Supporting Information
Computational Part

Ruthenium-Catalyzed Alkyne *trans*-Hydrometalation: Mechanistic Insights and Preparative Implications

Dragoş Adrian Roşca, Karin Radkowski, Larry M. Wolf, Minal Wagh, Richard Goddard, Walter Thiel, Alois Fürstner*

Max-Planck-Institut für Kohlenforschung, D-45470 Mülheim/Ruhr, Germany
E-mail: fuerstner@kofo.mpg.de

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1. Computational Methods

All geometry optimizations were performed using the M06[1] functional. The def2-SVP[2] basis set was used for all atoms. The 28 inner-shell core electrons of the ruthenium atom were described by the corresponding def2 effective core potential[3] accounting for scalar relativistic effects (def2-ecp).

Stationary points were characterized by evaluating the harmonic vibrational frequencies at the optimized geometries. Zero-point vibrational energies (ZPVE) were computed from the corresponding harmonic vibrational frequencies without scaling. Relative free energies (ΔG) were determined at standard pressure (1 bar) and at room temperature (298 K). The thermal and entropic contributions were evaluated within the rigid-rotor harmonic-oscillator approximation. Solvation contributions were included for dichloromethane on the optimized gas-phase geometries employing the SMD solvation model[4] using the same functional and the def2-TZVP basis set. All calculations were performed using Gaussian09 with the ultrafine grid.[5]

Decomposition analysis was performed on the M06/def2-TZVP optimized geometries of [Cp*Ru(Cl)($CH_3C{\equiv}CCH_3$)] and [Cp*Ru(Cl)(*E*-2-butene)] using the ADF2016[6] program package at the M06 level in conjunction with a triple-ζ-quality basis set using uncontracted Slater-type orbitals (STOs)[7] augmented with two sets of polarization functions for all atoms; all electrons were included (i.e., inner core electrons were not described by a frozen core). Scalar relativistic effects were accounted for using the zeroth-order regular approximation (ZORA).[8]

2. Orbital Interaction Diagram Construction (Figure 4).

The orbital interaction diagram from Figure was constructed using perturbation theory (Eq. 1). The relevant fragment orbitals are shown (Figure S1 and S2). The overlap integrals and Fock interaction elements were used in the diagram construction.

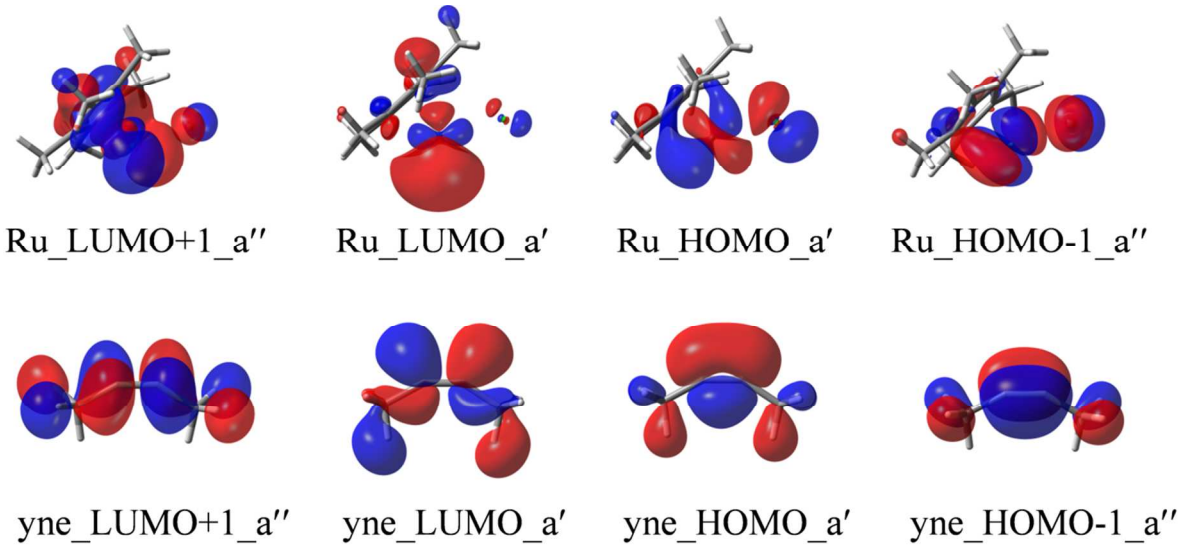

Figure S1. Fragment orbitals for the [Cp*Ru(Cl)($CH_3C{\equiv}CCH_3$)] complex.

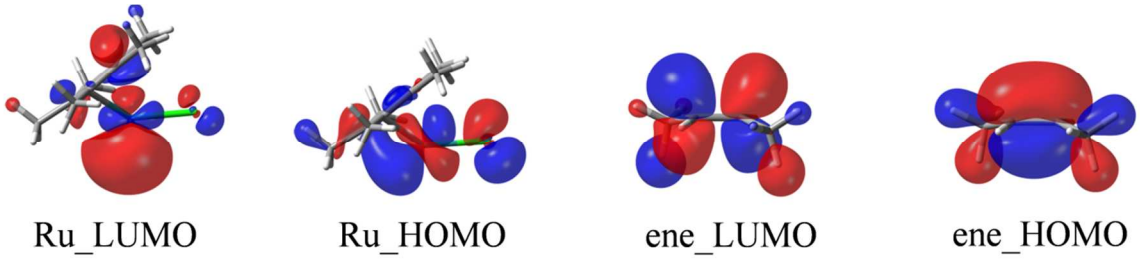

Figure S2. Fragment orbitals for the [Cp*Ru(Cl)(*E*-2-butene)] complex.

Eq 1. Perturbation theory derived expression for determining the interaction between two orbitals.

$$\text{Bonding:} \qquad \Delta\varepsilon_{ij} = \varepsilon_i - \left(\frac{-b}{2a} - \frac{1}{2a}(b^2 - 4ac)^{1/2} \right) \qquad \varepsilon_i \le \varepsilon_j$$

$$\text{Anti-bonding:} \qquad \Delta\varepsilon_{ij} = \left(\frac{-b}{2a} + \frac{1}{2a}(b^2 - 4ac)^{1/2} \right) - \varepsilon_i \qquad \varepsilon_i \ge \varepsilon_j$$

$$a = (1 - S_{ij}^2) \qquad b = 2S_{ij}F_{ij} - (\varepsilon_i + \varepsilon_j) \qquad c = \varepsilon_i\varepsilon_j - F_{ij}^2$$

where S_{ij} is the overlap integral between orbitals *i* and *j*, F_{ij} is the Fock matrix element between orbitals *i* and *j*, and ε_i is the orbital energy for *i*.

Table S1. Fragment orbital energies for the [Cp*Ru(Cl)($CH_3C{\equiv}CCH_3$)] complex.

	ε (eV)
Ru_LUMO_a′	-1.711
Ru_LUMO+1_a′′	-1.457
Ru_HOMO_a′	-5.194
Ru_HOMO-1_a′′	-5.533
yne_LUMO_a′	-0.52
yne_LUMO+1_a′′	1.158
yne_HOMO_a′	-6.849
yne_HOMO-1_a′′	-6.909

Table S2. Overlap integrals between the fragment orbitals for the [Cp*Ru(Cl)($CH_3C{\equiv}CCH_3$)] complex.

Overlap Matrix (S_{ij})				
	yne_LUMO_a′	yne_LUMO+1_a′′	yne_HOMO_a′	yne_HOMO-1_a′′
Ru_LUMO_a′	–	0	0.24	0
Ru_LUMO+1_a′′	0	–	0	0.21
Ru_HOMO_a′	0.22	0	–	0
Ru_HOMO-1_a′′	0	0.08	0	–

Table S3. The corresponding Fock interaction matrix elements for the [Cp*Ru(Cl)($CH_3C{\equiv}CCH_3$)] complex.

Fock Matrix (F_{ij} (eV))				
	yne_LUMO_a′	yne_LUMO+1_a′′	yne_HOMO_a′	yne_HOMO-1_a′′
Ru_LUMO_a′	–	0	-3.23	0
Ru_LUMO+1_a′′	0	–	0	-2.74
Ru_HOMO_a′	-3.22	0	–	0
Ru_HOMO-1_a′′	0	-0.80	0	–

Table S4. Orbital interaction matrix elements computed using eq. 1 for the [Cp*Ru(Cl)($CH_3C{\equiv}CCH_3$)] complex.

