.13584600	H	-2.09302700	-4.17755500	2.77127900
C	0.24015400	-4.66168400	0.72423800	C	2.72417800	1.12193200	-1.99116300
H	-0.05349900	-5.47456000	0.04952400	H	1.89304900	0.64768000	-2.50787100
H	-0.13410200	-4.88705300	1.73209800	C	3.72331900	1.78884100	-2.70611600
C	3.10103000	-2.31178500	0.45625300	H	3.67304100	1.82238700	-3.79397600
C	3.71146400	-2.21058500	-0.81722400	C	4.78277000	2.42420900	-2.03471600
C	5.04823900	-1.78877300	-0.87991200	H	5.55136700	2.95124200	-2.59896100
H	5.52386000	-1.70107200	-1.85781100	C	4.84410000	2.37680400	-0.63321400
C	5.78380500	-1.47570000	0.27699900	H	5.65952700	2.86695300	-0.10239900
C	5.14689600	-1.59314900	1.52280800	C	3.85717100	1.69177700	0.08366600
H	5.70276000	-1.35562700	2.43140800	H	3.91284400	1.64198100	1.17097000
C	3.81092400	-2.01819400	1.64174100	C	-0.98443500	2.89339000	-1.37853100
C	2.94503100	-2.54098400	-2.07829900	H	-0.84487900	2.13612100	-2.16794400
H	3.57797100	-2.39263400	-2.96072700	C	-2.19111800	3.78139100	-1.77561800
H	2.05155000	-1.90928900	-2.17838000	H	-3.11058300	3.18873800	-1.85798700
H	2.60350500	-3.58630700	-2.08151400	H	-2.36814700	4.54859100	-1.00581500
C	7.22050400	-1.00439200	0.17471500	C	-1.93018700	4.47463200	-3.13297600
H	7.71126300	-1.00639600	1.15554900	H	-1.85482400	3.70417900	-3.91708000
H	7.26650400	0.01918900	-0.22432300	H	-2.79107800	5.10928000	-3.39108100
H	7.80276700	-1.64464100	-0.50130800	C	-0.63503200	5.30673300	-3.11379100
C	3.16480000	-2.15819800	3.00324300	H	-0.45414300	5.75350200	-4.10245600
H	2.17432500	-1.68505600	3.02535800	H	-0.75074000	6.14148300	-2.40254800
H	3.79582300	-1.69955100	3.77400000	C	0.56283500	4.43946200	-2.68607700
H	3.03108200	-3.21617300	3.27649000	H	1.47590400	5.04922800	-2.62091900
C	-1.72861000	-3.37400600	-0.12148800	H	0.74798800	3.66630700	-3.44809200
C	-2.05717100	-3.62854800	-1.47689100	C	0.29988900	3.75695500	-1.32713000
C	-3.41206300	-3.76174700	-1.81970600	H	0.18451400	4.53837600	-0.55958300
H	-3.67039100	-3.95176700	-2.86253600	H	1.16498600	3.14714200	-1.04330200
C	-4.43416600	-3.69307800	-0.85704300	C	-0.91298700	2.82022800	1.71906800
C	-4.06841500	-3.49107100	0.48293800	H	-1.25891200	2.11328600	2.49064600
H	-4.84356900	-3.46832700	1.25078300	C	0.56437600	3.11747000	2.06560200
C	-2.72662000	-3.33763000	0.88034800	H	1.13955500	2.18571600	2.02429200

H	0.99907500	3.81512900	1.33621900
C	0.67145800	3.72869800	3.47887400
H	0.33494400	2.98174200	4.21511000
H	1.72481600	3.94975300	3.70671700
C	-0.18206400	5.00458000	3.61253900
H	-0.12442400	5.40008900	4.63724200
H	0.22270300	5.78497200	2.94665300
C	-1.64859800	4.72759100	3.23153700
H	-2.23967500	5.65442600	3.27834300
H	-2.08901200	4.03037000	3.96266600
C	-1.76165800	4.11122700	1.81881500
H	-1.40528800	4.84501500	1.07965600
H	-2.81815200	3.91308000	1.59040200
C	-3.03175600	1.46834100	0.20527300
H	-3.48978100	2.46373800	0.07988500
C	-3.49815000	0.58099000	-0.97479500
H	-3.08839500	0.93602100	-1.92927200
H	-3.10824400	-0.43890300	-0.83913600
C	-5.03948100	0.54358400	-1.03211200
H	-5.41867500	1.55819100	-1.24130700
H	-5.36430500	-0.09382400	-1.86766100
C	-5.63830000	0.03412000	0.29333100
H	-6.73723200	0.07829200	0.25870200
H	-5.36138200	-1.02252500	0.42264500
C	-5.11305900	0.83994500	1.49721200
H	-5.49228100	0.41111500	2.43663900
H	-5.49984600	1.87143400	1.44118800
C	-3.56863700	0.88998600	1.53523100
H	-3.15585900	-0.11579300	1.69584900
H	-3.25067100	1.49989600	2.39043100

**1a-Inact-C PPh<sub>3</sub>Cl<sub>2</sub>Ru=CHPh**

Ru	-0.86549800	-0.67211400	-0.83488000
Cl	-0.79200800	0.44474500	-2.86203600
Cl	-0.82214600	-2.81573300	0.03894900
P	1.00146300	0.07922700	0.09285100
C	-1.98625800	0.31471000	0.25946300
H	-1.60860900	1.11052800	0.91961900
C	-3.44174800	0.18643700	0.23731000
C	-4.23571500	1.21830900	0.80354100
C	-5.63188800	1.14790500	0.77153500
C	-6.26677500	0.04141600	0.18394800
C	-5.49641100	-0.99784900	-0.36646700

C	-4.10165000	-0.93005100	-0.33986000
H	-7.35386300	-0.01595200	0.16294500
H	-6.22543400	1.95110400	1.20565400
H	-3.74169300	2.07696600	1.25788700
H	-3.50934900	-1.75564700	-0.73468700
H	-5.98666200	-1.86405400	-0.80754600
C	1.06006500	1.89953600	0.42378600
C	1.65628100	2.41727200	1.59266200
C	0.49970200	2.78768800	-0.51858800
C	1.70050700	3.80280200	1.80733400
H	2.08127600	1.74434100	2.33432900
C	0.55314300	4.17128100	-0.29978600
H	0.02478000	2.39309200	-1.41602600
C	1.15146200	4.68171900	0.86231300
H	2.16063700	4.19127400	2.71465600
H	0.12007200	4.84722500	-1.03544100
H	1.18424700	5.75667300	1.03341400
C	1.48398800	-0.67514800	1.71056700
C	2.83591700	-0.90751300	2.03496500
C	0.48423700	-0.98525100	2.65312400
C	3.18010700	-1.43525400	3.28841900
H	3.61717700	-0.68355800	1.31069800
C	0.83281000	-1.50644000	3.90590600
H	-0.56318000	-0.84083500	2.39527900
C	2.18029400	-1.73277200	4.22582300
H	4.22704100	-1.61643400	3.52713700
H	0.05148900	-1.75013400	4.62380200
H	2.44857400	-2.14742200	5.19629600
C	2.43189900	-0.28029400	-1.01134400
C	2.66090800	-1.62644900	-1.37051900
C	3.26074800	0.73009100	-1.53357900
C	3.71470200	-1.95251300	-2.23314700
H	2.01549800	-2.41165700	-0.97631800
C	4.31251300	0.39610900	-2.40003800
H	3.08696400	1.77102000	-1.26862500
C	4.54136300	-0.94214300	-2.75006600
H	3.88518500	-2.99271900	-2.50556600
H	4.94907800	1.18322800	-2.80112100
H	5.35616000	-1.19723300	-3.42576700

**1b-Inact-C PCy<sub>3</sub>Cl<sub>2</sub>Ru=CHPh**

Ru	1.03435600	-1.02535200	-0.16289200
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C	-4.62494600	-2.22097300	-0.14814700
H	-4.53101700	-2.38764400	2.00485500
H	-4.36505600	-2.00172000	-2.28297700
C	3.00888600	-0.86327700	-0.03158300
C	3.61951400	-0.55146200	1.20618600
C	3.65659300	-0.58306700	-1.26105800
C	4.82822900	0.16787700	1.18395000
C	4.86498500	0.12917100	-1.22633300
C	5.45299500	0.53885200	-0.01635400
H	5.29243600	0.43497100	2.13439900
H	5.36024800	0.36523600	-2.16903800
C	-1.66141100	-1.81117500	-2.56096800
H	-0.95748900	-2.63618000	-2.73980300
H	-2.33235400	-1.75112700	-3.42533100
H	-1.07309800	-0.88518800	-2.51345100
C	-1.84785200	-2.27574200	2.50974400
H	-2.57729300	-2.35466400	3.32385200
H	-1.16690500	-3.13567900	2.58250800
H	-1.24567500	-1.37129100	2.66701100
C	3.07194300	-1.04175400	2.53029100
H	1.99243200	-1.21043000	2.49713400
H	3.56981900	-1.98292200	2.81269800
H	3.26577100	-0.31125300	3.32314100
C	3.10431400	-1.08686300	-2.57686600
H	2.07462300	-0.75010500	-2.73499900
H	3.71615300	-0.72310500	-3.41023800
H	3.11392800	-2.18691200	-2.60853800
C	-6.13568300	-2.32498800	-0.21847500
H	-6.44549300	-3.35944700	-0.42761700
H	-6.60081800	-2.02603800	0.72869000
H	-6.54264700	-1.69313300	-1.01785500
C	6.72606200	1.36052500	-0.01113300
H	7.31200000	1.18451700	0.89938800
H	7.35536800	1.12724500	-0.87902500
H	6.49298300	2.43461600	-0.05200200
C	-1.57507500	1.04441500	0.04354900
H	-2.24809100	0.18425400	0.11594900
C	-2.24828700	2.33880600	0.01440900
C	-1.56441600	3.55927100	-0.22994000
C	-3.64709000	2.39017000	0.25696100
C	-2.24930000	4.77585900	-0.21723100
H	-0.49834100	3.54419400	-0.45640000
C	-4.32876000	3.61078300	0.27164200

H	-4.18411100	1.45955300	0.43904500
C	-3.63199100	4.80742900	0.03626700
H	-1.71010200	5.70167500	-0.41046000
H	-5.40058500	3.63203300	0.46365600
H	-4.16268200	5.75823900	0.04464300

### PPh<sub>3</sub>

C	-0.93671300	-1.37935800	-0.41220000
C	1.66503800	-0.12126800	-0.41297000
C	-0.72563200	1.50219900	-0.41318000
C	-0.48883800	-2.08601000	0.72150700
C	-2.16060600	-1.75820200	-1.00595200
C	2.04839800	0.61288900	0.72743300
C	2.60850000	-0.98574700	-1.00938200
C	-0.42753800	2.75381800	-0.99486400
C	-1.57753700	1.46505200	0.70901400
C	-1.25121500	-3.13694300	1.25351000
H	0.45769700	-1.81688100	1.18714800
C	-2.92845600	-2.79820400	-0.46555200
H	-2.51023700	-1.23525800	-1.89631300
C	3.33851100	0.47722600	1.26225500
H	1.33963500	1.29335900	1.19662400
C	3.89185600	-1.13163500	-0.46626900
H	2.33429600	-1.54507000	-1.90402600
C	-0.94597400	3.93788600	-0.45429000
H	0.21252000	2.79778000	-1.87625300
C	-2.10816700	2.65025200	1.24105100
H	-1.82924900	0.50908500	1.16508900
C	-2.47339400	-3.49301200	0.66567300
H	-0.88927600	-3.67479900	2.12886800
H	-3.87238800	-3.07350000	-0.93388600
C	4.26147100	-0.39728200	0.67109100
H	3.61944400	1.05404300	2.14258000
H	4.60469700	-1.80724700	-0.93697200
C	-1.79126200	3.88869500	0.66506400
H	-0.70084800	4.89464200	-0.91329200
H	-2.76726300	2.60362200	2.10707100
H	-3.06291000	-4.30918100	1.08042900
H	5.26194400	-0.50108700	1.08819100
H	-2.20421700	4.80701500	1.07961500
P	0.00103400	0.00008900	-1.22710100

**PCy<sub>3</sub>**

P	-0.23506200	-0.06745100	-1.04691700
C	0.75263000	-1.50550100	-0.29247700
H	0.01572900	-2.32668200	-0.34717400
C	1.23555400	-1.42169100	1.17287300
H	0.41005500	-1.13817400	1.84147000
H	2.00277000	-0.63674500	1.25716900
C	1.85210300	-2.76280000	1.63068800
H	2.20397300	-2.67897300	2.66973300
H	1.07175000	-3.54153700	1.62057700
C	3.00850700	-3.18980100	0.70651800
H	3.41164700	-4.16225800	1.02487200
H	3.83026300	-2.46036600	0.79758500
C	2.55055900	-3.25555400	-0.76330000
H	3.39732400	-3.51529900	-1.41566100
H	1.80512600	-4.06032000	-0.87406500
C	1.92216500	-1.92229100	-1.22131200
H	1.56328100	-2.00555300	-2.25663000
H	2.69751200	-1.14074600	-1.21622200
C	-1.84091600	-0.12357400	-0.03396000
H	-1.61496300	-0.08554100	1.04594300
C	-2.61053100	-1.43635300	-0.32570300
H	-2.01319000	-2.30979200	-0.02961800
H	-2.77374600	-1.51792800	-1.41288700
C	-3.97112000	-1.48569800	0.40050700
H	-4.49230100	-2.42044800	0.14621800
H	-3.80069500	-1.50288800	1.48957100
C	-4.84445500	-0.26952700	0.04316800
H	-5.10094800	-0.30974600	-1.02807900
H	-5.79262600	-0.30111000	0.59943600
C	-4.09515000	1.04285500	0.33518300
H	-3.92950000	1.13223900	1.42148600
H	-4.70534900	1.90777000	0.03569900
C	-2.73439100	1.09111100	-0.39241000
H	-2.22265000	2.03271100	-0.14946000
H	-2.90469200	1.09565100	-1.48172600
C	0.55263700	1.56684900	-0.47452400
H	-0.05797700	2.30316400	-1.02859000
C	0.51730200	1.98610200	1.01534600
H	1.12845300	1.29799400	1.61574700
H	-0.50587100	1.92964600	1.41168800
C	1.06160100	3.42268600	1.19040700
H	0.39384700	4.12780800	0.66836400

H	1.04571500	3.70026700	2.25486800
C	2.48743000	3.56140400	0.62305400
H	2.83991400	4.59784600	0.72775700
H	3.17319900	2.93119000	1.21305500
C	2.54233900	3.12227700	-0.85250400
H	3.57417900	3.17740900	-1.22967000
H	1.94219500	3.81746200	-1.46194500
C	1.99211800	1.69252900	-1.03101900
H	2.01300900	1.40688900	-2.09275800
H	2.65020100	0.98967000	-0.49620400

**PBEh****1a-PC**

Ru	0.13997100	-0.08909800	0.04314400
Cl	0.15565900	0.18520900	-2.32693500
Cl	0.31804300	-1.17347900	2.16981700
P	-2.22723400	-0.53764800	0.02207900
P	2.50978900	-0.14291900	-0.04739300
C	0.10299300	1.59997000	0.75408800
H	0.71086100	1.73258700	1.66534900
C	-1.87566000	5.25319600	-0.20354300
C	-1.26678600	5.07445900	1.04000300
C	-0.62149000	3.87796300	1.32515500
C	-0.59442000	2.82575900	0.38586300
C	-1.20945700	3.02548900	-0.86399500
C	-1.83595300	4.23171900	-1.15362200
H	-2.37427000	6.19106800	-0.43363900
H	-1.28841200	5.87060100	1.77894900
H	-0.13146500	3.74009100	2.28679000
H	-1.16465100	2.23278000	-1.60352600
H	-2.30215800	4.37269700	-2.12467900
C	3.42666600	1.16267300	-0.95227200
C	4.82955800	1.14802200	-0.95802500
C	2.75138400	2.21078000	-1.58204800
C	5.54129500	2.15618900	-1.59979400
H	5.36595000	0.35074300	-0.44939500
C	3.46844900	3.22556500	-2.21647000
H	1.66702600	2.22302800	-1.58874800
C	4.86005800	3.19858800	-2.23036400
H	6.62758500	2.13299700	-1.60015400
H	2.93187100	4.03607300	-2.70161000
H	5.41618500	3.98922300	-2.72690000

C	3.42357600	-0.13368000	1.54770500
C	4.00143000	-1.27244700	2.11235100
C	3.52150000	1.08691300	2.22892700
C	4.66252900	-1.19282300	3.33737200
H	3.94553500	-2.22649400	1.59875300
C	4.17851300	1.16358200	3.45274700
H	3.10108400	1.98983700	1.79264300
C	4.75036300	0.02148100	4.01223900
H	5.10878500	-2.08731500	3.76314600
H	4.24833600	2.11809400	3.96719800
H	5.26447300	0.08023000	4.96753200
C	2.93402700	-1.72412800	-0.86917700
C	2.42280600	-2.91184800	-0.32363600
C	3.64915600	-1.77568400	-2.06972800
C	2.65746800	-4.13096300	-0.95404300
H	1.83445200	-2.87667600	0.59125900
C	3.87393400	-2.99819200	-2.69958100
H	4.01858500	-0.86174300	-2.52345200
C	3.38544400	-4.17747300	-2.14181400
H	2.26046100	-5.04448300	-0.51987000
H	4.42716400	-3.02516600	-3.63426900
H	3.56101900	-5.12850200	-2.63703800
C	-2.50118200	-2.27914300	-0.51151300
C	-1.72352500	-3.27116800	0.10263300
C	-3.45850100	-2.65518100	-1.45986300
C	-1.90018900	-4.61072500	-0.23254800
H	-0.99330500	-2.99193000	0.85912700
C	-3.62741000	-3.99795100	-1.79556900
H	-4.08000200	-1.90514800	-1.93849800
C	-2.84858700	-4.97833200	-1.18558400
H	-1.29383900	-5.36889400	0.25567000
H	-4.37379900	-4.27479100	-2.53518600
H	-2.98195900	-6.02387600	-1.44957800
C	-3.09344800	-0.47625100	1.64092000
C	-4.24223200	-1.24533300	1.86351400
C	-2.63858100	0.37765700	2.64878400
C	-4.92937500	-1.15174000	3.07090900
H	-4.59924400	-1.92350100	1.09314400
C	-3.33104500	0.47540400	3.85400800
H	-1.72945400	0.94993100	2.49856900
C	-4.47648100	-0.28788900	4.06751600
H	-5.81701600	-1.75691900	3.23352300
H	-2.96354400	1.13870700	4.63193200

H	-5.01061600	-0.21728500	5.01119000
C	-3.33346400	0.45397200	-1.05761700
C	-4.31454300	1.28990400	-0.51044700
C	-3.16929300	0.42272400	-2.45140700
C	-5.12120400	2.07010800	-1.33693800
H	-4.45250900	1.33642300	0.56517900
C	-3.98104700	1.20083900	-3.27268900
H	-2.39389500	-0.19511600	-2.89183700
C	-4.96003600	2.02577100	-2.71940900
H	-5.87734300	2.71256900	-0.89406800
H	-3.84266900	1.16218700	-4.34978800
H	-5.59265200	2.63072000	-3.36355600

### 1b-PC

Ru	-0.02827700	-0.00691800	0.08338000
Cl	-0.07382400	-0.27881800	-2.31548900
Cl	-0.01996200	0.82345200	2.35977100
P	2.34893100	0.45283000	0.03187800
P	-2.42746900	0.28319000	-0.00394300
C	-0.01184700	-1.70976700	0.76103900
H	-0.19849300	-1.74248900	1.84753700
C	3.25454300	0.15352900	1.63574900
H	2.72327800	0.84607400	2.30472200
C	4.74257500	0.52842100	1.62634000
H	4.89673300	1.53092200	1.21032600
H	5.29630000	-0.16873300	0.98294200
C	5.32383400	0.46502900	3.04158900
H	6.39239400	0.71270200	3.01487600
H	4.83882700	1.23209200	3.66268300
C	5.10789500	-0.90637500	3.67662300
H	5.49542300	-0.91472700	4.70273100
H	5.68487800	-1.65809000	3.11764300
C	3.62994400	-1.29065100	3.66022600
H	3.49153700	-2.29503200	4.07920400
H	3.06484300	-0.60077000	4.30296400
C	3.04876800	-1.23683800	2.24655100
H	1.97966300	-1.46145300	2.27920500
H	3.52689400	-2.00745500	1.63027000
C	2.61106200	2.28467200	-0.25498000
H	3.67888600	2.39300600	-0.49548500
C	2.32801900	3.17879200	0.95889000
H	2.93253600	2.87125300	1.81885300
H	1.28236000	3.06750000	1.27054300

C	2.63372200	4.64224400	0.63200800	C	-4.84051300	-0.44155400	-1.39531800
H	2.40573900	5.26748700	1.50384900	H	-5.33273900	-0.84094700	-0.49818800
H	3.71205400	4.75332100	0.44235800	H	-5.06375300	0.63139900	-1.42534500
C	1.85765900	5.12912800	-0.58878800	C	-3.24779600	0.07512600	1.66427300
H	0.78375500	5.13088200	-0.35294700	H	-2.47861500	0.50347700	2.32449200
H	2.12652300	6.16599100	-0.82523700	C	-3.40409500	-1.39766100	2.06446700
C	2.10648000	4.22623800	-1.79478000	H	-4.18886500	-1.86597500	1.45484300
H	3.15743800	4.31834100	-2.10744400	H	-2.47869000	-1.95086200	1.87035300
H	1.49918900	4.54859400	-2.64974600	C	-3.79077400	-1.51785500	3.53902100
C	1.80551300	2.76315900	-1.47087500	H	-2.97548700	-1.11570500	4.15661600
H	1.99027300	2.12927800	-2.34514300	H	-3.90249800	-2.57520300	3.80980500
H	0.73309200	2.65513600	-1.25502900	C	-5.07982000	-0.75431900	3.83336200
C	3.26510400	-0.34175400	-1.39492300	H	-5.32514600	-0.81239900	4.90085100
H	2.48635600	-0.35343800	-2.17234900	H	-5.91260600	-1.23029600	3.29435700
C	4.48352600	0.39417300	-1.97118200	C	-4.96437000	0.70369700	3.39575700
H	5.29026700	0.44140400	-1.22740300	H	-5.91197500	1.23057400	3.56399200
H	4.23272500	1.42683200	-2.23499000	H	-4.20935300	1.20770200	4.01577000
C	4.99603400	-0.31884100	-3.22666200	C	-4.55953800	0.83062300	1.92359700
H	4.22484400	-0.25787500	-4.00790700	H	-4.45847000	1.89279100	1.67799100
H	5.87735500	0.20721100	-3.61436000	H	-5.36528700	0.43368400	1.29195100
C	5.32363200	-1.78589600	-2.96087800	C	-2.83748800	2.04880600	-0.47429200
H	5.64515100	-2.27728400	-3.88731100	H	-3.92003700	2.14705500	-0.30466000
H	6.17166100	-1.84850700	-2.26275700	C	-2.57670700	2.38723500	-1.94783300
C	4.12342000	-2.51149400	-2.35833400	H	-3.12004100	1.70249700	-2.60707800
H	4.38038200	-3.55153300	-2.12232500	H	-1.51330600	2.25053600	-2.18140300
H	3.30826600	-2.54674100	-3.09501400	C	-3.00428000	3.82338400	-2.25812300
C	3.62706600	-1.80315500	-1.09772700	H	-2.78665300	4.05147700	-3.30871100
H	2.76719900	-2.33653300	-0.68108600	H	-4.09496000	3.90903000	-2.14029100
H	4.42230600	-1.83645600	-0.34081300	C	-2.31978300	4.83255100	-1.34076500
C	-3.33096000	-0.69906700	-1.30613800	H	-1.23961500	4.82799200	-1.54593500
H	-2.85476000	-0.32296300	-2.22351700	H	-2.67397900	5.84801600	-1.55666200
C	-3.04214800	-2.20392900	-1.28474000	C	-2.55365900	4.48713200	0.12785700
H	-3.46744600	-2.66651500	-0.38586600	H	-3.62165200	4.60758000	0.36399900
H	-1.96374000	-2.36816200	-1.25276500	H	-2.01170400	5.18485300	0.77824900
C	-3.63505600	-2.88008400	-2.52196000	C	-2.12606000	3.05339000	0.44208700
H	-3.12248300	-2.49712000	-3.41608700	H	-1.04019400	2.95907200	0.30701100
H	-3.43531200	-3.95799700	-2.48402400	H	-2.30451600	2.82225300	1.49780900
C	-5.13514400	-2.61969900	-2.64445800	C	0.60231900	-5.72823000	-0.56796400
H	-5.53145400	-3.07833000	-3.55873400	C	0.37099400	-5.43589500	0.77545300
H	-5.65644600	-3.09939300	-1.80255200	C	0.17362400	-4.11701200	1.17022300
C	-5.43503700	-1.12272800	-2.63056300	C	0.20672800	-3.06073100	0.23728700
H	-5.01235600	-0.65907000	-3.53378900	C	0.44398700	-3.37655900	-1.11374400
H	-6.51761500	-0.94744100	-2.66599600	C	0.63545100	-4.69512200	-1.50759200



H	0.75558100	-6.75698900	-0.88307200
H	0.34336600	-6.23337700	1.51285000
H	-0.00831900	-3.88811900	2.21817700
H	0.46315100	-2.57041200	-1.84136200
H	0.81301600	-4.92094500	-2.55567900

**pseudo E-2b-PC**

Ru	-0.01938300	-0.29975200	0.10529900
C	-0.26764600	-2.35457000	0.23157900
N	0.73775700	-3.25948300	0.26666800
N	-1.41018000	-3.02020900	0.51951700
C	0.30428900	-4.58220200	0.73176400
H	0.67589600	-4.75827700	1.74839700
H	0.70152800	-5.36612000	0.07978800
C	-1.21179700	-4.46497200	0.68130400
H	-1.69793900	-4.82105900	1.59364000
H	-1.65215900	-5.00027600	-0.17022100
Cl	0.43254000	-0.41630900	-2.25727500
Cl	0.07774200	-0.44294600	2.52559000
C	-2.75878500	-2.57306600	0.38589500
C	-3.52460300	-2.34137200	1.53894700
C	-3.33455900	-2.52797800	-0.89647800
C	-4.87287300	-2.00994900	1.37757100
C	-4.68555500	-2.20155800	-1.00338100
C	-5.47017800	-1.93092600	0.11963200
H	-5.47182800	-1.81615100	2.26554500
H	-5.13484500	-2.15079900	-1.99324300
C	2.11081300	-3.11565900	-0.10814500
C	3.09530600	-2.91502100	0.87326800
C	2.46251500	-3.38572900	-1.44507500
C	4.43509300	-2.90507800	0.47135600
C	3.81250100	-3.36286300	-1.79357900
C	4.81506300	-3.11688600	-0.85284900
H	5.20236400	-2.74510700	1.22670300
H	4.08776500	-3.56398700	-2.82710300
C	-2.51953700	-2.81765800	-2.12284300
H	-2.09028200	-3.82612700	-2.09555500
H	-3.13816200	-2.74533100	-3.02112800
H	-1.68215100	-2.11801200	-2.22376300
C	-2.92849700	-2.45677400	2.91216300
H	-3.61423700	-2.05484700	3.66321400
H	-2.73761800	-3.50473900	3.17689800

H	-1.97629300	-1.92098300	2.98253300
C	2.75440000	-2.77597500	2.32898800
H	1.86339600	-2.16322000	2.49097800
H	2.57469400	-3.76072100	2.77995200
H	3.58660700	-2.32271200	2.87519900
C	1.42570800	-3.73211600	-2.47281300
H	0.79305000	-2.86520100	-2.68816800
H	1.90218400	-4.05296600	-3.40296900
H	0.77418000	-4.54478800	-2.13102400
C	-6.91497700	-1.54529700	-0.03184000
H	-7.41940400	-2.17064600	-0.77557500
H	-7.45603100	-1.63796500	0.91422600
H	-7.00297600	-0.50495100	-0.36769400
C	6.26179300	-3.08866200	-1.26120100
H	6.92183400	-3.26565200	-0.40710300
H	6.47583000	-3.84656700	-2.02125500
H	6.53017800	-2.11462600	-1.68803000
C	-1.76352700	0.24168800	0.24824100
H	-2.14227400	0.22826600	1.28215100
C	-2.78005200	0.78594500	-0.65803500
C	-2.73547500	0.71735800	-2.06169000
C	-3.89627800	1.40394200	-0.05973200
C	-3.76197200	1.25395400	-2.82947200
H	-1.88711900	0.23270700	-2.53462100
C	-4.91368900	1.95900400	-0.82883900
H	-3.95521700	1.44402100	1.02550000
C	-4.84972400	1.88252700	-2.21959800
H	-3.71216100	1.18642300	-3.91312800
H	-5.75770200	2.44341700	-0.34488500
H	-5.64446900	2.30841500	-2.82665600
H	1.32986800	4.77452000	3.78416300
C	1.10791100	3.75006400	4.12068300
C	-0.35861400	3.66652600	4.53626500
C	1.43919200	2.76282600	2.99778600
H	1.76047400	3.55741900	4.98129500
C	-1.27602600	3.87996000	3.33465400
H	-0.55498800	2.67460400	4.96675000
H	-0.57594700	4.40225100	5.32060500
C	0.51986900	2.99446900	1.79245000
H	1.31689400	1.73660200	3.36014200
H	2.48903100	2.89063400	2.71076300
C	-0.95288000	2.89482100	2.20997900
H	-1.16077500	4.91102700	2.96720700