Interaction Energy ($\Delta\varepsilon_{ij}$)				
	yne_LUMO_a′	yne_LUMO+1_a′′	yne_HOMO_a′	yne_HOMO-1_a′′
Ru_LUMO_a′	–	0	0.40	0
Ru_LUMO+1_a′′	0	–	0	0.28
Ru_HOMO_a′	0.67	0	–	0
Ru_HOMO-1_a′′	0	0.02	0	–

Table S5. Fragment orbital energies for the [Cp*Ru(Cl)(*E*-2-butene)] complex.

	ε (eV)
Ru_LUMO	-1.558
Ru_HOMO	-5.393
ene_LUMO	0.075
ene_HOMO	-6.649

Table S6. Overlap integrals between the fragment orbitals for the [Cp*Ru(Cl)(*E*-2-butene)] complex.

Overlap Matrix (S_{ij})		
	ene_LUMO	ene_HOMO
Ru_LUMO	–	0.21
Ru_HOMO	0.17	–

Table S7. The corresponding Fock interaction matrix elements for the [Cp*Ru(Cl)(*E*-2-butene)] complex.

Fock Matrix (F_{ij}(eV))		
	ene_LUMO	ene_HOMO
Ru_LUMO	–	-2.95
Ru_HOMO	-2.25	–

Table S8. Orbital interaction matric elements computed using eq. 1 for the [Cp*Ru(Cl)(*E*-2-butene)] complex.

Interaction Energy ($\Delta\varepsilon_{ij}$)		
	ene_LUMO	ene_HOMO
Ru_LUMO	-	0.40
Ru_HOMO	0.30	-

3. Hydrostannation to Form the Minor Constitutional Isomer *Z*-prod′

The regioisomeric pathway leading to the constitutional isomer from addition of H and Sn on opposite carbon atoms was also investigated (Figure S3). The H---Cl hydrogen bond present in the complex of **INT1** is not feasible in this pathway (**INT1′**). In solution the hydrogen bond accounts for an additional 1.1 kcal/mol, while in the gas phase the interaction is ~2.8 kcal/mol. It is this interaction that accounts for the preference for the pathway from **INT1**.

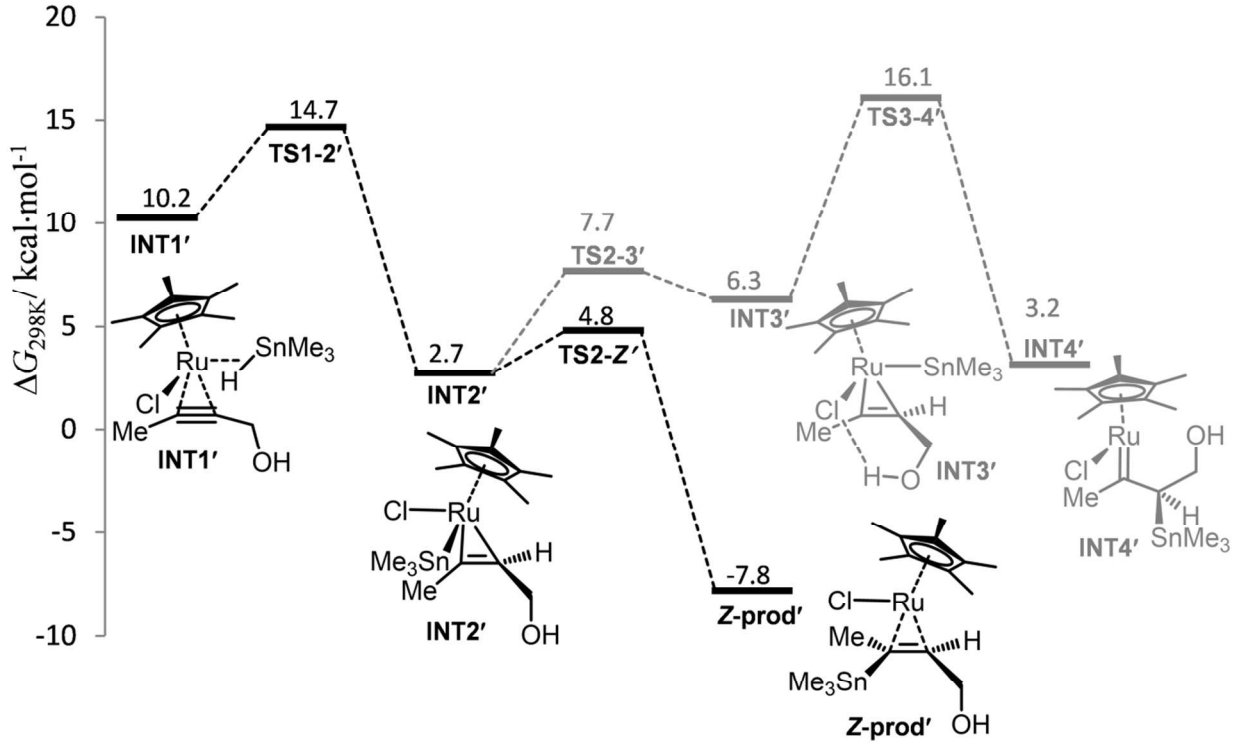

Figure S3. Gibbs free energy profile (in units of kcal·mol^{-1}) for the formation of the minor constitutional isomer *Z*-prod′

4. Energy table for Hydrostannation.

Table S9. Listed are the SCF energy, zero point vibrational energy (*ZPVE*), enthalpy correction (H_{corr}), and Gibbs free energy correction (G_{corr}) determined on the gas-phase geometries for all stationary points calculated. The single imaginary frequency (υ_i cm^{-1}) is also listed for all transition states. Single point solvent (DCM) corrected SCF energies on the gas phase geometries are also tabulated. All energies are in atomic units.

	SCF_{gas}	SCF_{DCM}	*ZPVE*	H_{corr}	G_{corr}	υ_i (cm^{-1})
INT-0	-1175.414755	-1176.300435	0.313615	0.336298	0.262974	
INT-0′	-1175.410334	-1176.293814	0.313457	0.336235	0.263991	
TS0-0′	-1175.395577	-1176.277645	0.311803	0.334349	0.263159	*i*50
INT-1	-1509.941825	-1510.966874	0.428589	0.461002	0.368079	
TS1-2	-1509.936209	-1510.960702	0.427989	0.459594	0.369781	*i*357
INT-2	-1509.960924	-1510.986417	0.431744	0.463391	0.373849	
TS2-*Z*	-1509.955835	-1510.980848	0.432264	0.463005	0.375293	*i*60
Z-prod	-1509.977168	-1511.004460	0.432620	0.464572	0.371992	
TS2-3	-1509.940287	-1510.969867	0.430124	0.461879	0.370981	*i*19
INT-3	-1509.941386	-1510.969479	0.431572	0.463632	0.371580	
TS3-5	-1509.931650	-1510.961553	0.430416	0.462230	0.371126	*i*135
INT-5	-1509.949109	-1510.977028	0.432007	0.463879	0.373126	
TS5-*E*	-1509.941168	-1510.969135	0.430289	0.462179	0.370534	*i*40
E-prod	-1509.981640	-1511.008570	0.433038	0.464812	0.373277	
TS2-5	-1509.934291	-1510.960006	0.430637	0.462455	0.371210	*i*139
TS3-4	-1509.922145	-1510.953201	0.430572	0.462265	0.371039	*i*23
INT-4	-1509.952860	-1510.979041	0.431088	0.463487	0.369015	
TS4-5	-1509.934235	-1510.960788	0.431226	0.462494	0.372426	*i*36
INT-1`	-1509.936521	-1510.964309	0.427633	0.460404	0.367256	
TS1-2`	-1509.922883	-1510.955087	0.425512	0.458276	0.365068	*i*358
INT-2`	-1509.959257	-1510.983735	0.432059	0.463637	0.374732	
TS2-*Z*`	-1509.951677	-1510.979847	0.432454	0.463366	0.374138	*i*84
Z-prod`	-1509.968267	-1510.998926	0.432775	0.464726	0.373121	
TS2-3`	-1509.948528	-1510.973666	0.430477	0.461882	0.372557	*i*42
INT-3`	-1509.951255	-1510.976535	0.431789	0.463477	0.373189	
TS3-4`	-1509.932208	-1510.961045	0.431842	0.462788	0.373295	*i*36
INT-4`	-1509.952332	-1510.978008	0.431634	0.463736	0.369709	
INT0-Si	-1544.545274	-1545.624670	0.386120	0.415060	0.329152	
INT0′-Si	-1544.546570	-1545.622976	0.385727	0.415111	0.326918	
$HSnMe_3$	-334.5022961	-334.6541988	0.112760	0.122697	0.078276	