H	-2.32678500	3.77036700	3.63119200	C	1.75693800	0.33808400	0.30398700
P	0.86051100	2.00761600	0.21924300	H	2.09916600	0.31235600	1.35045700
H	0.69230000	4.03249400	1.47304200	C	2.77496500	0.97274700	-0.54013000
H	-1.14594100	1.87188300	2.54999700	Cl	-0.21805200	-0.39367000	-2.29839100
H	-1.61528000	3.08133100	1.35495500	Cl	-0.13723700	-0.41654900	2.50868800
C	2.72387800	1.95351600	0.09667000	C	0.51583200	-2.36177100	0.21803600
C	0.30213100	3.35251800	-0.98136800	P	-1.11537000	1.80116100	0.14950000
C	3.25138600	1.79871900	-1.33746000	N	-0.40664400	-3.35187700	0.22383700
C	3.29608500	0.81513900	0.95539300	N	1.70813800	-2.93371800	0.50315300
H	3.08235500	2.91584000	0.49653300	C	1.63563400	-4.39427500	0.63019300
C	0.00212400	2.91891500	-2.41864900	H	2.13283500	-4.72522700	1.54631700
C	1.18377900	4.61479500	-0.99673200	H	2.14145400	-4.86832100	-0.22097800
H	-0.66475800	3.63765400	-0.53452800	C	0.13561100	-4.64893900	0.64175700
C	4.78076000	1.84030500	-1.35570800	H	-0.17609200	-5.43445500	-0.05368400
H	2.89374900	0.84675000	-1.74993800	H	-0.23752500	-4.90535500	1.64034800
H	2.86034700	2.58182700	-1.99185600	C	3.01552600	-2.36855500	0.43385500
C	4.82410100	0.85151000	0.96160800	C	3.64098800	-2.25132700	-0.82039400
H	2.96660100	-0.14289900	0.52680300	C	4.96583100	-1.82027900	-0.85911700
H	2.90819400	0.83925800	1.97653300	H	5.45309100	-1.71287100	-1.82625500
C	-0.68629900	4.04579500	-3.19012600	C	5.67668400	-1.51564900	0.30400600
H	0.92922600	2.63620800	-2.93149000	C	5.02914300	-1.65608800	1.53120200
H	-0.61857800	2.02464800	-2.41839100	H	5.56947300	-1.42803700	2.44823500
C	0.49458400	5.74748500	-1.76239700	C	3.70342500	-2.08943300	1.62434500
H	2.13932100	4.39030400	-1.48650800	C	2.90026700	-2.56702200	-2.08667300
H	1.42990300	4.96007800	0.01327800	H	3.55016600	-2.43409300	-2.95531200
C	5.38645500	0.76697300	-0.45518000	H	2.02476000	-1.91910700	-2.20924700
H	5.12026200	2.83256100	-1.02196200	H	2.53626000	-3.60118400	-2.09818800
H	5.13891900	1.71902200	-2.38556700	C	7.09772200	-1.03244600	0.22487800
H	5.16253800	1.78307200	1.43986600	H	7.14026700	-0.02725200	-0.21104600
H	5.21076600	0.02823500	1.57483000	H	7.70673000	-1.68682100	-0.40791800
C	0.14351500	5.32703900	-3.18751100	H	7.56204000	-0.98994400	1.21416900
H	-1.66823500	4.24486300	-2.73563800	C	3.04436200	-2.25051800	2.96391500
H	-0.88145300	3.71969300	-4.21922100	H	2.06627500	-1.75818600	2.99194800
H	-0.42416300	6.03478900	-1.23029300	H	3.67188700	-1.82760500	3.75322800
H	1.14110400	6.63406400	-1.77131400	H	2.88440300	-3.30830900	3.20825000
H	5.14527900	-0.22173500	-0.86822800	C	-1.79228000	-3.30014800	-0.12297300
H	6.48060500	0.85054100	-0.44112700	C	-2.14930400	-3.51877600	-1.46705800
H	1.07238300	5.15668100	-3.75145900	C	-3.50539600	-3.58390200	-1.79004700
H	-0.39076600	6.13511000	-3.70246100	H	-3.78721600	-3.74242400	-2.82907900
				C	-4.50197300	-3.48547100	-0.81798600
				C	-4.11079200	-3.32969200	0.51206800
				H	-4.87092600	-3.28989100	1.29046300
				C	-2.76749400	-3.24394700	0.88797900

***pseudo Z-2b-PC***

Ru 0.06890200 -0.34287600 0.09635400

C	-1.11016500	-3.72761400	-2.52880200
H	-0.55208000	-2.80392100	-2.71248300
H	-1.57896100	-4.04085300	-3.46538600
H	-0.38942300	-4.50031600	-2.23730900
C	-5.95639400	-3.54422100	-1.19287600
H	-6.35935100	-2.53639000	-1.35291100
H	-6.55411400	-4.01142500	-0.40430800
H	-6.10798300	-4.10863200	-2.11758500
C	-2.40535000	-3.16690700	2.34362100
H	-3.24538900	-2.77915200	2.92692500
H	-1.54159700	-2.52123700	2.52280600
H	-2.17640900	-4.16558300	2.73831700
C	2.74178700	1.05286400	-1.94439100
H	1.89780100	0.62043300	-2.47146900
C	3.76640500	1.68181100	-2.64104400
H	3.72480200	1.73004600	-3.72612000
C	4.83914100	2.26053100	-1.95903600
H	5.63133100	2.76022100	-2.51071600
C	4.88700000	2.19766400	-0.56728500
H	5.71513800	2.64792100	-0.02624500
C	3.87172000	1.55154800	0.12985900
H	3.91667600	1.48967200	1.21450100
C	-0.88300700	2.87831500	-1.36922500
H	-0.74697200	2.11716500	-2.15240700
C	-2.05257200	3.78143800	-1.78932300
H	-2.98165600	3.21107700	-1.88261100
H	-2.22846000	4.55345100	-1.02754600
C	-1.75877700	4.45488900	-3.13367700
H	-1.69754900	3.68031600	-3.91153800
H	-2.59661800	5.10814100	-3.40819200
C	-0.45276200	5.24429200	-3.10818900
H	-0.24818600	5.67476100	-4.09622100
H	-0.55456200	6.09026200	-2.41224600
C	0.70663100	4.36080200	-2.65619300
H	1.63238500	4.94523800	-2.58668400
H	0.88596700	3.57654000	-3.40490400
C	0.40885800	3.70557600	-1.30729700
H	0.30126900	4.49622600	-0.55213800
H	1.25517800	3.08448600	-1.00153700
C	-0.85427600	2.81316100	1.69724300
H	-1.21209600	2.11186000	2.46501800
C	0.61150000	3.08514300	2.05532700
H	1.17151500	2.14756800	2.02006000

H	1.06742300	3.76978600	1.33071000
C	0.71657300	3.69232600	3.45511000
H	0.36746100	2.95255700	4.18929600
H	1.76822300	3.89678700	3.69190600
C	-0.11317900	4.96826000	3.58100700
H	-0.05579500	5.36530000	4.60199500
H	0.30709600	5.74121900	2.92030800
C	-1.56789800	4.71552700	3.19263900
H	-2.14484900	5.64786400	3.23667800
H	-2.02358400	4.02962800	3.92150600
C	-1.68080200	4.10256900	1.79408400
H	-1.31736100	4.83034100	1.05607800
H	-2.73601500	3.91887900	1.56131400
C	-2.96281200	1.51081700	0.17647900
H	-3.40502400	2.50820200	0.03707500
C	-3.42726800	0.62757100	-0.98980800
H	-3.00517000	0.96344700	-1.94279500
H	-3.05017400	-0.39416600	-0.84674800
C	-4.95438700	0.60467300	-1.06137500
H	-5.32087000	1.61649500	-1.29239800
H	-5.27664800	-0.03883800	-1.88961300
C	-5.57005200	0.12730300	0.25256800
H	-6.66502700	0.18581400	0.20617900
H	-5.31286700	-0.92962800	0.39782200
C	-5.04873300	0.92852900	1.44363400
H	-5.44293100	0.51580500	2.38070100
H	-5.42150800	1.96197000	1.37856300
C	-3.51856800	0.95881800	1.49473200
H	-3.12001200	-0.04814100	1.67153800
H	-3.20155400	1.56789000	2.34734600

**1a-Inact-C PPh<sub>3</sub>-Cl<sub>2</sub>Ru=CHPh**

Ru	-0.87239900	-0.63597700	-0.86069300
Cl	-0.77808700	0.56701100	-2.82203900
Cl	-0.81639300	-2.79196500	-0.05474000
P	0.99321800	0.07347600	0.09303700
C	-1.95472700	0.30859900	0.25929400
H	-1.57653100	1.09181300	0.93022600
C	-3.40694600	0.17898400	0.24419200
C	-4.19202200	1.22460200	0.76654600
C	-5.57972800	1.15763300	0.73227100
C	-6.21036800	0.03832800	0.18805700
C	-5.44623100	-1.01571600	-0.31585000

C	-4.05902600	-0.95034100	-0.28794800	Cl	0.97530900	-1.36099800	-2.47868300
H	-7.29519100	-0.01730000	0.16539100	P	-0.92223800	0.05282900	0.01088000
H	-6.17154700	1.97594000	1.13297700	C	2.14658200	0.44316800	-0.03171700
H	-3.69876600	2.09636800	1.19011800	H	1.80879900	1.48420400	-0.02962700
H	-3.46919500	-1.79184900	-0.64449400	C	-1.16013400	0.93067600	1.64180000
H	-5.93548200	-1.89570400	-0.72357000	H	-1.15734200	0.07576200	2.33440700
C	1.05423200	1.86631900	0.48141500	C	0.00031400	1.82671500	2.09437500
C	1.61905900	2.33358100	1.67494500	H	0.10716100	2.68813200	1.42149800
C	0.53300700	2.78594900	-0.43916300	H	0.93404700	1.25847900	2.05710300
C	1.67091800	3.70152500	1.93770100	C	-0.23067000	2.32944700	3.52091200
H	2.01589800	1.63278400	2.40298900	H	-0.20158900	1.47178500	4.20787200
C	0.59444600	4.15148400	-0.17304500	H	0.59432000	2.98987800	3.81362900
H	0.07765400	2.42933500	-1.35978600	C	-1.56883200	3.04870200	3.66568300
C	1.16174000	4.61215100	1.01453000	H	-1.72258500	3.36542700	4.70413300
H	2.10825900	4.05241800	2.86832200	H	-1.55906700	3.96523300	3.05719700
H	0.19003900	4.85514300	-0.89532100	C	-2.71847800	2.15508800	3.20844700
H	1.20163800	5.67801700	1.22216600	H	-2.79694700	1.28953100	3.88191900
C	1.46145300	-0.73155000	1.67162300	H	-3.67343400	2.69071300	3.27390100
C	2.80596100	-0.95052400	1.99419800	C	-2.50479600	1.65935700	1.77629000
C	0.46770100	-1.08179900	2.59151500	H	-2.52598300	2.52333200	1.09827900
C	3.15007200	-1.50467200	3.22569500	H	-3.33682200	1.00786900	1.48475700
H	3.58566600	-0.69368100	1.28243500	C	-1.30899200	1.17892600	-1.44090200
C	0.81561500	-1.63022300	3.82279300	H	-0.87131100	0.61044000	-2.27434000
H	-0.57876000	-0.94913800	2.33301700	C	-0.56155800	2.51782300	-1.36052300
C	2.15599800	-1.84222700	4.14208700	H	-0.94862500	3.10648900	-0.51764200
H	4.19595700	-1.67569500	3.46503800	H	0.50321400	2.35112400	-1.17508700
H	0.03599700	-1.90676000	4.52680700	C	-0.72444800	3.32816700	-2.64736300
H	2.42468000	-2.27893900	5.10005100	H	-0.24818000	2.78452000	-3.47515100
C	2.40760300	-0.25684200	-1.01581200	H	-0.19278200	4.28261100	-2.55057700
C	2.61664800	-1.58185900	-1.42399500	C	-2.19522100	3.56397700	-2.97336000
C	3.25117800	0.75428900	-1.48267900	H	-2.29608100	4.11219300	-3.91753000
C	3.66614900	-1.88662600	-2.28488100	H	-2.64482700	4.19650600	-2.19364500
H	1.95828600	-2.37174200	-1.06741600	C	-2.94782300	2.23920700	-3.04687800
C	4.29898300	0.44206200	-2.34779300	H	-4.01328900	2.41131200	-3.24221100
H	3.09141000	1.78400200	-1.17662300	H	-2.56471300	1.65210500	-3.89363600
C	4.50789600	-0.87533100	-2.74872300	C	-2.79382700	1.41745800	-1.76273900
H	3.82253800	-2.91482100	-2.59849700	H	-3.32182900	0.46743800	-1.89120800
H	4.95016600	1.23288100	-2.70954300	H	-3.28449400	1.94623500	-0.93548300
H	5.32304100	-1.11480500	-3.42594500	C	-2.32773100	-1.18503900	-0.01003100

**1b-Inact-C PCy<sub>3</sub>-Cl<sub>2</sub>Ru=CHPh**

Ru	1.04901200	-0.99291500	-0.19608300	H	-3.23364700	-0.56946000	-0.11588700
Cl	1.03868100	-1.90036800	1.93500100	C	-2.48916600	-2.01357200	1.27178600
				H	-2.61323700	-1.36366800	2.14474400
				H	-1.58226600	-2.60302700	1.45080400

C	-3.70367300	-2.94014200	1.16771200	H	-4.45248400	-2.33234400	2.01005700
H	-3.78098000	-3.53958600	2.08269700	H	-4.35413400	-1.96941200	-2.26113600
H	-4.61995800	-2.33309700	1.11426800	C	2.98322500	-0.84431500	-0.02041500
C	-3.63050200	-3.84497800	-0.05878700	C	3.59081200	-0.53955000	1.20921300
H	-2.77836400	-4.53137400	0.04703000	C	3.61922000	-0.54553400	-1.24114300
H	-4.52980100	-4.46900100	-0.12601200	C	4.78257600	0.19044400	1.19102900
C	-3.45477600	-3.02168600	-1.33173800	C	4.80924900	0.17850500	-1.20413100
H	-4.35599100	-2.41290300	-1.50023200	C	5.39290600	0.57972100	0.00037000
H	-3.35284600	-3.67740000	-2.20452200	H	5.24568900	0.45329800	2.14013400
C	-2.23452400	-2.10676800	-1.23506200	H	5.29544300	0.43297800	-2.14366700
H	-1.32835500	-2.72184500	-1.15723200	C	-1.66585900	-1.80136100	-2.57213800
H	-2.11590100	-1.53077600	-2.15923900	H	-0.94131600	-2.60484100	-2.74541500
C	6.39284600	0.02768000	-0.08810100	H	-2.33989200	-1.77113600	-3.43182300
C	5.79259300	1.23396600	-0.45084800	H	-1.10372400	-0.86063100	-2.54470100
C	4.40972700	1.36239400	-0.40623600	C	-1.77448700	-2.23555500	2.46056900
C	3.59702500	0.28247900	-0.01115600	H	-2.48244400	-2.34380200	3.28608500
C	4.21961800	-0.92329800	0.36682600	H	-1.06273300	-3.06692300	2.51861800
C	5.60304000	-1.04587500	0.32559700	H	-1.20361400	-1.31251400	2.61500100
H	7.47425400	-0.07218500	-0.11764100	C	3.05907000	-1.04562600	2.51998300
H	6.40484600	2.07476800	-0.76479900	H	1.99083700	-1.26035700	2.48427300
H	3.94155200	2.30218600	-0.68954600	H	3.59513400	-1.95939600	2.80922600
H	3.61340400	-1.74863900	0.73310400	H	3.21031500	-0.30702400	3.31080800
H	6.06930400	-1.97949600	0.62701500	C	3.08171600	-1.04988100	-2.54930200

**2b-Inact-C NHC-Cl<sub>2</sub>Ru=CHPh**

Ru	0.25236400	0.85526700	0.07666000	H	2.01419300	-0.84985300	-2.65452700
C	0.50310100	-1.05695300	-0.01085400	H	3.59541100	-0.56944300	-3.38567900
N	1.75892900	-1.58167800	-0.04959500	H	3.24213900	-2.13222400	-2.64103600
N	-0.36190800	-2.10145000	-0.01757200	C	-6.07639100	-2.26045500	-0.17628500
C	1.77764500	-3.03840200	0.05030100	H	-6.40244400	-3.29001300	-0.36743100
H	2.14304900	-3.34431500	1.03940600	H	-6.52377700	-1.94580700	0.77088800
H	2.43846800	-3.46932700	-0.70776200	H	-6.48874900	-1.63503000	-0.97379200
C	0.31055600	-3.39560000	-0.16508500	C	6.64474800	1.41134600	0.00802800
H	-0.07019300	-4.10963200	0.57149200	H	7.21318300	1.27172100	0.93205700
H	0.12103700	-3.80571200	-1.16543900	H	7.29523800	1.16326900	-0.83614200
Cl	0.75554700	1.39670800	-2.12523200	H	6.40017500	2.47754700	-0.06999300
Cl	0.59786900	1.14502800	2.35184000	C	-1.55871600	1.01157700	0.03021700
C	-1.78476700	-2.08709200	-0.06073700	H	-2.23439700	0.15801900	0.10627600
C	-2.49452600	-2.20864600	1.14268900	C	-2.22875000	2.30428900	0.00059400
C	-2.43853300	-2.00275500	-1.30014200	C	-1.56367400	3.50496300	-0.31764400
C	-3.88949800	-2.24831900	1.08251500	C	-3.59792600	2.36212800	0.32687300
C	-3.83357600	-2.04702200	-1.30857900	C	-2.24187700	4.71632300	-0.29028800
C	-4.57584400	-2.17607900	-0.13162600	H	-0.52015200	3.48045700	-0.62256300
				C	-4.27258400	3.57659700	0.35748000
				H	-4.12172000	1.43869900	0.56296900

C	-3.59503400	4.75709700	0.05098400
H	-1.71723700	5.63316400	-0.54325900
H	-5.32735100	3.60503000	0.61666400
H	-4.12189200	5.70714700	0.07033100

**PPH<sub>3</sub>**

C	0.64843900	1.52229500	-0.41805400
C	-1.64445600	-0.19829500	-0.41623400
C	0.99316900	-1.32382900	-0.41778500
C	0.07450900	2.12446900	0.70740800
C	1.77767800	2.11735100	-0.99772300
C	-1.87830300	-0.99693200	0.70885900
C	-2.72565300	0.47973900	-0.99681100
C	0.94896500	-2.59943500	-0.99755700
C	1.79990900	-1.12519400	0.70853200
C	0.62417700	3.28756400	1.24547300
H	-0.80731200	1.68433900	1.16477300
C	2.33480900	3.27070000	-0.45218400
H	2.22224500	1.67171800	-1.88501200
C	-3.16062800	-1.10500900	1.24612200
H	-1.05578100	-1.53911600	1.16705100
C	-4.00308400	0.38319000	-0.45193400
H	-2.56322900	1.08706900	-1.88469900
C	1.67315700	-3.65584700	-0.45167200
H	0.34221500	-2.76385700	-1.88543100
C	2.53615200	-2.17985700	1.24694200
H	1.85556700	-0.14144700	1.16627100
C	1.75661400	3.86080900	0.67103600
H	0.16551700	3.74469200	2.11828200
H	3.21348700	3.71546200	-0.91133300
C	-4.22426100	-0.41298000	0.67131900
H	-3.32640400	-1.73145900	2.11859300
H	-4.82839100	0.91995900	-0.91178800
C	2.47178800	-3.44729800	0.67208000
H	1.62311800	-4.63925400	-0.91114500
H	3.16022600	-2.00888300	2.12009900
H	2.18326800	4.76694300	1.09215200
H	-5.22237500	-0.49856300	1.09188200
H	3.04620400	-4.26777200	1.09316800
P	-0.00174900	-0.00056500	-1.22731800

**PCy<sub>3</sub>**

P	-0.23089200	-0.07198700	-1.03455000
C	0.76503000	-1.48638700	-0.30033500
H	0.04690800	-2.31872600	-0.37882600
C	1.22003700	-1.41780300	1.16055400
H	0.38187000	-1.16081100	1.81980400
H	1.96530900	-0.61852300	1.27036400
C	1.85395700	-2.73898400	1.60480000
H	2.18970600	-2.66358500	2.64671300
H	1.09223300	-3.53208600	1.57835900
C	3.01892900	-3.12896700	0.69732600
H	3.43777900	-4.09412000	1.00746100
H	3.82465800	-2.38845100	0.80920300
C	2.58642000	-3.18200200	-0.76668300
H	3.44374600	-3.41687400	-1.40969600
H	1.86288200	-3.99979100	-0.90006700
C	1.94214600	-1.86814800	-1.21181700
H	1.59827100	-1.94358200	-2.25008300
H	2.70099500	-1.07444400	-1.19282800
C	-1.81955600	-0.13622900	-0.03420700
H	-1.59561000	-0.06872000	1.04200100
C	-2.56434700	-1.45513900	-0.28681400
H	-1.96112500	-2.30943200	0.04055000
H	-2.71514300	-1.57642600	-1.36988200
C	-3.91870400	-1.49985400	0.42215900
H	-4.42607700	-2.44488300	0.19171500
H	-3.75814300	-1.48907500	1.51025100
C	-4.79644300	-0.31404900	0.03295700
H	-5.04667700	-0.38430100	-1.03565700
H	-5.74658000	-0.34378600	0.58014700
C	-4.07181300	1.00327400	0.29273600
H	-3.91729700	1.12439500	1.37507700
H	-4.68894800	1.85094100	-0.03014500
C	-2.71870300	1.04872600	-0.41891600
H	-2.22092600	2.00000700	-0.19796600
H	-2.88030600	1.02906800	-1.50709300
C	0.53052100	1.55432000	-0.47078000
H	-0.08093300	2.28154300	-1.03114500
C	0.47481200	1.97277900	1.00455100
H	1.08003200	1.29026800	1.61284300
H	-0.54917300	1.90659300	1.38992400

C	1.00133600	3.39996800	1.18621100
H	0.33225600	4.10014700	0.66443300
H	0.97358100	3.67614800	2.24777300
C	2.41728100	3.55365300	0.63412700
H	2.75850900	4.59038000	0.74303100
H	3.10475300	2.93434100	1.22902800
C	2.49028700	3.11828500	-0.82768500
H	3.52177700	3.18520500	-1.19531500
H	1.89318900	3.80717100	-1.44271900
C	1.95986500	1.69646000	-1.01077300
H	1.99478800	1.41007700	-2.06935500
H	2.62073800	1.00172900	-0.47413200

## PBE

### 1a-PC

Ru	0.15396300	-0.02643000	0.07471900
Cl	0.15276000	0.24283300	-2.30079500
Cl	0.33943300	-1.17241200	2.17099100
P	-2.20104000	-0.58316900	0.04741800
P	2.53758200	-0.03940600	-0.02621900
C	0.07064100	1.71435700	0.71049800
H	0.79896900	1.95904000	1.51300300
C	-2.27906200	5.19884900	-0.15636500
C	-1.58337600	5.08197000	1.06124000
C	-0.82226400	3.93840700	1.32109300
C	-0.76830300	2.86576300	0.38675600
C	-1.47245600	3.00415200	-0.83670200
C	-2.20831800	4.16412600	-1.10489900
H	-2.86537900	6.09889500	-0.36759200
H	-1.62544400	5.88968000	1.79885800
H	-0.25750400	3.85618900	2.25696000
H	-1.40171000	2.20393200	-1.57684000
H	-2.73563300	4.25761400	-2.05936400
C	3.42442400	1.40192800	-0.78175100
C	4.82847400	1.51232000	-0.67371900
C	2.70348600	2.41304900	-1.44706700
C	5.49784300	2.61079200	-1.23196000
H	5.40004300	0.74417200	-0.14339500
C	3.37796100	3.51431400	-1.99911500
H	1.61854100	2.32759900	-1.54742000
C	4.77325500	3.61561700	-1.89470700
H	6.58632800	2.68436500	-1.14173100

H	2.80534900	4.29362000	-2.51169200
H	5.29625900	4.47591400	-2.32453300
C	3.51593800	-0.29064100	1.52827000
C	4.50363500	-1.28661800	1.65547600
C	3.28779000	0.58640000	2.60888700
C	5.25021500	-1.39913700	2.84049800
H	4.69241500	-1.98105400	0.83188100
C	4.03571900	0.47564500	3.78793900
H	2.51538600	1.35727900	2.53450000
C	5.02020900	-0.51918500	3.90793600
H	6.01361200	-2.17931600	2.92451100
H	3.84177700	1.16137500	4.61860500
H	5.60112900	-0.60952900	4.83114200
C	2.97537600	-1.49902400	-1.06729700
C	2.54587700	-2.77175900	-0.62862700
C	3.62340300	-1.37708600	-2.31096200
C	2.78344200	-3.90591700	-1.41782000
H	2.02566400	-2.86976200	0.33118500
C	3.85383900	-2.51632200	-3.09851000
H	3.93863300	-0.39347300	-2.67007500
C	3.43784000	-3.78094300	-2.65464900
H	2.44845600	-4.88774300	-1.06846200
H	4.35502300	-2.41080100	-4.06587900
H	3.61581100	-4.66609200	-3.27339000
C	-2.39511900	-2.35564700	-0.49123200
C	-1.55349900	-3.32556400	0.09701900
C	-3.36023700	-2.77097000	-1.43175200
C	-1.67457400	-4.67769600	-0.25504200
H	-0.81591500	-3.02091800	0.84705100
C	-3.47338000	-4.12579500	-1.78401100
H	-4.03168900	-2.04148800	-1.89190700
C	-2.63038600	-5.08305800	-1.19993300
H	-1.01714900	-5.41624400	0.21513300
H	-4.22787900	-4.42968700	-2.51674500
H	-2.71987300	-6.13820300	-1.47718100
C	-3.06062600	-0.56645700	1.68959900
C	-4.13301100	-1.44124000	1.95962600
C	-2.66788100	0.36378200	2.67076600
C	-4.80557700	-1.37865000	3.18949100
H	-4.44143700	-2.17696900	1.21039400
C	-3.34676000	0.42964300	3.89693200
H	-1.81860600	1.02410100	2.47798400
C	-4.41564300	-0.44119600	4.15966500

H	-5.63336100	-2.06647900	3.38949200
H	-3.02863000	1.15441100	4.65289800
H	-4.93862600	-0.39531200	5.12022100
C	-3.40178600	0.32577800	-1.03416600
C	-4.46909300	1.06647000	-0.48395700
C	-3.22685700	0.31945500	-2.43796600
C	-5.34637300	1.77796500	-1.31740600
H	-4.61950700	1.09134000	0.59857800
C	-4.10826700	1.03071800	-3.26540500
H	-2.38919700	-0.22665200	-2.87897300
C	-5.17135800	1.76159300	-2.70942000
H	-6.16907900	2.34642600	-0.87196800
H	-3.95897000	1.01258900	-4.34976700
H	-5.85857100	2.31443600	-3.35796900

### 1b-PC

Ru	-0.02859100	-0.02455600	0.08375600
Cl	-0.07043400	-0.29297300	-2.32993300
Cl	-0.03203900	0.82109700	2.37512900
P	2.34953700	0.46777600	0.03018200
P	-2.43589700	0.27274600	-0.00671400
C	-0.00941200	-1.74029400	0.77560600
H	-0.22267600	-1.77419000	1.86743300
C	3.27055400	0.16250500	1.64951400
H	2.72906800	0.85539800	2.32379200
C	4.76580500	0.54974500	1.64237000
H	4.91549500	1.56270700	1.22913100
H	5.32790400	-0.14581200	0.99067700
C	5.35098600	0.48126000	3.06797400
H	6.42593000	0.73744100	3.04214200
H	4.85790000	1.24896400	3.69635200
C	5.14060800	-0.90270500	3.70238800
H	5.52952700	-0.91236000	4.73662200
H	5.72771600	-1.65425100	3.13766200
C	3.65519500	-1.29971800	3.68134000
H	3.52113400	-2.31471700	4.09740000
H	3.08076100	-0.61205900	4.33211700
C	3.07080300	-1.24078900	2.25747500
H	1.99530200	-1.47514000	2.28658300
H	3.55870700	-2.01008800	1.63270000
C	2.60055100	2.32437500	-0.24633500
H	3.67568100	2.43593600	-0.49168200
C	2.31810600	3.21498700	0.98255700

H	2.93106100	2.90143500	1.84472900
H	1.26648400	3.09586000	1.29925700
C	2.61758800	4.69259900	0.66248000
H	2.38792000	5.31499400	1.54610000
H	3.70282000	4.81116400	0.46914600
C	1.83103400	5.18802700	-0.56131100
H	0.74991600	5.18566200	-0.32010800
H	2.09783100	6.23479900	-0.79415100
C	2.07861800	4.28733900	-1.78235600
H	3.13522400	4.38729600	-2.10232900
H	1.46128100	4.61464700	-2.63878600
C	1.78552500	2.80984200	-1.46585600
H	1.97511800	2.17892700	-2.35117000
H	0.70691900	2.69040400	-1.24668600
C	3.28990400	-0.31278300	-1.41697400
H	2.50626100	-0.31383200	-2.20183600
C	4.51810800	0.43492100	-1.98467400
H	5.32950300	0.46931600	-1.23349100
H	4.26905700	1.47970500	-2.23592000
C	5.03662800	-0.26754400	-3.25718100
H	4.26075500	-0.19653300	-4.04440200
H	5.92459700	0.26798700	-3.63974800
C	5.36605400	-1.74794800	-3.00739600
H	5.69066700	-2.23192000	-3.94620400
H	6.22037800	-1.81899600	-2.30483500
C	4.15833700	-2.48663500	-2.40915200
H	4.41849500	-3.53623600	-2.18112100
H	3.33879800	-2.51695200	-3.15330800
C	3.65178700	-1.78758600	-1.13432000
H	2.78324000	-2.32945000	-0.72610100
H	4.44811900	-1.82970000	-0.36718700
C	-3.34822400	-0.72121100	-1.32616000
H	-2.86172500	-0.34148900	-2.24680800
C	-3.05729200	-2.23611500	-1.30031700
H	-3.49336700	-2.69893700	-0.39673300
H	-1.97151700	-2.40355900	-1.25873500
C	-3.64682700	-2.92054800	-2.54811300
H	-3.12433600	-2.53741700	-3.44650300
H	-3.44554600	-4.00629100	-2.50575400
C	-5.15621500	-2.65830700	-2.68321000
H	-5.54890000	-3.12074900	-3.60683800
H	-5.68742600	-3.14163600	-1.83887000
C	-5.45953600	-1.15145000	-2.67084900