5. Coordinates

Cartesian coordinates (Å)

INT0

Ru	-0.18454	0.02086	-0.10065
Cl	-1.38806	-2.04897	-0.52122
C	-2.06220	0.82685	-0.23698
C	-1.20641	1.78136	-0.26180
C	-0.97730	3.23545	-0.30413
C	-3.45508	0.31793	-0.31755
C	1.33755	-0.52815	1.32904
C	1.47831	0.86372	0.94955
C	1.73903	0.90265	-0.46234
C	1.76715	-0.46475	-0.94399
C	1.60099	-1.33010	0.17677
C	1.06049	-1.02464	2.70294
H	0.49552	-1.96864	2.67670
H	0.46158	-0.29962	3.27441
H	1.99617	-1.20456	3.26237
C	1.46459	1.99788	1.91408
H	0.56169	1.97896	2.54652
H	1.49805	2.97275	1.40578
H	2.33937	1.94891	2.58570
C	2.06609	2.08963	-1.29801
H	1.50292	2.08355	-2.24575
H	3.14003	2.10052	-1.55369
H	1.84183	3.03425	-0.78150
C	2.00903	-0.88706	-2.34873
H	1.43452	-1.79400	-2.59127
H	3.07731	-1.10452	-2.52720
H	1.70313	-0.10405	-3.05875
C	1.63403	-2.81477	0.13962
H	0.98108	-3.25792	0.90488
H	2.66444	-3.16838	0.32021
H	1.30147	-3.20702	-0.83184
H	-4.14175	1.18220	-0.25490
H	-3.59482	-0.12440	-1.32748
O	-3.79337	-0.56430	0.70035
H	-3.20184	-1.32911	0.58492
H	-1.92727	3.78744	-0.38798
H	-0.33896	3.52340	-1.15504
H	-0.46825	3.58335	0.60975

INT0′

Ru	-0.08487	0.37920	0.01176
Cl	-1.68734	2.11116	-0.46993
C	1.14825	2.00668	0.25496
C	1.87232	0.94926	0.16440
C	3.25844	0.42939	0.19716
C	1.01276	3.46635	0.31867
C	-1.82286	-0.94623	0.34715
C	-0.78438	-1.20428	1.30101
C	0.37543	-1.67678	0.58605
C	0.07505	-1.61795	-0.81452
C	-1.28698	-1.15089	-0.96223
C	-3.20625	-0.51375	0.67594
H	-3.66074	0.04806	-0.15140
H	-3.22440	0.14606	1.55661
H	-3.83842	-1.39249	0.89446
C	-0.91280	-1.10761	2.77868
H	-1.63456	-0.32903	3.06663
H	0.05018	-0.85997	3.25016
H	-1.26096	-2.06410	3.20866
C	1.60157	-2.22912	1.22379
H	2.46972	-2.17913	0.55114
H	1.44410	-3.28509	1.50606
H	1.85363	-1.68287	2.14698
C	0.93807	-2.06946	-1.93903
H	0.93254	-1.33567	-2.76197
H	0.56686	-3.02374	-2.35258
H	1.97762	-2.21478	-1.61631
C	-2.01836	-0.96673	-2.24426
H	-2.59349	-0.02766	-2.23044
H	-2.71840	-1.79951	-2.43275
H	-1.32355	-0.91381	-3.09591
H	3.46129	-0.01627	1.18758
O	3.54376	-0.55945	-0.75710
H	3.23679	-0.23557	-1.61250
H	3.95580	1.28821	0.10233
H	0.33847	3.76791	1.13499
H	0.54302	3.84221	-0.60377
H	1.99188	3.95526	0.45328

TS0-0′

Ru	-0.02282	-0.28281	-0.20004
Cl	-0.57300	-1.08587	-2.33767
C	-2.16229	-0.25209	0.49271
C	-1.81729	-1.44558	0.52529
C	-1.74774	-2.90055	0.59353
C	-2.97775	0.96505	0.35415
C	2.08980	0.15990	-0.29617
C	1.72061	-0.46923	0.96393
C	0.81639	0.40422	1.66336
C	0.56570	1.52678	0.80579
C	1.36801	1.37899	-0.39420
C	3.01664	-0.41952	-1.30641
H	2.82441	-0.01152	-2.30977
H	2.89337	-1.51191	-1.37724
H	4.07192	-0.21744	-1.05150
C	2.26362	-1.76165	1.46298
H	2.39546	-2.48341	0.64118
H	1.59336	-2.22088	2.20582
H	3.24892	-1.62465	1.94432
C	0.22735	0.17090	3.01056
H	-0.77282	0.62509	3.09565
H	0.85503	0.59100	3.81576
H	0.10352	-0.90539	3.21221
C	-0.25264	2.73306	1.11356
H	-0.94730	2.97006	0.29183
H	0.39997	3.60983	1.27201
H	-0.84483	2.59973	2.03159
C	1.36418	2.34074	-1.52717
H	1.71750	1.87308	-2.45782
H	2.00972	3.21169	-1.31492
H	0.34579	2.71941	-1.71087
H	-4.04423	0.65467	0.38739
H	-2.82579	1.63728	1.21800
O	-2.68629	1.69977	-0.80160
H	-2.46574	1.07710	-1.51042
H	-2.71159	-3.33640	0.90618
H	-0.96702	-3.23807	1.29542
H	-1.49205	-3.30010	-0.40131

INT1

Ru	0.52346	0.01054	0.14742
Cl	-0.06388	-1.28185	-1.91579
C	1.31326	-1.96104	0.71137
C	0.48280	-1.68350	1.60785
C	-0.33912	-1.86379	2.80802
C	2.25546	-2.84314	-0.02591
C	2.17042	1.10423	-0.96824
C	2.62892	0.82347	0.34843
C	1.71771	1.43254	1.28387
C	0.72458	2.14712	0.51646
C	0.97773	1.91695	-0.87358
C	2.81268	0.71479	-2.25139
H	2.07122	0.28514	-2.94517
H	3.60222	-0.03465	-2.10250
H	3.25581	1.59824	-2.74380
C	3.86221	0.08186	0.72623
H	4.16108	-0.62650	-0.05926
H	3.71748	-0.48657	1.65867
H	4.69537	0.78516	0.89990
C	1.89512	1.46394	2.76302
H	0.95610	1.72185	3.27705
H	2.65361	2.20768	3.06596
H	2.22388	0.48514	3.14799
C	-0.32838	3.04188	1.07630
H	-1.21565	3.08774	0.42499
H	0.05563	4.07133	1.18227
H	-0.66580	2.70890	2.06997
C	0.28060	2.51223	-2.04606
H	0.10125	1.75159	-2.82281
H	0.88525	3.31724	-2.50078
H	-0.69423	2.94144	-1.77137
H	3.10327	-3.08309	0.64240
H	1.72261	-3.80338	-0.19595
H	-0.25722	-1.00531	3.49579
H	-0.04033	-2.77175	3.35719
H	-1.40732	-1.96628	2.54770
O	2.78212	-2.32704	-1.20282
H	2.01840	-2.06444	-1.75164
H	-0.70503	0.18676	1.20775
Sn	-2.26867	-0.12387	-0.08646
C	-3.42646	0.81941	1.51591
H	-3.36911	1.91865	1.46470
H	-4.48593	0.52773	1.42587
H	-3.06277	0.49833	2.50643
C	-2.84053	-2.20915	-0.07629
H	-3.63275	-2.38894	0.66773
H	-3.20795	-2.48944	-1.07491
H	-1.96382	-2.83443	0.14950
C	-2.89349	0.90046	-1.88558
H	-2.84423	1.99287	-1.75421
H	-2.26203	0.59440	-2.73136
H	-3.93941	0.62248	-2.09324