H	-5.03021200	-0.68420700	-3.57903600
H	-6.55002400	-0.97515500	-2.71150400
C	-4.86711000	-0.46243600	-1.42516000
H	-5.36686200	-0.86328600	-0.52292000
H	-5.09310900	0.61795600	-1.45864400
C	-3.27355200	0.06193700	1.67662200
H	-2.50549300	0.51553400	2.33609000
C	-3.40252200	-1.41825100	2.09691800
H	-4.18101200	-1.91334100	1.48556700
H	-2.45846600	-1.95841200	1.91266900
C	-3.79506200	-1.52790500	3.58214600
H	-2.98199000	-1.10118900	4.20062000
H	-3.88850500	-2.59160700	3.86765800
C	-5.10654000	-0.77887600	3.86823500
H	-5.35345100	-0.82806300	4.94414300
H	-5.93626700	-1.28086700	3.33136000
C	-5.01880000	0.68509900	3.40772800
H	-5.98422700	1.19941600	3.56650900
H	-4.27045900	1.21679700	4.02718900
C	-4.60906700	0.80004000	1.92434400
H	-4.53080700	1.86771100	1.65887000
H	-5.41026500	0.37188000	1.29324100
C	-2.85851600	2.05612600	-0.48436400
H	-3.95364000	2.13447900	-0.33086300
C	-2.57744200	2.40233000	-1.96261800
H	-3.10305700	1.70504300	-2.63631000
H	-1.50068800	2.27955500	-2.17959100
C	-3.02081400	3.84344700	-2.28158600
H	-2.78567400	4.07686600	-3.33576100
H	-4.12259200	3.91522500	-2.18309000
C	-2.36281300	4.86751700	-1.34412400
H	-1.27111000	4.87867000	-1.53117700
H	-2.72967900	5.88588800	-1.56638600
C	-2.61827200	4.51424200	0.12982600
H	-3.69951600	4.62216600	0.34939300
H	-2.09285000	5.22315200	0.79532700
C	-2.17575900	3.07547600	0.45401800
H	-1.07848300	2.99253700	0.34261500
H	-2.37695100	2.84003500	1.51298300
C	0.67618600	-5.77437900	-0.56358800
C	0.44534500	-5.48138700	0.79082900
C	0.22435200	-4.15741600	1.18944100
C	0.23673800	-3.09048300	0.24909500

C	0.47355500	-3.40841900	-1.11362100
C	0.68502200	-4.73319900	-1.51023400
H	0.84666500	-6.80811900	-0.88107200
H	0.43525300	-6.28445800	1.53467600
H	0.04003800	-3.92848600	2.24538600
H	0.47305500	-2.59607600	-1.84711400
H	0.86007700	-4.95803400	-2.56741800

### ***Pseudo E- 2b-PC***

Ru	-0.03851600	-0.30753100	0.09958900
C	-0.28571800	-2.35154900	0.22530400
N	0.72753000	-3.27174400	0.26472300
N	-1.44279500	-3.02067600	0.52399700
C	0.28227900	-4.60098500	0.74451300
H	0.65919300	-4.77470800	1.76903400
H	0.67808700	-5.39539200	0.09028300
C	-1.24306200	-4.47812000	0.69634500
H	-1.73202000	-4.82772600	1.61978900
H	-1.69114600	-5.02272400	-0.15662800
Cl	0.42169600	-0.41548000	-2.27702800
Cl	0.06765200	-0.44342400	2.54075000
C	-2.80112700	-2.57336700	0.38697000
C	-3.57319300	-2.34068000	1.55031500
C	-3.38335500	-2.53374300	-0.90568200
C	-4.93268800	-2.01290500	1.38700000
C	-4.74605900	-2.21062600	-1.01046600
C	-5.53694800	-1.93772200	0.12062300
H	-5.53558900	-1.81696300	2.28184300
H	-5.20021700	-2.16553600	-2.00737600
C	2.11114600	-3.14054200	-0.11218700
C	3.10403800	-2.95027500	0.88019600
C	2.46559200	-3.42136700	-1.45837200
C	4.45436300	-2.96259500	0.47795200
C	3.82758900	-3.41912500	-1.80376700
C	4.83904100	-3.18489100	-0.85439600
H	5.22760300	-2.81111100	1.24080700
H	4.10459000	-3.62963000	-2.84360100
C	-2.56750300	-2.82685100	-2.14020000
H	-2.12756900	-3.83962100	-2.11058800
H	-3.19380400	-2.76203800	-3.04342900
H	-1.72644200	-2.11991200	-2.24911000
C	-2.97240600	-2.44808300	2.93061700

H	-3.66473400	-2.04617700	3.68727700	C	-0.93075700	2.92454500	2.22921900
H	-2.76993400	-3.50080800	3.20288300	H	-1.12666900	4.95434400	2.99738700
H	-2.01528600	-1.90292700	2.99922300	H	-2.30760100	3.81051300	3.66379500
C	2.75846500	-2.79837200	2.34162600	P	0.88636000	2.00503400	0.21971300
H	1.87047000	-2.16449300	2.49905200	H	0.73689400	4.05329100	1.48106000
H	2.55416300	-3.78331700	2.80199300	H	-1.13618700	1.89409400	2.56627700
H	3.60295300	-2.35700700	2.89477000	H	-1.59574100	3.12168900	1.36835000
C	1.42264800	-3.75201700	-2.49628200	C	2.76945400	1.93767300	0.09235500
H	0.80022000	-2.86755100	-2.71566200	C	0.33551700	3.37817400	-0.99028200
H	1.89988700	-4.08380400	-3.43158600	C	3.29545100	1.77408600	-1.35222200
H	0.74677300	-4.55651700	-2.15617500	C	3.34760700	0.79956900	0.96503600
C	-6.99100900	-1.55492700	-0.03046100	H	3.12989900	2.91028000	0.48838700
H	-7.49980100	-2.18657000	-0.77799000	C	0.02210100	2.94990800	-2.43662700
H	-7.53538400	-1.64643800	0.92312300	C	1.23472700	4.64040300	-1.00340000
H	-7.08604800	-0.50798800	-0.37157600	H	-0.63359400	3.67033800	-0.53260700
C	6.29522200	-3.17966100	-1.26027300	C	4.83568200	1.81108000	-1.37761200
H	6.95600200	-3.36458200	-0.39807900	H	2.93047600	0.81401300	-1.76118700
H	6.50345900	-3.94704500	-2.02418100	H	2.90050500	2.56116200	-2.01354200
H	6.58357200	-2.20413700	-1.69247800	C	4.88649000	0.83363600	0.96344200
C	-1.79223000	0.25611900	0.25133600	H	3.01049400	-0.16852400	0.54577700
H	-2.17374100	0.23981800	1.29491800	H	2.96259100	0.83606300	1.99537100
C	-2.80297400	0.81713500	-0.65917700	C	-0.66390600	4.09404300	-3.20651200
C	-2.76123800	0.75541600	-2.07479900	H	0.95157800	2.66013600	-2.95874300
C	-3.92416700	1.44840100	-0.05444300	H	-0.61072500	2.05403000	-2.43656500
C	-3.79036800	1.30843600	-2.84485800	C	0.54948000	5.79073700	-1.76854800
H	-1.91183900	0.25985700	-2.55364500	H	2.19374200	4.40580600	-1.50042500
C	-4.94302100	2.01973200	-0.82685300	H	1.48820000	4.98142000	0.01535500
H	-3.98245600	1.48411600	1.03908000	C	5.44804300	0.73739100	-0.46432700
C	-4.88060500	1.94938700	-2.22855000	H	5.18175400	2.81277100	-1.05170600
H	-3.74117700	1.24343400	-3.93687900	H	5.19088400	1.67986700	-2.41598300
H	-5.78848100	2.51330300	-0.33633400	H	5.23101500	1.77531700	1.43648800
H	-5.67756600	2.38819600	-2.83779500	H	5.27703900	0.00888000	1.58688900
H	1.38227300	4.79784700	3.81640600	C	0.18300900	5.37655000	-3.20288800
C	1.15179800	3.76684400	4.15440700	H	-1.64903100	4.30209400	-2.74320800
C	-0.32492800	3.69362500	4.57403900	H	-0.86889800	3.77088900	-4.24334100
C	1.47822600	2.77248800	3.02141900	H	-0.37004200	6.08806800	-1.22641900
H	1.80953600	3.56729700	5.01994100	H	1.21037800	6.67686400	-1.77711700
C	-1.24839800	3.91530600	3.36526700	H	5.20376400	-0.26188100	-0.87188600
H	-0.52969400	2.69570400	5.00768100	H	6.55038700	0.82094500	-0.45456300
H	-0.53774900	4.43585400	5.36485700	H	1.11371500	5.19882000	-3.77751400
C	0.55254300	3.01109100	1.80981000	H	-0.35042100	6.19790000	-3.71509400
H	1.34958900	1.73837100	3.38444400				
H	2.53604800	2.89564000	2.73089200				

**Pseudo Z- 2b-PC**

Ru	0.09376700	-0.34108900	0.08879200	C	-2.77707900	-3.28150800	0.88492300
C	1.79063900	0.36237000	0.30303200	C	-1.06618700	-3.74837900	-2.53945400
H	2.13965600	0.33001100	1.35752200	H	-0.53336100	-2.80123800	-2.73261400
C	2.79664200	1.02101300	-0.54581700	H	-1.51959700	-4.09201100	-3.48228600
Cl	-0.20214900	-0.37912000	-2.31902900	H	-0.31263700	-4.49411900	-2.23087600
Cl	-0.11564700	-0.41008400	2.51995500	C	-5.95941500	-3.66481300	-1.24082200
C	0.53924400	-2.34761100	0.22259600	H	-6.39448400	-2.65761200	-1.37784400
P	-1.14590400	1.79552000	0.15480900	H	-6.55548600	-4.17188100	-0.46424100
N	-0.39001300	-3.35452800	0.24045600	H	-6.09120500	-4.21140400	-2.18850200
N	1.74504600	-2.91924500	0.53203900	C	-2.43121500	-3.16989600	2.35028800
C	1.67111500	-4.39263500	0.66993500	H	-3.30841500	-2.84010200	2.92961400
H	2.18571800	-4.72049300	1.58754100	H	-1.60959100	-2.45781500	2.53188300
H	2.16792100	-4.87544000	-0.19338400	H	-2.12665400	-4.15063600	2.76164000
C	0.16263500	-4.64764400	0.70404300	C	2.76315800	1.10852100	-1.96115400
H	-0.15860400	-5.46239300	0.03401800	H	1.91863800	0.66228500	-2.49331700
H	-0.20336700	-4.87004100	1.72303200	C	3.78506800	1.75976100	-2.66062900
C	3.06324800	-2.35770000	0.44293000	H	3.74134900	1.81085000	-3.75368300
C	3.68410600	-2.25361600	-0.82789500	C	4.85800900	2.35655200	-1.97342100
C	5.02318300	-1.83359100	-0.87889400	H	5.64832800	2.87342200	-2.52770000
H	5.50724400	-1.73949500	-1.85821800	C	4.90735400	2.28731300	-0.57134500
C	5.75306700	-1.52586500	0.28417600	H	5.73534500	2.75050000	-0.02454400
C	5.10901900	-1.65376900	1.52651700	C	3.89614500	1.61908000	0.12962700
H	5.66343100	-1.42299000	2.44422800	H	3.94358000	1.55200000	1.22207000
C	3.77030000	-2.07603700	1.63585600	C	-0.94562700	2.88842800	-1.38397900
C	2.92895900	-2.57136100	-2.09437400	H	-0.81216600	2.11788200	-2.17051400
H	3.58176000	-2.45986600	-2.97383100	C	-2.13755500	3.78427200	-1.79425900
H	2.05743400	-1.90535100	-2.22233100	H	-3.06928900	3.20069600	-1.87544500
H	2.54023300	-3.60526100	-2.09457100	H	-2.31287300	4.56232600	-1.02675700
C	7.18478300	-1.05120800	0.19045300	C	-1.86508900	4.46412400	-3.15256600
H	7.23164000	-0.02894500	-0.22642200	H	-1.80387500	3.68382600	-3.93632800
H	7.78257700	-1.69903000	-0.47314700	H	-2.72005800	5.11205800	-3.41950500
H	7.67104300	-1.03386100	1.17893400	C	-0.55859100	5.27305600	-3.14246900
C	3.11804300	-2.22189800	2.98929600	H	-0.36883200	5.70963700	-4.13981100
H	2.13560700	-1.71944200	3.02174400	H	-0.66289600	6.12392700	-2.43983700
H	3.75977200	-1.79594700	3.77667900	C	0.62404600	4.39713000	-2.70088100
H	2.94724200	-3.28366200	3.24686100	H	1.55070900	4.99635500	-2.64073300
C	-1.78170700	-3.32465000	-0.12435100	H	0.80556200	3.61047600	-3.45858200
C	-2.12386100	-3.55938700	-1.48164000	C	0.34949800	3.73050300	-1.34012200
C	-3.48586600	-3.65489500	-1.81883000	H	0.24788700	4.52314800	-0.57431500
H	-3.75553400	-3.82618000	-2.86764500	H	1.21094600	3.10975600	-1.04805600
C	-4.50202000	-3.57452900	-0.85092200	C	-0.88475900	2.82722400	1.71400000
C	-4.12347200	-3.40250700	0.49204500	H	-1.23440000	2.11661500	2.48915600
H	-4.89784100	-3.37614900	1.26843700	C	0.58980900	3.11813900	2.06451300

H	1.16661800	2.18106400	2.02544300
H	1.03416200	3.81276300	1.32978800
C	0.69834600	3.73345000	3.47231300
H	0.36202300	2.98463700	4.21562300
H	1.75713500	3.95222000	3.70225000
C	-0.15219400	5.00762000	3.60532300
H	-0.09386100	5.40765900	4.63384200
H	0.25843900	5.79211300	2.93838700
C	-1.61579900	4.73714900	3.22083200
H	-2.20743200	5.66989900	3.26584300
H	-2.06472600	4.04248800	3.95799200
C	-1.73049300	4.11628200	1.81371600
H	-1.37464100	4.85194200	1.06773800
H	-2.79279000	3.92120300	1.58409700
C	-3.00851700	1.47489000	0.19822600
H	-3.46263800	2.47614600	0.05742500
C	-3.47277900	0.57981200	-0.97251300
H	-3.05696500	0.92319000	-1.93483400
H	-3.07935000	-0.44411400	-0.82910000
C	-5.01070300	0.53836600	-1.03627800
H	-5.39264900	1.55242000	-1.27168700
H	-5.33170600	-0.11673200	-1.86682400
C	-5.61957400	0.05689300	0.29155000
H	-6.72340500	0.10415300	0.24965300
H	-5.34920600	-1.00491400	0.44014900
C	-5.09734400	0.87353400	1.48540000
H	-5.48564300	0.45834100	2.43335200
H	-5.48386700	1.91051300	1.41667200
C	-3.55629400	0.92053500	1.53045100
H	-3.14424800	-0.08855200	1.71258000
H	-3.23921100	1.54205300	2.38454600

**1a-Inact-C PPh<sub>3</sub>Cl<sub>2</sub>Ru=CHPh**

Ru	-0.86535500	-0.91279100	-0.55538900
Cl	-0.82120000	-0.54910500	-2.83520300
Cl	-0.81361900	-2.64945500	0.96673000
P	0.99484100	0.09978600	0.05718100
C	-1.97969000	0.37717900	0.15478700
H	-1.59678800	1.34865700	0.52193100
C	-3.43448500	0.25232400	0.17119500
C	-4.22426300	1.41414000	0.38300200
C	-5.62205000	1.34391000	0.37533200
C	-6.26354100	0.11116700	0.16570100