TS1-2

Ru	-0.53045	0.02977	0.10617
Cl	-0.02696	1.11921	-2.07166
C	-1.37347	1.94168	0.49715
C	-0.44335	1.90369	1.36357
C	0.32451	2.52379	2.46213
C	-2.45015	2.69278	-0.19575
C	-2.10060	-1.30729	-0.80358
C	-2.54473	-0.95006	0.49972
C	-1.54900	-1.37570	1.44533
C	-0.51577	-2.07524	0.71952
C	-0.83452	-1.99869	-0.67755
C	-2.81788	-1.10027	-2.09008
H	-2.13251	-0.71292	-2.86146
H	-3.64060	-0.37874	-1.98655
H	-3.23360	-2.05341	-2.46203
C	-3.82043	-0.25850	0.83398
H	-4.12862	0.42000	0.02383
H	-3.72872	0.33315	1.75849
H	-4.62789	-0.99327	0.99664
C	-1.63236	-1.23439	2.92713
H	-0.63111	-1.25913	3.38677
H	-2.22655	-2.04544	3.38374
H	-2.10267	-0.28025	3.21485
C	0.59189	-2.85984	1.33511
H	1.42499	-3.01587	0.63224
H	0.23230	-3.85721	1.64447
H	1.00457	-2.36665	2.22857
C	-0.13730	-2.65344	-1.81838
H	-0.03347	-1.95694	-2.66580
H	-0.70551	-3.53090	-2.17491
H	0.87175	-2.99505	-1.54615
H	-2.05673	3.71052	-0.40684
H	-0.08838	3.51549	2.70198
H	1.38741	2.65142	2.19162
Sn	2.19386	0.12137	-0.11130
H	0.41874	0.62710	1.31795
C	2.99866	-1.09774	-1.71233
H	4.03165	-0.76544	-1.90498
H	3.02123	-2.16611	-1.44524
H	2.40374	-0.95537	-2.62640
C	3.19360	-0.52318	1.73309
H	4.13742	0.03673	1.84210
H	2.56709	-0.31353	2.61767
H	3.43262	-1.59858	1.72410
C	2.84706	2.16821	-0.41033
H	3.68765	2.41006	0.26037
H	3.16813	2.29701	-1.45520
H	2.01415	2.86473	-0.22866
H	-3.29462	2.83659	0.50414
H	0.29384	1.90811	3.37814
O	-2.95016	2.07843	-1.33810
H	-2.17677	1.82689	-1.87898

INT2

Ru	-0.64109	0.41181	0.00893
Cl	0.16206	0.94532	-2.24976
C	0.10281	2.03168	0.59565
C	-0.23242	1.44777	1.83561
C	0.79061	1.12435	2.89409
C	0.91446	3.22439	0.30147
C	-2.78492	0.07905	0.55695
C	-1.96627	-0.91094	1.22192
C	-1.42958	-1.79906	0.22849
C	-1.81488	-1.30059	-1.03862
C	-2.65415	-0.13230	-0.84287
C	-3.65261	1.07875	1.23469
H	-4.01128	1.84544	0.53246
H	-3.13286	1.59975	2.05657
H	-4.53714	0.59303	1.68252
C	-1.91884	-1.16993	2.68687
H	-2.15963	-0.27377	3.27789
H	-0.92598	-1.52731	3.00504
H	-2.64879	-1.95250	2.96181
C	-0.73563	-3.08237	0.52596
H	-0.15310	-3.44993	-0.33148
H	-1.47453	-3.86347	0.78065
H	-0.04984	-2.99576	1.38248
C	-1.53730	-1.91504	-2.36339
H	-0.82778	-2.75214	-2.28934
H	-1.11306	-1.17694	-3.06364
H	-2.47061	-2.30134	-2.80856
C	-3.31594	0.61282	-1.94716
H	-3.76759	1.55131	-1.59339
H	-4.11410	0.00747	-2.41203
H	-2.58825	0.87064	-2.73353
H	1.81149	3.14849	0.96368
H	0.84496	1.93799	3.64019
H	1.80086	0.99469	2.47209
H	0.54390	0.20330	3.44861
Sn	1.86453	-0.63887	-0.02334
C	2.13849	-2.03789	-1.66232
H	3.21802	-2.11361	-1.87258
H	1.76587	-3.04326	-1.40806
H	1.62838	-1.66846	-2.56422
C	2.32957	-1.78018	1.79155
H	3.18967	-1.32096	2.30610
H	1.48566	-1.81258	2.50012
H	2.59699	-2.81429	1.51788
C	3.41041	0.87198	-0.21084
H	3.02343	1.75862	-0.73739
H	3.78146	1.17273	0.78285
H	4.25300	0.45513	-0.78540
H	-1.20770	1.74023	2.26572
H	0.33408	4.07165	0.73813
O	1.29066	3.50142	-0.99559
H	0.94290	2.80317	-1.57915

TS2-*Z*

Ru	0.66616	-0.36844	0.18685
Cl	0.16625	-1.96492	-1.61531
C	-0.54569	-1.36014	1.23860
C	0.09900	-0.59823	2.23790
H	0.86012	-1.15679	2.81762
C	-0.59078	0.45203	3.07259
C	-1.43054	-2.54509	1.32784
C	2.80512	-0.40553	-0.45012
C	2.69280	0.19432	0.83466
C	1.90896	1.40822	0.69136
C	1.62688	1.58547	-0.70480
C	2.13827	0.46771	-1.39701
C	3.54652	-1.64519	-0.80606
H	3.83310	-2.21481	0.09042
H	4.47026	-1.41029	-1.36367
H	2.92824	-2.30442	-1.43664
C	3.33390	-0.29836	2.08334
H	3.30802	-1.39845	2.14314
H	2.83838	0.09264	2.98504
H	4.39300	0.00965	2.12956
C	1.70481	2.45394	1.73155
H	0.68371	2.86595	1.71319
H	2.39886	3.29750	1.56873
H	1.88933	2.07016	2.74504
C	0.99078	2.77324	-1.33621
H	0.31886	2.49139	-2.16332
H	1.76290	3.43830	-1.76358
H	0.40846	3.36478	-0.61558
C	2.08447	0.28417	-2.87186
H	2.36941	-0.73353	-3.17038
H	2.76981	0.99482	-3.36702
H	1.07177	0.46449	-3.26683
H	-2.22748	-2.31805	2.06681
H	-0.79465	-3.31574	1.83182
H	-1.21570	1.13737	2.47758
H	0.12395	1.06798	3.64164
H	-1.25319	-0.02862	3.81821
O	-2.03668	-3.00818	0.17785
H	-1.39115	-2.93592	-0.55041
Sn	-1.89970	0.54639	-0.28995
C	-2.19067	0.45976	-2.43195
H	-1.31879	0.88005	-2.95774
H	-2.30614	-0.58842	-2.74255
H	-3.09117	1.03359	-2.70439
C	-2.05617	2.65589	0.28371
H	-2.02840	3.29204	-0.61579
H	-3.03413	2.79143	0.77477
H	-1.27480	2.99754	0.98015
C	-3.67982	-0.27064	0.64031
H	-3.64727	-0.13421	1.73387
H	-4.54979	0.28123	0.24779
H	-3.78116	-1.33973	0.40336

Z-prod

Ru	-1.01313	-0.10474	-0.07893
Cl	0.08317	-2.11336	0.70612
C	0.90195	0.23906	-1.09317
C	0.14604	1.41251	-1.20745
H	-0.37853	1.56710	-2.16902
C	0.46457	2.68327	-0.47080
C	0.99216	-0.64090	-2.33283
C	-2.96185	-0.03636	-0.92181
C	-2.71156	1.26308	-0.36764
C	-2.41685	1.08614	1.02537
C	-2.61045	-0.31272	1.35810
C	-2.95600	-1.00085	0.15950
C	-3.29239	-0.33051	-2.34095
H	-2.94230	-1.33285	-2.63287
H	-2.82658	0.39710	-3.02363
H	-4.38362	-0.29683	-2.51248
C	-2.87832	2.54782	-1.10073
H	-2.39253	2.53970	-2.08910
H	-2.48295	3.40553	-0.53802
H	-3.95184	2.74069	-1.27147
C	-2.09668	2.14605	2.01837
H	-1.29429	1.82191	2.70037
H	-2.97918	2.38214	2.63937
H	-1.76560	3.07770	1.53726
C	-2.46369	-0.88535	2.72260
H	-1.58202	-0.46910	3.23536
H	-2.32953	-1.97551	2.69207
H	-3.34953	-0.66239	3.34278
C	-3.23478	-2.45233	-0.00411
H	-4.32015	-2.63516	-0.08863
H	-2.84930	-3.03946	0.84066
H	-2.75430	-2.84753	-0.91321
H	0.02415	-0.58588	-2.88770
H	1.74091	-0.17425	-3.00816
H	-0.39381	3.36937	-0.40834
H	1.26865	3.23281	-0.99464
H	0.81716	2.49275	0.55628
Sn	2.64127	0.12211	0.24398
C	3.67099	-1.76457	0.18705
H	3.74297	-2.10793	-0.85462
H	4.67882	-1.65600	0.61739
H	3.09932	-2.50709	0.76246
C	2.10621	0.65744	2.27414
H	2.07445	1.75120	2.40479
H	1.12160	0.22742	2.51634
H	2.84662	0.24515	2.97705
C	3.97758	1.65302	-0.53753
H	3.86369	1.73149	-1.63135
H	3.75170	2.63521	-0.09237
H	5.02733	1.40339	-0.31722
O	1.40455	-1.95071	-2.12548
H	0.96123	-2.28352	-1.32474

TS2-3

Ru	-0.57329	0.01500	-0.12268
Cl	0.08483	0.34529	-2.43772
C	-1.34527	1.68178	0.02525
C	-0.31616	1.91743	0.95800
H	-0.52590	1.72005	2.02455
C	0.61233	3.09157	0.74038
C	-2.35014	2.46306	-0.70347
C	-2.52839	-0.94185	0.58663
C	-1.47476	-1.13732	1.55527
C	-0.48608	-2.00841	0.97723
C	-0.85523	-2.21425	-0.38355
C	-2.13466	-1.56701	-0.62244
C	-3.80312	-0.22032	0.86099
H	-4.36816	-0.01640	-0.06084
H	-3.64208	0.74612	1.36817
H	-4.45526	-0.82353	1.51618
C	-1.52530	-0.70704	2.98011
H	-2.05683	0.25159	3.09846
H	-0.51481	-0.58201	3.40137
H	-2.05441	-1.44735	3.60664
C	0.60823	-2.67096	1.74014
H	1.40042	-3.05600	1.08231
H	0.20944	-3.52914	2.31031
H	1.07855	-1.99066	2.46749
C	-0.15383	-3.05023	-1.39770
H	-0.01194	-2.49039	-2.33706
H	-0.73728	-3.95808	-1.63051
H	0.84040	-3.36709	-1.05041
C	-2.87653	-1.63023	-1.91077
H	-3.76768	-0.98430	-1.90213
H	-3.21325	-2.65867	-2.13040
H	-2.23625	-1.30161	-2.74670
H	-1.78395	2.84574	-1.59060
H	-3.11677	1.79944	-1.13987
H	0.82300	3.25015	-0.33011
H	1.57846	2.96170	1.25528
H	0.17096	4.02313	1.14401
Sn	2.12567	0.16215	0.05505
C	3.06332	-1.58201	-0.85491
H	2.65790	-1.71804	-1.86978
H	4.14404	-1.37719	-0.93354
H	2.92873	-2.51159	-0.28025
C	2.77677	0.25067	2.14576
H	3.30806	-0.67089	2.43380
H	3.46300	1.10228	2.28548
H	1.91497	0.38721	2.82061
C	3.10570	1.79421	-0.99147
H	3.41810	2.59863	-0.30780
H	4.00168	1.37962	-1.48144
H	2.44436	2.20111	-1.77112
O	-2.99672	3.46600	0.02315
H	-2.32580	4.03629	0.41643

INT-3

Ru	-0.58002	0.03782	-0.27267
Cl	0.43929	-0.20894	-2.45408
C	-1.31494	1.72369	-0.29123
C	-0.07377	2.10845	0.26881
C	0.73351	3.12787	-0.50992
C	-2.53234	2.47678	-0.64215
C	-2.58345	-0.79336	0.45756
C	-1.59754	-0.77152	1.51471
C	-0.59378	-1.75874	1.21017
C	-0.86786	-2.24236	-0.09667
C	-2.10431	-1.64639	-0.56630
C	-3.91025	-0.12388	0.53007
H	-4.39290	-0.04919	-0.45630
H	-3.85827	0.88826	0.96176
H	-4.58499	-0.71500	1.17423
C	-1.73290	-0.06090	2.81724
H	-2.26849	0.89584	2.70393
H	-0.74593	0.16165	3.25398
H	-2.28970	-0.66608	3.55562
C	0.39077	-2.27757	2.20112
H	1.07028	-3.01878	1.75904
H	-0.14646	-2.77522	3.02807
H	1.00716	-1.48494	2.65553
C	-0.11371	-3.27532	-0.85903
H	0.79803	-3.59176	-0.33209
H	0.19151	-2.89240	-1.84742
H	-0.73997	-4.16893	-1.02481
C	-2.74584	-1.97046	-1.86886
H	-3.56968	-1.27833	-2.10009
H	-3.15560	-2.99616	-1.87565
H	-2.01353	-1.89705	-2.68966
H	-2.22080	3.14803	-1.47783
H	-3.32646	1.83668	-1.05521
H	0.24465	4.12015	-0.45299
H	0.80496	2.85299	-1.57456
H	1.75516	3.25598	-0.12158
Sn	2.10470	0.16170	0.18619
O	-3.08031	3.18886	0.43896
H	-2.36692	3.68426	0.86157
C	3.03171	-1.78942	-0.10205
H	4.12161	-1.63633	-0.02844
H	2.73722	-2.55505	0.62977
H	2.79744	-2.14149	-1.11890
C	2.48879	0.82226	2.23681
H	2.72487	1.89939	2.22607
H	1.61976	0.67139	2.89805
H	3.35025	0.28286	2.66287
C	3.37668	1.37191	-1.09001
H	2.86570	1.63565	-2.02677
H	3.72109	2.28673	-0.58276
H	4.25622	0.75556	-1.33757
H	-0.03026	2.25670	1.36610

TS3-5

Ru	-0.56215	-0.12429	-0.05919
Cl	0.10307	0.74587	-2.26621
C	-1.95033	1.32477	-0.16406
C	-1.16228	2.13745	0.54058
H	-0.05796	1.91726	0.44962
C	-1.48446	3.18621	1.56211
C	-3.36110	1.42287	-0.58706
C	-1.76909	-1.85922	-0.48959
C	-1.90201	-1.52732	0.90395
C	-0.59671	-1.66062	1.50843
C	0.31223	-2.17589	0.52500
C	-0.38688	-2.21383	-0.72278
C	-2.83615	-1.93659	-1.52665
H	-2.53518	-1.40377	-2.44345
H	-3.78047	-1.49090	-1.17900
H	-3.04517	-2.98428	-1.80648
C	-3.14705	-1.23489	1.67176
H	-4.03230	-1.19630	1.01932
H	-3.08499	-0.27278	2.20850
H	-3.33502	-2.01843	2.42624
C	-0.31302	-1.47560	2.95942
H	0.75603	-1.29257	3.14544
H	-0.60512	-2.36829	3.54207
H	-0.87321	-0.61990	3.37010
C	1.64971	-2.77304	0.79464
H	2.29482	-2.77049	-0.09588
H	1.52582	-3.82731	1.10156
H	2.18865	-2.26337	1.60673
C	0.15789	-2.69012	-2.02295
H	-0.24682	-2.10385	-2.86120
H	-0.09499	-3.75257	-2.18848
H	1.25324	-2.59182	-2.06309
H	-3.40225	1.10101	-1.65230
H	-3.97752	0.68895	-0.03667
H	-1.25091	2.82191	2.57856
H	-2.55449	3.43685	1.52997
H	-0.89276	4.10474	1.41114
O	-3.95320	2.68017	-0.39926
H	-3.40250	3.32776	-0.85661
Sn	2.11624	0.58344	0.02894
C	2.33961	2.71078	-0.34638
H	2.05515	3.28808	0.54910
H	3.39369	2.92964	-0.58304
H	1.70652	3.00859	-1.19481
C	3.41732	-0.49545	-1.32436
H	4.23626	0.18096	-1.61699
H	3.85323	-1.39650	-0.86702
H	2.84802	-0.76209	-2.22765
C	2.84998	0.44694	2.09186
H	3.09775	-0.57119	2.42962
H	3.76006	1.06563	2.16585
H	2.09249	0.87231	2.77182