C	-5.49722300	-1.05266800	-0.03024700
C	-4.10107900	-0.98641200	-0.02573300
H	-7.35648800	0.05467100	0.16345200
H	-6.21376000	2.25067400	0.53575400
H	-3.72295400	2.37467000	0.54549600
H	-3.51085100	-1.90247400	-0.14039500
H	-5.99380500	-2.01659300	-0.17785200
C	1.05235700	1.92776400	-0.24227700
C	1.60921200	2.81368200	0.70506000
C	0.53177000	2.44129400	-1.44997000
C	1.65583400	4.19153700	0.43901600
H	2.00387000	2.43273100	1.65084300
C	0.58952500	3.81807200	-1.71147600
H	0.07793000	1.76132900	-2.17896300
C	1.15043500	4.69585700	-0.76913700
H	2.08650400	4.87023400	1.18199300
H	0.18608600	4.20416300	-2.65275600
H	1.18709600	5.77065200	-0.97305700
C	1.48723800	-0.05942000	1.83541900
C	2.84494300	-0.13617200	2.20932700
C	0.49307400	-0.05028400	2.83461100
C	3.20097500	-0.19097600	3.56633400
H	3.62562000	-0.15695400	1.44283400
C	0.85375400	-0.10029300	4.18875600
H	-0.56299400	-0.02812300	2.54877900
C	2.20719200	-0.16941500	4.55742600
H	4.25721800	-0.25454600	3.84624100
H	0.07359500	-0.10061000	4.95611800
H	2.48606500	-0.21670400	5.61477800
C	2.42529700	-0.61373200	-0.86413400
C	2.64560300	-2.00494600	-0.75502400
C	3.26335100	0.16283800	-1.68723800
C	3.70017200	-2.60488300	-1.45604500
H	1.99086400	-2.61607200	-0.12369300
C	4.31658500	-0.44597100	-2.38861600
H	3.09628400	1.23984800	-1.78207800
C	4.53632400	-1.82718100	-2.27524700
H	3.86480500	-3.68302400	-1.36657200
H	4.96360800	0.16359400	-3.02711600
H	5.35516200	-2.29905200	-2.82721300

**1b-Inact-C PCy<sub>3</sub>Cl<sub>2</sub>Ru=CHPh**

Ru	1.02652700	-1.02680700	-0.11618400	H	-2.55588300	-1.32803400	2.22967200
Cl	1.04967900	-1.83011200	2.06148300	H	-1.60103200	-2.61094800	1.47962700
Cl	0.95134100	-1.61397500	-2.35815100	C	-3.75869400	-2.87530000	1.30019000
P	-0.91742400	0.06324100	0.01897300	H	-3.81382800	-3.47565200	2.22593400
C	2.17960900	0.40754100	-0.06441100	H	-4.66164600	-2.23225800	1.28873600
H	1.84486400	1.45873200	-0.08618400	C	-3.77479300	-3.78826500	0.06442700
C	-1.15903800	1.03626600	1.62268300	H	-2.93964600	-4.51225600	0.13473700
H	-1.16027000	0.20863700	2.36052100	H	-4.70586700	-4.38241900	0.03747900
C	0.01534400	1.95431300	2.02608400	C	-3.62236300	-2.96830300	-1.22625000
H	0.11405600	2.79042000	1.30762600	H	-4.51556900	-2.32520500	-1.36044400
H	0.95680500	1.38256700	2.00107400	H	-3.57959500	-3.63399800	-2.10676600
C	-0.20184700	2.52564300	3.44050700	C	-2.36017000	-2.08830200	-1.18602100
H	-0.16742100	1.69329900	4.17024700	H	-1.46399800	-2.73413300	-1.14616200
H	0.63372600	3.20104400	3.69751100	H	-2.26623800	-1.51415700	-2.12345500
C	-1.54605500	3.25939500	3.56738000	C	6.45540400	0.00719000	-0.11507500
H	-1.69349500	3.61816200	4.60173000	C	5.84925400	1.25442000	-0.34225200
H	-1.53613500	4.15965300	2.92093700	C	4.45499800	1.37174200	-0.31103400
C	-2.71140200	2.35005800	3.14755500	C	3.63136700	0.24189400	-0.05901400
H	-2.79441300	1.50735500	3.86170300	C	4.26450900	-1.00776600	0.18024600
H	-3.66973500	2.89829000	3.19380700	C	5.65713300	-1.12090200	0.14946300
C	-2.50609000	1.78591800	1.72735700	H	7.54566400	-0.08535000	-0.13619400
H	-2.51940200	2.62370600	1.00478200	H	6.46585000	2.13658900	-0.54158000
H	-3.35109500	1.12514600	1.46612500	H	3.98268400	2.34422500	-0.48886400
C	-1.29142900	1.13584200	-1.50608700	H	3.65457800	-1.88613300	0.41968500
H	-0.89728300	0.48624300	-2.31296200	H	6.12650600	-2.09087100	0.34014000
C	-0.47806000	2.44985000	-1.53712000	<b>2b-Inact-C NHCCl<sub>2</sub>Ru=CHPh</b>			
H	-0.83056300	3.12258200	-0.73167300	Ru	0.25204600	0.87031800	0.06608700
H	0.58939900	2.25038700	-1.35125600	C	0.51170300	-1.03385000	-0.00345600
C	-0.62801600	3.16990500	-2.89111400	N	1.78464000	-1.57453400	-0.06643900
H	-0.18427400	2.53760000	-3.68431400	N	-0.36159600	-2.09877000	0.03959800
H	-0.04854700	4.11063800	-2.87603100	C	1.79146400	-3.03418200	0.13110400
C	-2.10132400	3.44868300	-3.22285500	H	2.11266400	-3.28108500	1.16171400
H	-2.19105100	3.92270700	-4.21657400	H	2.48694900	-3.51858700	-0.57377000
H	-2.51125200	4.17237400	-2.49035500	C	0.32501200	-3.39809000	-0.12329900
C	-2.92437200	2.15292100	-3.17161100	H	-0.07140300	-4.13400100	0.59524700
H	-3.99234900	2.36272000	-3.36265600	H	0.16185700	-3.79019000	-1.14588200
H	-2.58691400	1.47348500	-3.97853500	Cl	0.77094700	1.46099100	-2.12105000
C	-2.78026400	1.42996600	-1.81602900	Cl	0.62671200	1.25730600	2.32422600
H	-3.37183200	0.50041100	-1.84690100	C	-1.79375200	-2.09924700	-0.01843300
H	-3.21735700	2.06304300	-1.02217100	C	-2.51790800	-2.20380200	1.19217800
C	-2.37024800	-1.15678400	0.04718600	C	-2.44569500	-2.06091500	-1.27473800
H	-3.26606100	-0.50610000	-0.02099300	C	-3.92130100	-2.27236800	1.12124600
C	-2.50088100	-1.98461200	1.34460500				

C	-3.85017100	-2.13349700	-1.29041200
C	-4.60563200	-2.24640900	-0.10794600
H	-4.49382800	-2.34288600	2.05367300
H	-4.36814100	-2.09255400	-2.25603200
C	3.02439900	-0.84374000	-0.03695100
C	3.63661400	-0.52447300	1.20064900
C	3.67936600	-0.57892600	-1.26863100
C	4.85060500	0.18779800	1.17431300
C	4.89505400	0.12352400	-1.23611100
C	5.48315800	0.54238300	-0.02815300
H	5.31698300	0.46127800	2.12825500
H	5.39924400	0.34502000	-2.18406700
C	-1.66624300	-1.88492300	-2.55633800
H	-0.97108600	-2.72329400	-2.73857000
H	-2.34668600	-1.82503500	-3.41957300
H	-1.05920300	-0.96330100	-2.53140500
C	-1.80440700	-2.19332400	2.52301400
H	-2.52484700	-2.25569700	3.35308000
H	-1.10431500	-3.04202600	2.61978200
H	-1.20924800	-1.27207100	2.64823000
C	3.08585300	-0.99769100	2.52539300
H	1.99847600	-1.15076800	2.50151700
H	3.57079200	-1.94801900	2.81875400
H	3.29161500	-0.26327400	3.31914900
C	3.11679400	-1.06669700	-2.58131300
H	2.17980100	-0.54271500	-2.83113200
H	3.83600000	-0.89211800	-3.39671300
H	2.89429500	-2.14777900	-2.55077700
C	-6.11190800	-2.36562900	-0.16014900
H	-6.41963300	-3.42039300	-0.27936500
H	-6.57997700	-1.99128400	0.76454900
H	-6.53342000	-1.80556300	-1.01071700
C	6.76032500	1.35012600	-0.02799900
H	7.32787200	1.21118400	0.90628600
H	7.41281300	1.07561000	-0.87302200
H	6.54095500	2.42912000	-0.12218300
C	-1.58215600	1.03014000	0.01248500
H	-2.24652600	0.15368000	0.02174200
C	-2.27615000	2.31266300	-0.00167600
C	-1.60561700	3.56265300	-0.09036000
C	-3.69520200	2.31759400	0.08135900
C	-2.32483800	4.76061200	-0.08929300
H	-0.51373000	3.59023400	-0.17507900

C	-4.41202800	3.51928600	0.08317500
H	-4.22287200	1.35962800	0.14773100
C	-3.72933000	4.74477900	-0.00149500
H	-1.79181300	5.71362700	-0.16090300
H	-5.50460300	3.50292900	0.14898700
H	-4.28857400	5.68562900	-0.00238700

### PPh<sub>3</sub>

C	-1.15798800	-1.20096700	-0.41544900
C	1.61910900	-0.40355700	-0.41531100
C	-0.45940000	1.60318800	-0.41430200
C	-0.82980100	-1.98611000	0.70901000
C	-2.43711300	-1.34942700	-0.99615700
C	2.13103100	0.27089500	0.71205300
C	2.39047200	-1.43348200	-0.99780900
C	0.05060100	2.78546100	-0.99521900
C	-1.30392200	1.71087200	0.70977800
C	-1.76247700	-2.88947600	1.24427000
H	0.15961800	-1.89327200	1.16769100
C	-3.37299000	-2.24051700	-0.45191500
H	-2.69900400	-0.76115400	-1.88300000
C	3.37983600	-0.08302900	1.24816800
H	1.55196100	1.07803700	1.17131100
C	3.63041400	-1.79664900	-0.45274600
H	2.01445400	-1.95265500	-1.88675300
C	-0.25484600	4.04134500	-0.45159500
H	0.69123600	2.71849400	-1.88194900
C	-1.62154400	2.97013500	1.24445900
H	-1.71720400	0.80705000	1.16825200
C	-3.03646700	-3.01634300	0.66960800
H	-1.49095000	-3.49367500	2.11614500
H	-4.36163700	-2.33826000	-0.91182500
C	4.13054800	-1.11897500	0.67126800
H	3.76460500	0.45254800	2.12228200
H	4.21223500	-2.60102600	-0.91419200
C	-1.09553700	4.13721800	0.66952500
H	0.15375400	4.94669100	-0.91189900
H	-2.28092500	3.03682000	2.11608100
H	-3.76159400	-3.72097500	1.08876500
H	5.10358100	-1.39306200	1.09092400
H	-1.34469000	5.11743800	1.08799700

P	0.00033400	-0.00043300	-1.23104300
<b>PCy<sub>3</sub></b>			
P	-0.23295000	-0.06929800	-1.04538500
C	0.76007200	-1.50489500	-0.29514900
H	0.02286600	-2.33281600	-0.36207400
C	1.22992500	-1.43246700	1.17163300
H	0.39399400	-1.15982700	1.84097200
H	1.99010900	-0.63452100	1.27094800
C	1.85833700	-2.76666700	1.62289200
H	2.20561900	-2.68734800	2.66941800
H	1.08153200	-3.55695700	1.60817600
C	3.01863900	-3.17988100	0.70224700
H	3.43083100	-4.15553900	1.01744800
H	3.84101900	-2.44397100	0.80478900
C	2.57239100	-3.23598400	-0.76845000
H	3.42860800	-3.48508700	-1.42153300
H	1.83413400	-4.05319100	-0.89296700
C	1.93258400	-1.90964500	-1.21994000
H	1.57748700	-1.98800300	-2.26285600
H	2.70494300	-1.11707100	-1.21168800
C	-1.83947700	-0.12898000	-0.03289600
H	-1.60926900	-0.08216600	1.05179200
C	-2.60129600	-1.44543000	-0.30941800
H	-1.99995400	-2.31757700	0.00186900
H	-2.75563900	-1.54593400	-1.40245400
C	-3.96497900	-1.49289700	0.40452000
H	-4.48396800	-2.43628400	0.15480700
H	-3.80217000	-1.50470000	1.50064200
C	-4.83882800	-0.28408000	0.03704500
H	-5.09449700	-0.33372700	-1.03994600
H	-5.79511400	-0.31520300	0.58988200
C	-4.09742100	1.03133000	0.31920300
H	-3.94036400	1.13409900	1.41147700
H	-4.71177300	1.89626800	0.00902900
C	-2.73398200	1.07904700	-0.39636800
H	-2.22441200	2.02858500	-0.15557700
H	-2.89735700	1.08213100	-1.49282000
C	0.54723900	1.56771400	-0.46980400
H	-0.07525600	2.30235400	-1.02485200
C	0.51037800	1.98502100	1.01716400
H	1.12502500	1.29289700	1.61998900
H	-0.51640300	1.92092700	1.41827900

C	1.04931100	3.41932500	1.19891800
H	0.37181800	4.12927200	0.68372500
H	1.03463700	3.69396400	2.26961500
C	2.46854100	3.57055700	0.62629400
H	2.81787800	4.61324000	0.73517700
H	3.16558700	2.94238600	1.21606400
C	2.52417500	3.13560000	-0.84739400
H	3.55945100	3.19842800	-1.22932000
H	1.91989300	3.83523600	-1.45815000
C	1.97918600	1.70799200	-1.03249400
H	1.99779300	1.42531900	-2.10090700
H	2.64844700	1.00031500	-0.50619300

### BP86

#### 1a-PC

Ru	0.14976000	-0.03908800	0.06643400
Cl	0.15039300	0.26268800	-2.30820800
Cl	0.32513500	-1.21704800	2.14947500
P	-2.21754200	-0.57522600	0.04001300
P	2.54329100	-0.06011800	-0.03119600
C	0.08248000	1.70078800	0.71712400
H	0.81391300	1.92984400	1.52243400
C	-2.19698400	5.24361600	-0.12716400
C	-1.49062400	5.10972000	1.08442200
C	-0.75511900	3.94604800	1.33680800
C	-0.73715200	2.87043400	0.40130000
C	-1.45237900	3.02607100	-0.81597400
C	-2.16264700	4.20560500	-1.07667300
H	-2.76294100	6.15865600	-0.33320200
H	-1.50401700	5.91916100	1.82229300
H	-0.18175500	3.85041700	2.26688800
H	-1.40923700	2.22469700	-1.55799100
H	-2.69742700	4.31278700	-2.02610600
C	3.43537000	1.39981900	-0.75372300
C	4.83657500	1.52597200	-0.60889800
C	2.71997300	2.40836000	-1.43267600
C	5.50846700	2.63694000	-1.14328100
H	5.40339000	0.76014800	-0.06920000
C	3.39668900	3.52177400	-1.96150000
H	1.63840600	2.31090400	-1.56203300
C	4.78917000	3.63876600	-1.81971000
H	6.59406000	2.72212900	-1.02411300