INT-5

Ru	-0.59600	-0.02682	-0.31158
Cl	0.46032	-0.49485	-2.44189
C	-1.37851	1.60061	-0.73592
C	-0.10347	2.10317	-0.40516
C	0.11128	3.03872	0.76263
H	0.54951	2.30091	-1.27453
C	-2.68583	2.22195	-1.02972
C	-0.89018	-2.28580	0.07461
C	-2.15409	-1.66804	-0.24856
C	-2.43301	-0.71195	0.77172
C	-1.30752	-0.67961	1.67439
C	-0.39174	-1.72186	1.28052
C	-0.28713	-3.39566	-0.71449
H	0.62765	-3.78363	-0.24253
H	-0.02389	-3.06237	-1.73293
H	-0.99885	-4.23344	-0.80775
C	-3.01325	-2.06492	-1.39796
H	-2.41077	-2.18515	-2.31251
H	-3.78455	-1.30907	-1.61125
H	-3.52771	-3.02472	-1.21074
C	-3.71163	0.01615	1.00725
H	-3.56536	1.08724	1.22173
H	-4.23195	-0.42368	1.87631
H	-4.39725	-0.06455	0.15034
C	-1.26346	0.08328	2.95336
H	-0.23077	0.31173	3.25886
H	-1.72952	-0.48984	3.77585
H	-1.80673	1.03821	2.87159
C	0.73452	-2.22793	2.11488
H	1.50064	-2.74317	1.51781
H	0.35613	-2.94994	2.86112
H	1.23319	-1.42141	2.67430
H	-3.49919	1.48261	-1.08289
H	-2.59250	2.64059	-2.05797
H	1.15460	3.02961	1.12001
H	-0.53067	2.76602	1.61723
H	-0.10802	4.09011	0.49130
O	-3.07048	3.19366	-0.08857
H	-2.36394	3.84662	-0.01735
Sn	2.09753	0.25566	0.05289
C	2.59316	0.85288	2.10629
H	3.18636	0.06229	2.59502
H	3.20714	1.76828	2.06897
H	1.70634	1.06233	2.72537
C	3.13356	-1.62398	-0.31659
H	2.45541	-2.37582	-0.74646
H	3.93176	-1.42738	-1.05022
H	3.59101	-2.01361	0.60736
C	3.12183	1.70425	-1.19202
H	4.20197	1.48579	-1.15730
H	2.77571	1.61188	-2.23260
H	2.96279	2.73659	-0.84159

TS5-*E*

Ru	-0.60077	0.08593	-0.11745
Cl	0.05867	0.44349	-2.43981
C	-0.90280	1.91484	-0.05177
C	-0.09005	1.83796	1.10297
C	-0.62229	1.98342	2.50659
H	0.89399	2.33813	0.99788
C	-1.40172	2.99374	-0.91423
C	-1.13725	-2.06380	-0.69820
C	-2.32078	-1.22451	-0.68016
C	-2.51300	-0.78631	0.66405
C	-1.42507	-1.30052	1.45823
C	-0.61605	-2.14480	0.61913
C	-0.65128	-2.80051	-1.89616
H	0.34163	-3.24496	-1.72974
H	-0.57034	-2.13043	-2.76665
H	-1.34860	-3.61598	-2.15641
C	-3.20365	-0.97474	-1.85235
H	-2.60880	-0.71471	-2.74293
H	-3.89897	-0.14178	-1.66395
H	-3.81051	-1.86390	-2.10122
C	-3.67563	0.00591	1.15950
H	-3.45051	0.52862	2.10116
H	-4.54297	-0.64984	1.35084
H	-3.99424	0.76584	0.42853
C	-1.27836	-1.23714	2.93956
H	-0.23533	-1.03871	3.23616
H	-1.56921	-2.20028	3.39594
H	-1.90752	-0.45776	3.39218
C	0.44400	-3.06249	1.12113
H	1.10492	-3.41420	0.31590
H	-0.01329	-3.95566	1.58440
H	1.07602	-2.59249	1.89095
H	-2.42354	2.74445	-1.25666
H	-0.78459	2.93110	-1.84269
H	-0.01022	1.42736	3.23638
H	-1.66023	1.62876	2.59303
H	-0.61318	3.04474	2.81512
O	-1.43169	4.26401	-0.33327
H	-0.52898	4.50658	-0.09729
Sn	2.08710	0.01102	0.05364
C	2.78418	-0.17124	2.11599
H	3.87865	-0.30024	2.13442
H	2.53633	0.75477	2.66110
H	2.33128	-1.02021	2.65267
C	2.95718	-1.57911	-1.14602
H	2.42515	-1.61627	-2.10912
H	4.01734	-1.34406	-1.33416
H	2.89992	-2.56177	-0.65300
C	2.93960	1.87870	-0.66460
H	3.83078	1.66053	-1.27417
H	2.20788	2.40037	-1.30196
H	3.23979	2.53251	0.17011

E-prod

Ru	0.95593	0.24537	-0.08594
Cl	0.51984	2.39776	0.92226
C	-0.93670	0.52583	-1.12128
C	-0.16010	-0.29550	-1.94430
C	-1.39874	1.90577	-1.53853
C	2.90774	-0.38375	-0.69546
C	2.12799	-1.57013	-0.45908
C	1.68080	-1.52304	0.90054
C	2.26030	-0.35620	1.53156
C	3.02070	0.34302	0.55052
C	3.62852	-0.01662	-1.94383
H	3.51795	1.05584	-2.17053
H	3.26578	-0.58258	-2.81379
H	4.70960	-0.21942	-1.84123
C	1.90131	-2.68855	-1.41309
H	1.89023	-2.34662	-2.45955
H	0.94613	-3.20349	-1.22205
H	2.70096	-3.44432	-1.32312
C	0.88810	-2.55782	1.61459
H	0.19107	-2.10325	2.33659
H	1.55582	-3.22926	2.18426
H	0.29720	-3.17745	0.92476
C	2.04825	0.02188	2.95494
H	0.98897	-0.08577	3.23928
H	2.32256	1.06915	3.14212
H	2.64450	-0.61907	3.62778
C	3.81014	1.58951	0.73090
H	3.69015	2.26267	-0.13239
H	4.88518	1.35943	0.83378
H	3.49028	2.15038	1.61987
H	-0.55602	2.53561	-1.89318
H	-2.07899	1.78400	-2.40678
Sn	-2.42017	-0.37013	0.22818
O	-2.13096	2.55191	-0.53641
H	-1.47826	2.79087	0.14721
C	-2.19427	0.20264	2.29690
H	-3.17817	0.38517	2.75517
H	-1.68657	-0.59699	2.86087
H	-1.58794	1.12016	2.35111
C	-2.26447	-2.53388	0.02877
H	-1.40128	-2.83148	-0.58979
H	-2.17019	-3.01472	1.01543
H	-3.17635	-2.91652	-0.45636
C	-4.36083	0.16787	-0.55644
H	-4.46570	1.26168	-0.52261
H	-4.44827	-0.17108	-1.60103
H	-5.16302	-0.30251	0.03330
C	0.39805	0.17985	-3.25737
H	1.17911	-0.49180	-3.64880
H	-0.39855	0.22034	-4.02414
H	0.82656	1.19308	-3.18547
H	-0.29539	-1.38408	-1.87135

TS2-5

Ru	-0.58549	0.04022	0.00302
Cl	0.09685	0.78637	-2.24661
C	-1.69407	1.72793	0.01023
C	-0.72869	2.36888	0.66784
H	0.31269	1.97282	0.50584
C	-0.81704	3.45491	1.69530
C	-3.10577	2.10687	-0.24786
C	-1.88541	-1.58627	-0.55002
C	-2.19862	-1.19823	0.79781
C	-1.02539	-1.42604	1.59908
C	-0.02581	-2.05265	0.77912
C	-0.52866	-2.09323	-0.55811
C	-2.79737	-1.64922	-1.72535
H	-2.28480	-1.29242	-2.63345
H	-3.69420	-1.03195	-1.57896
H	-3.11525	-2.69017	-1.91501
C	-3.52579	-0.76189	1.31484
H	-4.14016	-0.32056	0.51603
H	-3.42221	-0.01591	2.11960
H	-4.07963	-1.61905	1.73643
C	-0.91922	-1.18124	3.06450
H	0.12008	-0.97660	3.36548
H	-1.26679	-2.05301	3.64772
H	-1.52862	-0.31621	3.37047
C	1.19804	-2.72787	1.29427
H	1.60945	-2.22556	2.18162
H	1.99914	-2.79578	0.54283
H	0.94735	-3.76157	1.59350
C	0.12233	-2.70528	-1.74884
H	-0.39864	-3.63345	-2.04238
H	1.17623	-2.95593	-1.55916
H	0.09527	-2.01491	-2.60751
H	-3.71578	1.94925	0.66296
H	-3.15194	3.19744	-0.45719
H	-0.64866	3.05901	2.71271
H	-1.81234	3.92720	1.68792
H	-0.06235	4.24128	1.52921
O	-3.69590	1.36774	-1.28147
H	-3.01467	1.23333	-1.95572
Sn	2.18430	0.30755	-0.03982
C	3.22092	-0.98423	-1.43286
H	2.68759	-0.96994	-2.39455
H	4.23366	-0.57535	-1.58059
H	3.31253	-2.02048	-1.07192
C	3.02443	0.02893	1.96864
H	3.56673	-0.92453	2.06505
H	3.73323	0.85422	2.14747
H	2.24299	0.07650	2.74483
C	2.73069	2.36075	-0.48624
H	2.61915	2.98874	0.41317
H	3.78533	2.39091	-0.80532
H	2.09460	2.75238	-1.29312

TS3-4

Ru	-0.87337	0.17100	-0.29084
Cl	-0.48715	-0.40322	-2.57928
C	-0.21570	1.86664	-0.23135
C	1.25125	1.63067	-0.24533
C	1.84157	2.17735	-1.54483
C	-0.73713	3.25915	-0.18313
C	-2.64805	0.38175	0.87220
C	-1.69302	-0.33890	1.66537
C	-1.55877	-1.68103	1.10308
C	-2.30642	-1.74754	-0.06842
C	-2.91436	-0.43254	-0.29031
C	-3.34593	1.63990	1.25099
H	-3.70587	2.19238	0.36887
H	-2.69774	2.31761	1.83099
H	-4.22781	1.41955	1.87878
C	-1.16685	0.06493	3.00095
H	-1.10520	1.16134	3.09667
H	-0.15525	-0.33481	3.17390
H	-1.80916	-0.30242	3.82276
C	-0.76252	-2.76261	1.74241
H	-0.72525	-3.67250	1.12540
H	-1.19901	-3.03917	2.71872
H	0.27609	-2.45000	1.94137
C	-2.40817	-2.87839	-1.02771
H	-1.93386	-2.61257	-1.98953
H	-3.46240	-3.12825	-1.23635
H	-1.91493	-3.78596	-0.64888
C	-3.86963	-0.12730	-1.39034
H	-3.99494	0.95872	-1.51973
H	-4.86524	-0.56553	-1.19334
H	-3.50276	-0.52760	-2.34785
H	-0.56130	3.70590	-1.18132
H	-1.83458	3.26134	-0.04697
H	1.38688	1.67707	-2.41624
H	2.93290	2.05077	-1.60252
H	1.64075	3.26083	-1.62943
Sn	2.40511	-0.44317	0.14353
C	2.53653	-0.54173	2.30728
H	3.58305	-0.72538	2.59797
H	2.22239	0.42292	2.73816
H	1.91355	-1.33993	2.73916
C	4.37305	0.16285	-0.52128
H	4.44516	0.18348	-1.61908
H	4.63445	1.15659	-0.12470
H	5.10340	-0.56815	-0.13800
C	1.90666	-2.31066	-0.80766
H	1.64442	-2.10283	-1.85515
H	2.76851	-2.99417	-0.75320
H	1.03268	-2.76787	-0.32170
O	-0.07904	4.08123	0.75035
H	-0.21281	3.69802	1.62527
H	1.71553	2.11518	0.63986

INT-4

Ru	-1.17891	-0.12215	-0.06800
Cl	0.14935	-1.66262	-1.28569
C	0.37035	0.92354	0.57295
C	1.36798	0.38760	1.45117
H	1.93870	1.15413	2.01730
C	1.09647	-0.85433	2.27263
C	0.55775	2.36552	0.21678
C	-3.02388	0.70666	-0.78600
C	-2.80461	1.15150	0.56719
C	-2.72413	-0.02422	1.38373
C	-3.00060	-1.18446	0.53659
C	-3.22084	-0.72727	-0.78046
C	-3.20092	1.57838	-1.98001
H	-2.73530	1.13454	-2.87451
H	-2.76476	2.57754	-1.82994
H	-4.27423	1.71583	-2.20505
C	-2.73870	2.56876	1.02128
H	-2.17621	3.19483	0.30965
H	-2.24374	2.65321	2.00168
H	-3.74890	3.00215	1.12634
C	-2.55717	-0.06627	2.86224
H	-2.06121	-0.99518	3.18480
H	-3.53229	-0.01778	3.38008
H	-1.94679	0.77778	3.22216
C	-2.98527	-2.59256	1.01546
H	-2.91532	-3.30379	0.17955
H	-3.89289	-2.83458	1.59608
H	-2.11563	-2.77355	1.66908
C	-3.46425	-1.54688	-1.99878
H	-2.80301	-1.23805	-2.82467
H	-4.50653	-1.44867	-2.34963
H	-3.26743	-2.61352	-1.81722
H	0.13240	2.93214	1.07874
H	1.63290	2.64940	0.19943
H	0.37362	-0.64165	3.08006
H	2.01341	-1.23507	2.75362
H	0.67207	-1.66472	1.65439
Sn	2.98440	-0.10695	-0.12118
C	2.63761	0.67344	-2.09509
H	2.23723	-0.12678	-2.73270
H	1.90120	1.49114	-2.05330
H	3.58236	1.05825	-2.50894
C	3.48385	-2.19436	0.05031
H	4.38909	-2.40002	-0.54199
H	3.68604	-2.45549	1.10025
H	2.64966	-2.80063	-0.32958
C	4.57635	1.05113	0.79841
H	4.74044	0.71631	1.83536
H	5.51820	0.93208	0.23968
H	4.31604	2.12181	0.81306
O	-0.04485	2.76676	-0.97829
H	-0.54708	1.99325	-1.28997

TS4-5

Ru	-0.85836	0.12353	-0.09502
Cl	-0.94310	0.96873	-2.37327
C	-0.07378	1.72978	0.38820
C	1.37694	1.56721	0.66146
H	1.93132	2.40445	0.18249
C	1.67701	1.56083	2.16031
C	-0.61952	3.10495	0.26269
C	-2.34271	-0.24281	1.36943
C	-1.34661	-1.26371	1.51179
C	-1.40292	-2.10951	0.32166
C	-2.36752	-1.60140	-0.55413
C	-2.90561	-0.38374	0.04175
C	-2.75469	0.76887	2.38302
H	-3.02756	1.72014	1.90006
H	-1.93665	0.98301	3.08989
H	-3.62317	0.41975	2.96915
C	-0.57384	-1.59889	2.74081
H	-0.49949	-0.73635	3.42159
H	0.45130	-1.92750	2.50570
H	-1.05573	-2.41850	3.30532
C	-0.55281	-3.31586	0.13633
H	-0.62421	-3.72331	-0.88271
H	-0.85111	-4.11417	0.83895
H	0.50926	-3.09861	0.33671
C	-2.71529	-2.08635	-1.91741
H	-2.47301	-1.32411	-2.67917
H	-3.79298	-2.30881	-1.99943
H	-2.16485	-3.00283	-2.17778
C	-4.01044	0.42988	-0.53175
H	-3.99318	1.45766	-0.13853
H	-4.99204	-0.01431	-0.28577
H	-3.93084	0.48725	-1.62791
H	-0.52713	3.61276	1.24594
H	0.07614	3.65992	-0.41380
H	1.30989	2.48130	2.65007
H	2.76052	1.49806	2.36190
H	1.19060	0.70748	2.66174
Sn	2.49806	-0.16929	-0.23501
C	1.83846	-1.16188	-2.03389
H	2.69036	-1.72188	-2.45182
H	1.00918	-1.85388	-1.82220
H	1.47887	-0.41814	-2.75958
C	2.96338	-1.60187	1.32698
H	2.34035	-2.50713	1.26072
H	4.01676	-1.90406	1.21498
H	2.83919	-1.16026	2.32806
C	4.35124	0.87177	-0.65650
H	4.69120	1.41524	0.24013
H	5.14032	0.16368	-0.95416
H	4.20828	1.59809	-1.47173
O	-1.93903	3.19060	-0.15799
H	-1.98953	2.65728	-0.97250