H	2.82832900	4.29801700	-2.48473800
H	5.31356400	4.50824300	-2.23085300
C	3.51370700	-0.34009700	1.52806600
C	4.50528200	-1.33637400	1.64202600
C	3.27495400	0.51366100	2.62721600
C	5.24412200	-1.47271600	2.83150500
H	4.70351300	-2.01229400	0.80469200
C	4.01519600	0.37974700	3.81076300
H	2.50046500	1.28429500	2.56364500
C	5.00288200	-0.61589200	3.91728000
H	6.00989200	-2.25272600	2.90427800
H	3.81257500	1.04742400	4.65492000
H	5.57723600	-0.72454000	4.84349700
C	3.00143200	-1.49853700	-1.09863000
C	2.57432600	-2.78489800	-0.69341600
C	3.67511400	-1.34759400	-2.32730300
C	2.84139400	-3.90321600	-1.49881600
H	2.03415700	-2.90654500	0.25313500
C	3.93439000	-2.47064500	-3.13210200
H	3.98917100	-0.35422100	-2.66123700
C	3.52225900	-3.74894700	-2.71987900
H	2.50960700	-4.89531200	-1.17453700
H	4.45588600	-2.34173900	-4.08664000
H	3.72357300	-4.62156500	-3.35045900
C	-2.44330500	-2.35236100	-0.48619100
C	-1.64295400	-3.33872300	0.13575800
C	-3.39740300	-2.75464600	-1.44603300
C	-1.79572700	-4.69360000	-0.19997300
H	-0.91228600	-3.04341000	0.89716800
C	-3.54125100	-4.11227300	-1.78300200
H	-4.03748500	-2.01341800	-1.93244800
C	-2.74100000	-5.08599700	-1.16334600
H	-1.17153000	-5.44412200	0.29723600
H	-4.28650700	-4.40487900	-2.53073800
H	-2.85506500	-6.14297100	-1.42724900
C	-3.07988300	-0.54000400	1.68484000
C	-4.17518500	-1.39038700	1.95121700
C	-2.66439900	0.37548400	2.67270100
C	-4.84732600	-1.31786800	3.18259200
H	-4.50160100	-2.11469700	1.19767700
C	-3.34227900	0.45140800	3.90092900
H	-1.79882100	1.01638500	2.48396800
C	-4.43383400	-0.39478200	4.15932600

H	-5.69275300	-1.98632200	3.37850300
H	-3.00593200	1.16429300	4.66130000
H	-4.95603000	-0.34107900	5.12074700
C	-3.40933900	0.34236200	-1.05053500
C	-4.48290300	1.08270000	-0.50778100
C	-3.22481100	0.33655000	-2.45489300
C	-5.35822400	1.79151000	-1.34856000
H	-4.64028000	1.10864200	0.57421100
C	-4.10421800	1.04481900	-3.29000200
H	-2.38148000	-0.20650500	-2.89026300
C	-5.17469700	1.77337600	-2.74112600
H	-6.18563000	2.35887100	-0.90867500
H	-3.94733500	1.02630100	-4.37400600
H	-5.86011200	2.32346600	-3.39513700

### 1b-PC

Ru	-0.02662700	-0.02698400	0.08318300
Cl	-0.06602400	-0.29360300	-2.33420200
Cl	-0.03025400	0.82414600	2.37698600
P	2.35757900	0.46104000	0.03020900
P	-2.43880300	0.28059300	-0.00569100
C	-0.00887200	-1.74508200	0.77858800
H	-0.21047600	-1.77725500	1.87330700
C	3.28063800	0.15133600	1.65327900
H	2.74200900	0.84567300	2.32943600
C	4.78045400	0.53380000	1.64435200
H	4.93295200	1.54850100	1.23442300
H	5.33827200	-0.16217000	0.98793500
C	5.37174000	0.45828500	3.07075600
H	6.44840500	0.71089700	3.04143500
H	4.88342200	1.22612600	3.70403400
C	5.15843600	-0.93005900	3.70243500
H	5.55028200	-0.94423500	4.73652400
H	5.74196100	-1.68239900	3.13339100
C	3.66834700	-1.32239800	3.68432700
H	3.53204700	-2.33946600	4.09690300
H	3.09818100	-0.63485300	4.34019200
C	3.07852500	-1.25586700	2.25927300
H	2.00166600	-1.48785600	2.29058100
H	3.56315400	-2.02436600	1.62945100
C	2.62008500	2.32005800	-0.24473300
H	3.69843100	2.42469600	-0.48200900
C	2.33313200	3.21434600	0.98433900



H	2.93318800	2.89327400	1.85376000	H	-5.03298900	-0.64212900	-3.60316200
H	1.27596700	3.10579100	1.28890500	H	-6.56076000	-0.91915200	-2.74195500
C	2.65277900	4.69213500	0.66786600	C	-4.87589100	-0.42666000	-1.44455100
H	2.41817400	5.31727000	1.54940700	H	-5.38395700	-0.82535900	-0.54501000
H	3.74247400	4.79911800	0.48854000	H	-5.09096400	0.65678700	-1.47621800
C	1.88581000	5.19782100	-0.56840400	C	-3.28060600	0.05966400	1.67940500
H	0.80111200	5.20996800	-0.34040200	H	-2.51751500	0.51964500	2.34149500
H	2.16981500	6.24157700	-0.79880800	C	-3.40044700	-1.42448000	2.09970700
C	2.13485300	4.29101900	-1.78863100	H	-4.17134600	-1.92606900	1.48250400
H	3.19695900	4.37553200	-2.09754800	H	-2.44982800	-1.95659100	1.92134300
H	1.53078800	4.62639500	-2.65227600	C	-3.80236800	-1.53868300	3.58570200
C	1.81738000	2.81496700	-1.47238200	H	-2.99579200	-1.10649000	4.21012500
H	2.00455000	2.18077900	-2.35670100	H	-3.88984800	-2.60430400	3.86947500
H	0.73513300	2.71028700	-1.25868000	C	-5.12399300	-0.79848900	3.86573300
C	3.30041700	-0.32153500	-1.42049000	H	-5.37606100	-0.85026400	4.94129200
H	2.51980800	-0.31379000	-2.20929200	H	-5.94776300	-1.30685800	3.32394300
C	4.53912300	0.42345700	-1.97805700	C	-5.04492000	0.66955800	3.40545400
H	5.34604500	0.44865000	-1.22060800	H	-6.01635500	1.17636400	3.55822400
H	4.29752300	1.47189300	-2.22441500	H	-4.30418000	1.20778200	4.02981400
C	5.06480300	-0.27580600	-3.25334400	C	-4.62668600	0.78703900	1.92120500
H	4.29443000	-0.19829400	-4.04644000	H	-4.55760500	1.85546800	1.65322600
H	5.95826200	0.25894000	-3.62685800	H	-5.42053400	0.34894600	1.28620400
C	5.38803000	-1.76138900	-3.00661600	C	-2.86168500	2.07134200	-0.47101600
H	5.71756900	-2.24342800	-3.94582200	H	-3.96030400	2.14202300	-0.33395100
H	6.23776600	-1.83846000	-2.29778600	C	-2.55755700	2.43149800	-1.94464700
C	4.17024100	-2.49919900	-2.41939800	H	-3.06404000	1.73352800	-2.63335400
H	4.42535300	-3.55128200	-2.19330600	H	-1.47493300	2.31973800	-2.14210600
H	3.35657600	-2.52331400	-3.17113000	C	-3.00874700	3.87400900	-2.26268100
C	3.65371000	-1.80265900	-1.14297300	H	-2.75527900	4.11753300	-3.31126400
H	2.77765300	-2.34316200	-0.74640000	H	-4.11367200	3.93481100	-2.18482800
H	4.44280600	-1.85274300	-0.36757600	C	-2.37761700	4.89955400	-1.30311500
C	-3.35689500	-0.70052600	-1.33813900	H	-1.28193000	4.92377500	-1.46920000
H	-2.86142400	-0.32118000	-2.25496400	H	-2.75167300	5.91654000	-1.52439400
C	-3.08224800	-2.22173400	-1.31557400	C	-2.65618700	4.53086000	0.16608000
H	-3.52889600	-2.68148300	-0.41443400	H	-3.74329000	4.62382400	0.36704100
H	-1.99785300	-2.40241300	-1.26881100	H	-2.15096000	5.24108000	0.84686500
C	-3.67438900	-2.89885400	-2.57041200	C	-2.20053800	3.09157300	0.48666600
H	-3.14371300	-2.51893700	-3.46624000	H	-1.10023900	3.02116800	0.38951500
H	-3.48469200	-3.98750000	-2.52918900	H	-2.41531500	2.84628600	1.54141600
C	-5.18346600	-2.62068700	-2.71224700	C	0.61813300	-5.79038900	-0.57233300
H	-5.57641800	-3.07684600	-3.64001500	C	0.40035600	-5.49659000	0.78582400
H	-5.72425800	-3.10121400	-1.87127900	C	0.20019500	-4.16891000	1.18881900
C	-5.47147500	-1.10750500	-2.69744700	C	0.22008800	-3.09912900	0.24893500

C	0.44471500	-3.41783700	-1.11746500	H	2.38957847	-3.42822628	3.41815120
C	0.63554800	-4.74628200	-1.51818000	H	3.68914367	-2.35055455	2.86450647
H	0.77166800	-6.82650000	-0.89327400	H	1.99748973	-1.80377663	2.76363847
H	0.38406300	-6.30147600	1.52869800	C	2.29202523	3.02711178	2.17096211
H	0.02580700	-3.93945700	2.24690600	H	1.75853145	2.07611905	2.33878666
H	0.44952200	-2.60338400	-1.84972400	H	3.32177801	2.90694947	2.55969622
H	0.80004600	-4.97186300	-2.57750800	H	1.81045876	3.80963461	2.78025115

**Pseudo E- 2b-PC**

Ru	0.00000000	0.00000000	0.00000000	H	3.07020589	1.93444818	-2.76700118
C	2.06652971	0.00000000	0.00000000	H	2.24961170	1.21694838	-2.94492922
N	2.86203986	1.11746009	0.00000000	H	3.27744374	2.47028795	-3.70755242
N	2.88861025	-1.07330467	0.23381511	H	3.97083722	1.35048939	-2.50337816
C	4.26905160	0.82885869	0.38066516	C	2.15770994	-6.77358703	-0.32078452
H	4.46825337	1.21608788	1.39707257	H	2.96590833	-7.20631631	-0.93739585
H	4.96242045	1.32233815	-0.32133310	H	2.16863173	-7.28237450	0.65725715
C	4.32437267	-0.70221818	0.31615288	H	1.20257471	-7.01856980	-0.81967538
H	4.78786534	-1.15478537	1.20823192	C	2.06446273	6.68819945	-1.32860691
H	4.86086420	-1.07578272	-0.57749033	H	2.26768819	7.34151351	-0.46362936
Cl	-0.08820427	0.50862982	-2.37113176	H	2.73456542	6.98913924	-2.15203198
Cl	0.26744516	0.07892178	2.43479601	H	1.02927130	6.89316562	-1.65970036
C	2.60294225	-2.47816541	0.10231865	C	-0.34095850	-1.81525315	0.13497159
C	2.54398882	-3.28337170	1.26637319	H	-0.22455702	-2.21254942	1.16694103
C	2.55823908	-3.05112636	-1.19628957	C	-0.82453977	-2.87034483	-0.77268176
C	2.39061469	-4.67534023	1.10132809	C	-0.85329354	-2.79044070	-2.18964189
C	2.41239778	-4.44511377	-1.30343408	C	-1.27690183	-4.07558592	-0.16493572
C	2.32205787	-5.27553429	-0.16861534	C	-1.32105713	-3.86492096	-2.95714898
H	2.33083752	-5.30615588	1.99717706	H	-0.49634351	-1.87438620	-2.67078290
H	2.36504860	-4.89326578	-2.30363664	C	-1.76620437	-5.14106786	-0.93356433
C	2.54371209	2.48747926	-0.32414195	H	-1.23958557	-4.16156651	0.92714564
C	2.30964225	3.42694293	0.71249928	C	-1.78757220	-5.04009721	-2.33619069
C	2.69538020	2.90753741	-1.67374108	H	-1.32706212	-3.78556112	-4.04993926
C	2.15010199	4.78253363	0.35637179	H	-2.12293700	-6.05185021	-0.44001315
C	2.52379983	4.27177626	-1.97199635	H	-2.16234361	-5.87208146	-2.94271353
C	2.24540808	5.22636341	-0.97470529	H	-4.99827478	0.77110792	4.05785994
H	1.96726007	5.51380520	1.15384896	C	-3.92700779	0.65426349	4.32420650
H	2.63589640	4.59867143	-3.01331583	C	-3.66034273	-0.81324073	4.70831858
C	2.66679052	-2.19160883	-2.43480992	C	-3.05079775	1.10729426	3.13411266
H	3.62802877	-1.64659247	-2.47153066	H	-3.74525094	1.31931132	5.18928905
H	2.60112019	-2.81057793	-3.34401810	C	-3.85687878	-1.74155039	3.49467833
H	1.86761752	-1.42976353	-2.47363671	H	-2.61885496	-0.90976837	5.07355632
C	2.65545318	-2.68356008	2.64992887	H	-4.32139022	-1.11964184	5.54070225
				C	-3.26361229	0.17546649	1.91811009
				H	-1.98613464	1.09102428	3.42678110
				H	-3.31068855	2.14914628	2.87428586

C	-2.98420980	-1.29731584	2.30113387	Ru	0.09862700	-0.33655800	0.08199500
H	-4.92598458	-1.73412771	3.19715603	C	1.79566100	0.37566100	0.29893500
H	-3.61334283	-2.78657349	3.76404493	H	2.14529300	0.34016400	1.35368300
P	-2.40028623	0.64441770	0.27436154	C	2.79939000	1.04569700	-0.54711300
H	-4.33923731	0.24634375	1.65768496	Cl	-0.18537200	-0.36916900	-2.33044400
H	-1.91599991	-1.39047660	2.56555905	Cl	-0.11226100	-0.41304100	2.51714500
H	-3.16447959	-1.96802853	1.44000954	C	0.55405600	-2.34527100	0.20459000
C	-2.56570899	2.52724988	0.18112703	P	-1.15824000	1.79551600	0.15500500
C	-3.77010832	-0.05450680	-0.86900929	N	-0.37006700	-3.36027900	0.21191100
C	-2.56380340	3.09025464	-1.26205971	N	1.76568100	-2.91402100	0.50679800
C	-1.44718628	3.22849722	0.99183492	C	1.70215900	-4.39330600	0.63094800
H	-3.54567473	2.76366080	0.64811418	H	2.21654800	-4.72468900	1.54816700
C	-3.39292680	-0.28079038	-2.34884460	H	2.20624000	-4.86414100	-0.23537200
C	-5.13566785	0.68076578	-0.78443449	C	0.19297500	-4.66018100	0.65726600
H	-3.91026494	-1.06237521	-0.42163651	H	-0.12142200	-5.46623500	-0.02732600
C	-2.78642090	4.61837278	-1.25238792	H	-0.17433300	-4.90115500	1.67203800
H	-1.59617043	2.84842126	-1.74070578	C	3.08472800	-2.34487800	0.43173000
H	-3.34263103	2.61220912	-1.87836635	C	3.71764600	-2.23441100	-0.83437300
C	-1.67101187	4.75420459	1.02893092	C	5.06141600	-1.82272900	-0.87119900
H	-0.47505826	3.02035163	0.50117346	H	5.55540800	-1.72768600	-1.84612200
H	-1.36721344	2.82489031	2.01345817	C	5.78448200	-1.52914400	0.30198800
C	-4.49111367	-1.08395754	-3.07810412	C	5.12684700	-1.65742100	1.53893100
H	-3.24837888	0.68971800	-2.85829935	H	5.67500300	-1.43630100	2.46355900
H	-2.42774716	-0.79975328	-2.41744127	C	3.78291100	-2.07236400	1.63383900
C	-6.23887574	-0.12325035	-1.50932174	C	2.97089000	-2.54331600	-2.11142000
H	-5.05003792	1.67542019	-1.26100001	H	3.62876100	-2.41746100	-2.98621000
H	-5.44542907	0.86147982	0.26032211	H	2.09436800	-1.88211300	-2.23705300
C	-1.73646906	5.34581353	-0.39187163	H	2.59060000	-3.58123600	-2.12507700
H	-3.80050318	4.83658989	-0.85837080	C	7.22779300	-1.07653100	0.22508800
H	-2.76463769	5.00106041	-2.29003677	H	7.30123600	-0.06552000	-0.21602500
H	-2.61661977	4.97138526	1.56725369	H	7.82880100	-1.75136600	-0.40985800
H	-0.86201197	5.23544577	1.60918073	H	7.69457900	-1.04298400	1.22346700
C	-5.86681937	-0.39901343	-2.97842454	C	3.11775800	-2.22510000	2.98352200
H	-4.55285448	-2.09877809	-2.63534334	H	2.13450900	-1.72195900	3.00995600
H	-4.20527363	-1.22177842	-4.13762867	H	3.75363800	-1.80288000	3.77890100
H	-6.38964079	-1.08695094	-0.98191683	H	2.94470100	-3.28907900	3.23434500
H	-7.19855765	0.42383094	-1.44706689	C	-1.76992800	-3.33803400	-0.13523400
H	-0.74201820	5.23296675	-0.86610861	C	-2.12928100	-3.57144000	-1.49005500
H	-1.95397843	6.42987200	-0.35176196	C	-3.49597200	-3.69141800	-1.80716600
H	-5.83645062	0.56163821	-3.53167027	H	-3.77835900	-3.86484300	-2.85300200
H	-6.64639051	-1.01655421	-3.46271427	C	-4.49977000	-3.63338800	-0.82258100
				C	-4.10397700	-3.45455500	0.51627500
				H	-4.86727100	-3.44311500	1.30479800

**Pseudo Z- 2b-PC**



C	-5.51241700	-1.01817800	-0.26306500	Cl	1.04243600	-1.84339100	2.06756500
C	-4.11456300	-0.94971900	-0.25245600	Cl	0.96038500	-1.63038800	-2.35187200
H	-7.37429700	0.01209800	0.18551100	P	-0.91908600	0.06272500	0.01762300
H	-6.23288300	2.07482800	1.03462400	C	2.18718200	0.40306000	-0.05810000
H	-3.74053700	2.20262800	1.05818900	H	1.85113700	1.45486600	-0.07634100
H	-3.52209500	-1.81413600	-0.57423700	C	-1.16718200	1.04472700	1.62021900
H	-6.00820600	-1.92702400	-0.61993600	H	-1.17322700	0.22019800	2.36251700
C	1.07978800	1.93572100	0.22615700	C	0.00871500	1.96657400	2.02313000
C	1.66821600	2.56592500	1.34540700	H	0.10978600	2.79861600	1.29898000
C	0.55061500	2.72898400	-0.81734100	H	0.95087600	1.39442500	2.00414600
C	1.73493900	3.96844300	1.41290200	C	-0.21273000	2.54873800	3.43615000
H	2.07397700	1.96550800	2.16498300	H	-0.18217300	1.72085000	4.17224700
C	0.62708700	4.12964000	-0.74582400	H	0.62355900	3.22538400	3.69152800
H	0.07810900	2.24717000	-1.68096300	C	-1.55906600	3.28701100	3.55342100
C	1.21713800	4.75261300	0.36816200	H	-1.71000900	3.65235700	4.58595100
H	2.19051700	4.44577000	2.28712600	H	-1.54520400	4.18415800	2.90129900
H	0.21614100	4.73338500	-1.56196800	C	-2.72673400	2.37493000	3.13398100
H	1.26758700	5.84531100	0.42458300	H	-2.81483000	1.53681900	3.85415100
C	1.46455300	-0.50161000	1.78368000	H	-3.68494000	2.92585600	3.17198200
C	2.81604400	-0.70583100	2.13834000	C	-2.51628400	1.79896500	1.71556900
C	0.45643300	-0.70995600	2.74847400	H	-2.52601500	2.63185100	0.98605500
C	3.15193400	-1.10372600	3.44402200	H	-3.36162000	1.13664800	1.45599200
H	3.60660600	-0.56022400	1.39507800	C	-1.28862700	1.13290400	-1.51564200
C	0.79680600	-1.10154200	4.05299000	H	-0.89941100	0.47699000	-2.32063300
H	-0.59536300	-0.59070200	2.46983400	C	-0.46676600	2.44515000	-1.55371300
C	2.14406300	-1.29894400	4.40363800	H	-0.81438600	3.12279000	-0.74915500
H	4.20292300	-1.26461100	3.70712500	H	0.60092400	2.24041600	-1.36906700
H	0.00552400	-1.26849200	4.79130000	C	-0.61648500	3.16347400	-2.91258300
H	2.40664300	-1.61426200	5.41911200	H	-0.17658300	2.52682800	-3.70548500
C	2.43573400	-0.40649000	-0.96549800	H	-0.03244000	4.10250500	-2.90085600
C	2.63722800	-1.78674100	-1.19928600	C	-2.09236300	3.44881000	-3.24309500
C	3.29555600	0.53592300	-1.56593200	H	-2.18161500	3.91964600	-4.23939100
C	3.69472600	-2.21343800	-2.01677000	H	-2.49762800	4.17809800	-2.51226500
H	1.96454400	-2.52326100	-0.74391700	C	-2.92378300	2.15480600	-3.18535100
C	4.35096000	0.10088600	-2.38657900	H	-3.99209500	2.36996300	-3.37392100
H	3.14296800	1.60612300	-1.39598000	H	-2.59220100	1.47031500	-3.99150400
C	4.55245900	-1.27094700	-2.61296400	C	-2.77950200	1.43455800	-1.82446700
H	3.84396000	-3.28381700	-2.19329800	H	-3.37621700	0.50711600	-1.84928700
H	5.01391200	0.83882200	-2.85075100	H	-3.21109400	2.07356500	-1.03117200
H	5.37297200	-1.60596200	-3.25633700	C	-2.37650300	-1.15835100	0.04581300
				H	-3.27152700	-0.50619500	-0.03280800
				C	-2.51471300	-1.97727900	1.35195700
				H	-2.57314400	-1.31257600	2.23173600
<b>1b-Inact-C PCy<sub>3</sub>-Cl<sub>2</sub>Ru=CHPh</b>							
Ru	1.02854300	-1.03139000	-0.10985300				

H	-1.61500900	-2.60306300	1.49628900	C	-4.61959800	-2.27178500	-0.10346200
C	-3.77512000	-2.87018900	1.30926300	H	-4.50302200	-2.37189600	2.05978600
H	-3.83398400	-3.46338200	2.24047600	H	-4.38559300	-2.11238500	-2.25365200
H	-4.67875600	-2.22688600	1.28873400	C	3.02775100	-0.84739900	-0.03706200
C	-3.78564500	-3.79537700	0.07845200	C	3.64368800	-0.53693300	1.20293300
H	-2.95092900	-4.52007800	0.15871200	C	3.68584200	-0.58337800	-1.26922800
H	-4.71797400	-4.38933600	0.05184200	C	4.86642400	0.16368100	1.17909700
C	-3.62660600	-2.98424700	-1.22089900	C	4.91010400	0.10749100	-1.23421400
H	-4.51987800	-2.34191800	-1.36472400	C	5.50378000	0.51563800	-0.02348100
H	-3.57950700	-3.65769400	-2.09641700	H	5.33512300	0.43012200	2.13467100
C	-2.36188800	-2.10183000	-1.18227700	H	5.41620100	0.32794300	-2.18219400
H	-1.46492100	-2.74726500	-1.13403700	C	-1.68368400	-1.88356300	-2.56007900
H	-2.26534900	-1.53396200	-2.12418800	H	-0.98158000	-2.71770600	-2.74035200
C	6.46971100	0.01456800	-0.10488100	H	-2.36696500	-1.83308800	-3.42281400
C	5.86030300	1.26599000	-0.30954500	H	-1.08407300	-0.95630000	-2.53994900
C	4.46389500	1.37909800	-0.28153800	C	-1.81268900	-2.20192800	2.52847200
C	3.64133300	0.24090800	-0.05439700	H	-2.53325300	-2.27546400	3.35872500
C	4.27794900	-1.01330700	0.16094300	H	-1.10562200	-3.04638600	2.62013100
C	5.67249100	-1.12243700	0.13324400	H	-1.22461700	-1.27633900	2.65961400
H	7.56101300	-0.07473800	-0.12367700	C	3.08578600	-1.00664500	2.52918100
H	6.47563100	2.15422200	-0.48893500	H	1.99572000	-1.14474100	2.50336100
H	3.98960300	2.35442200	-0.44160600	H	3.55810000	-1.96458000	2.82209300
H	3.66891900	-1.89920700	0.37642700	H	3.30105200	-0.27580400	3.32484300
H	6.14418000	-2.09562300	0.30490000	C	3.11752000	-1.05922400	-2.58701000

**2b-Inact-C PCy<sub>3</sub>-Cl<sub>2</sub>Ru=CHPh**

Ru	0.25070700	0.87829500	0.06174100	H	3.83943400	-0.88748100	-3.40188200
C	0.50752500	-1.03030400	-0.00508800	H	2.88383300	-2.13891400	-2.56222800
N	1.78174900	-1.57418700	-0.06844400	C	-6.12756500	-2.40901900	-0.15413500
N	-0.36966100	-2.09525300	0.03839400	H	-6.42361600	-3.46792600	-0.27479100
C	1.78590300	-3.03830700	0.12619100	H	-6.59910700	-2.04107800	0.77242300
H	2.10783600	-3.28799500	1.15641100	H	-6.55696000	-1.85177800	-1.00375000
H	2.48037700	-3.52175400	-0.58117700	C	6.79228200	1.31119200	-0.02052700
C	0.31597200	-3.39945800	-0.12782100	H	7.35909200	1.16167200	0.91366200
H	-0.08199900	-4.13562400	0.59038600	H	7.44211300	1.03233100	-0.86737400
H	0.15052500	-3.78903600	-1.15158500	H	6.58516700	2.39392900	-0.11024700
Cl	0.76574500	1.46447400	-2.13102500	C	-1.58658400	1.04547400	0.01632500
Cl	0.64323600	1.27258600	2.31855800	H	-2.25403300	0.16992200	0.02920700
C	-1.80531200	-2.09654000	-0.01738000	C	-2.27640000	2.33262700	0.00329800
C	-2.52799200	-2.21049600	1.19520300	C	-1.59834200	3.58034700	-0.08857100
C	-2.46056300	-2.06218700	-1.27393300	C	-3.69685500	2.34590600	0.09062000
C	-3.93246400	-2.29254800	1.12606800	C	-2.31132500	4.78387900	-0.08735600
C	-3.86596200	-2.14833000	-1.28795300	H	-0.50585400	3.60119100	-0.17533600
				C	-4.40760300	3.55312500	0.09244200

H	-4.23030400	1.39098100	0.16035200
C	-3.71739200	4.77613500	0.00391000
H	-1.77261400	5.73430700	-0.16154300
H	-5.50080800	3.54307000	0.16115300
H	-4.27168900	5.72074800	0.00290300

**PPh<sub>3</sub>**

C	-1.14690900	-1.21998600	-0.41344300
C	1.62980900	-0.38472500	-0.40557800
C	-0.47961100	1.59710000	-0.40834300
C	-0.80447800	-2.02649700	0.69320300
C	-2.43147200	-1.36584600	-0.98741100
C	2.10625300	0.25716700	0.75865300
C	2.44960800	-1.35372400	-1.02925400
C	0.00395700	2.78759300	-0.99918000
C	-1.32045500	1.69462900	0.72133200
C	-1.72839900	-2.94712300	1.21901600
H	0.18882800	-1.93699200	1.14515000
C	-3.35876000	-2.27378900	-0.45251100
H	-2.70452500	-0.76306600	-1.86187300
C	3.36538200	-0.07133000	1.29098600
H	1.49422400	1.02151500	1.24909000
C	3.70107900	-1.69138800	-0.48928000
H	2.10386600	-1.84361000	-1.94731500
C	-0.32431400	4.04174900	-0.46057700
H	0.64102600	2.72864200	-1.88975300
C	-1.66180700	2.95167600	1.25103600
H	-1.71355600	0.78430200	1.18579200
C	-3.00797700	-3.07036900	0.65223000
H	-1.44554900	-3.56728000	2.07678100
H	-4.35100100	-2.36858800	-0.90677900
C	4.16372700	-1.04832400	0.67244800
H	3.72145700	0.43867500	2.19289400
H	4.32054900	-2.44751900	-0.98362500
C	-1.16205800	4.12725300	0.66569600
H	0.06344700	4.95295100	-0.92880300
H	-2.31843600	3.01001800	2.12613400
H	-3.72601000	-3.78754500	1.06393900
H	5.14454300	-1.30201800	1.08850000

H	-1.42921700	5.10524300	1.07992500
P	0.00326000	-0.00327500	-1.22428000

**PCy<sub>3</sub>**

P	-0.23449800	-0.06733500	-1.04758700
C	0.75610100	-1.51045200	-0.29683600
H	0.01674100	-2.33724800	-0.36756500
C	1.22469400	-1.44237600	1.17386200
H	0.38729000	-1.17136500	1.84327100
H	1.98523100	-0.64397800	1.27627000
C	1.85378900	-2.78047800	1.62427800
H	2.20023800	-2.70274400	2.67215700
H	1.07639300	-3.57124200	1.60746700
C	3.01771000	-3.19303900	0.70252100
H	3.42877100	-4.17073200	1.01605500
H	3.84117400	-2.45760700	0.80839600
C	2.57285300	-3.24515900	-0.77210000
H	3.43095400	-3.49246300	-1.42493500
H	1.83426600	-4.06259600	-0.90041500
C	1.93264000	-1.91462000	-1.22197600
H	1.57989400	-1.99059800	-2.26675600
H	2.70554900	-1.12142900	-1.20951600
C	-1.84477800	-0.12333000	-0.03257900
H	-1.61473700	-0.07699600	1.05287600
C	-2.60999700	-1.44137000	-0.31061900
H	-2.00888800	-2.31502900	-0.00006100
H	-2.76475100	-1.54075000	-1.40452500
C	-3.97683300	-1.48806800	0.40459200
H	-4.49739600	-2.43128600	0.15348300
H	-3.81419600	-1.50119200	1.50155100
C	-4.85095600	-0.27532800	0.03702600
H	-5.10726300	-0.32422000	-1.04068300
H	-5.80786500	-0.30547800	0.59066600
C	-4.10642900	1.04181700	0.32043400
H	-3.94948000	1.14421400	1.41355800
H	-4.72022500	1.90819800	0.00992500
C	-2.73966500	1.08836600	-0.39614900
H	-2.22854400	2.03754600	-0.15354100
H	-2.90284100	1.09300900	-1.49346800
C	0.55255200	1.57071900	-0.46999600
H	-0.07257800	2.30819000	-1.01979300
C	0.52302600	1.98333500	1.02160400

H	1.13987100	1.28682400	1.61874700
H	-0.50287700	1.91889900	1.42710200
C	1.06619400	3.41899600	1.20819700
H	0.38715200	4.13301300	0.69899800
H	1.05681500	3.68869300	2.28114100
C	2.48617900	3.57060600	0.62900400
H	2.83773600	4.61323100	0.74044900
H	3.18536200	2.93867200	1.21370300
C	2.53495500	3.14076800	-0.84983300
H	3.56970400	3.20298600	-1.23590300
H	1.92931600	3.84479700	-1.45567800
C	1.98504700	1.71196800	-1.03963600
H	1.99840300	1.43482600	-2.11036300
H	2.65575100	0.99973500	-0.51955700