INT1′

Ru	-0.68819	0.26107	-0.37491
Cl	-0.07653	-1.19446	-2.23266
C	0.04217	1.65693	-1.38773
C	-0.20568	2.33060	-0.17650
C	0.87967	2.98072	0.65279
C	0.74282	1.95642	-2.64150
C	-2.77759	0.57619	0.36624
C	-1.88527	0.49676	1.50048
C	-1.38416	-0.84549	1.59139
C	-1.86510	-1.55740	0.46648
C	-2.73035	-0.67909	-0.30015
C	-3.63238	1.74301	0.02009
H	-4.06558	1.64285	-0.98587
H	-3.07679	2.69597	0.04707
H	-4.46645	1.84723	0.73592
C	-1.73149	1.52004	2.57055
H	-1.97083	2.53405	2.21639
H	-0.70579	1.53700	2.97462
H	-2.40711	1.29860	3.41648
C	-0.61858	-1.37943	2.75169
H	-0.13390	-2.33946	2.52356
H	-1.29522	-1.54721	3.60901
H	0.16407	-0.68304	3.09173
C	-1.64961	-2.99344	0.14813
H	-0.87340	-3.44522	0.78300
H	-1.33466	-3.11734	-0.90081
H	-2.58324	-3.56482	0.29180
C	-3.48921	-1.10417	-1.50663
H	-3.95769	-0.24942	-2.01651
H	-4.28780	-1.81933	-1.24120
H	-2.82078	-1.59733	-2.23102
H	0.16821	2.72248	-3.19342
H	1.72503	2.40868	-2.41509
H	0.72770	2.76132	1.72977
Sn	1.83357	-0.55508	0.19007
C	1.95910	-2.71361	0.44058
H	3.02295	-2.99775	0.37976
H	1.56583	-3.05755	1.41051
H	1.41549	-3.20998	-0.37731
C	2.56337	0.23199	2.12533
H	1.88371	0.96979	2.58924
H	2.67424	-0.60533	2.83427
H	3.56440	0.68675	2.01270
C	3.37867	-0.11818	-1.25957
H	3.05941	-0.47347	-2.25089
H	3.58506	0.96129	-1.30386
H	4.29711	-0.65460	-0.96897
H	-1.15364	2.89561	-0.10217
H	0.86619	1.07331	-3.28264
O	2.16967	2.62989	0.23651
H	2.62365	2.16933	0.95105
H	0.75651	4.08042	0.55827

TS1-2′

Ru	-0.60333	-0.04459	-0.08052
Cl	0.22251	0.06323	-2.40334
C	-1.58553	1.74344	-0.73446
C	-0.77647	2.14675	0.15630
C	-0.23621	3.28376	0.93190
C	-2.58129	1.98860	-1.77788
C	-2.16546	-1.57311	-0.42703
C	-2.54391	-0.80168	0.71917
C	-1.52134	-0.94389	1.71541
C	-0.54089	-1.87046	1.21724
C	-0.91340	-2.22862	-0.11799
C	-2.91306	-1.75945	-1.70181
H	-2.26894	-1.53254	-2.56813
H	-3.79327	-1.10183	-1.76166
H	-3.26746	-2.79943	-1.81101
C	-3.78865	-0.00473	0.90676
H	-4.40402	0.01548	-0.00478
H	-3.56911	1.03957	1.18636
H	-4.40667	-0.43610	1.71270
C	-1.55713	-0.34177	3.07855
H	-0.54297	-0.20373	3.48604
H	-2.11613	-0.97574	3.79020
H	-2.04542	0.64589	3.06569
C	0.56875	-2.45789	2.01969
H	1.39601	-2.81765	1.38869
H	0.20122	-3.32236	2.60079
H	0.98760	-1.73592	2.73710
C	-0.23663	-3.20095	-1.01938
H	-0.15147	-2.79194	-2.03897
H	-0.80547	-4.14576	-1.07679
H	0.78077	-3.44006	-0.67626
H	-2.75294	3.07000	-1.90471
H	0.83417	3.41890	0.65663
Sn	2.14077	0.06078	-0.01273
H	0.27143	1.13341	0.69977
C	3.04242	-1.67255	-0.94687
H	4.10598	-1.45495	-1.13622
H	2.97922	-2.56129	-0.29854
H	2.53807	-1.87036	-1.90365
C	2.90375	0.14004	2.04525
H	3.78826	0.79820	2.07110
H	2.14697	0.55835	2.73139
H	3.20419	-0.85206	2.41849
C	2.87754	1.88600	-0.91900
H	3.12990	2.62420	-0.13962
H	3.78532	1.67555	-1.50612
H	2.11162	2.29608	-1.59432
H	-3.54722	1.51108	-1.54339
H	-0.23838	3.01545	2.01434
H	-2.22365	1.56806	-2.73269
O	-1.00580	4.41621	0.66101
H	-0.55083	5.18898	1.01036

INT2′

Ru	-0.68819	0.26107	-0.37491
Cl	-0.07653	-1.19446	-2.23266
C	0.04217	1.65693	-1.38773
C	-0.20568	2.33060	-0.17650
C	0.87967	2.98072	0.65279
C	0.74282	1.95642	-2.64150
C	-2.77759	0.57619	0.36624
C	-1.88527	0.49676	1.50048
C	-1.38416	-0.84549	1.59139
C	-1.86510	-1.55740	0.46648
C	-2.73035	-0.67909	-0.30015
C	-3.63238	1.74301	0.02009
H	-4.06558	1.64285	-0.98587
H	-3.07679	2.69597	0.04707
H	-4.46645	1.84723	0.73592
C	-1.73149	1.52004	2.57055
H	-1.97083	2.53405	2.21639
H	-0.70579	1.53700	2.97462
H	-2.40711	1.29860	3.41648
C	-0.61858	-1.37943	2.75169
H	-0.13390	-2.33946	2.52356
H	-1.29522	-1.54721	3.60901
H	0.16407	-0.68304	3.09173
C	-1.64961	-2.99344	0.14813
H	-0.87340	-3.44522	0.78300
H	-1.33466	-3.11734	-0.90081
H	-2.58324	-3.56482	0.29180
C	-3.48921	-1.10417	-1.50663
H	-3.95769	-0.24942	-2.01651
H	-4.28780	-1.81933	-1.24120
H	-2.82078	-1.59733	-2.23102
H	0.16821	2.72248	-3.19342
H	1.72503	2.40868	-2.41509
H	0.72770	2.76132	1.72977
Sn	1.83357	-0.55508	0.19007
C	1.95910	-2.71361	0.44058
H	3.02295	-2.99775	0.37976
H	1.56583	-3.05755	1.41051
H	1.41549	-3.20998	-0.37731
C	2.56337	0.23199	2.12533
H	1.88371	0.96979	2.58924
H	2.67424	-0.60533	2.83427
H	3.56440	0.68675	2.01270
C	3.37867	-0.11818	-1.25957
H	3.05941	-0.47347	-2.25089
H	3.58506	0.96129	-1.30386
H	4.29711	-0.65460	-0.96897
H	-1.15364	2.89561	-0.10217
H	0.86619	1.07331	-3.28264
O	2.16967	2.62989	0.23651
H	2.62365	2.16933	0.95105
H	0.75651	4.08042	0.55827

TS2-*Z′*

Ru	-0.71599	0.10183	-0.38764
Cl	-0.26943	-1.84790	-1.79952
C	0.68622	0.88881	-1.43561
C	0.07982	2.03000	-0.86506
H	-0.51374	2.62584	-1.58645
C	0.78437	2.88113	0.15642
C	1.36407	0.73445	-2.74073
C	-2.83792	-0.44631	-0.31448
C	-2.68062	0.93073	0.02936
C	-1.91324	0.98963	1.25330
C	-1.66792	-0.35644	1.68719
C	-2.21395	-1.24042	0.72673
C	-3.59812	-1.00368	-1.46438
H	-3.78556	-0.23973	-2.23365
H	-4.57600	-1.39690	-1.13359
H	-3.04161	-1.82596	-1.94054
C	-3.25157	2.08827	-0.70969
H	-3.22228	1.92153	-1.79835
H	-2.69489	3.01573	-0.50527
H	-4.30463	2.26159	-0.42693
C	-1.67082	2.18936	2.10041
H	-0.69751	2.14022	2.61453
H	-2.44530	2.26656	2.88510
H	-1.69694	3.12256	1.51944
C	-1.01359	-0.70510	2.97730
H	-0.81461	-1.78267	3.06340
H	-1.66377	-0.41850	3.82287
H	-0.05731	-0.17360	3.11459
C	-2.21824	-2.72648	0.77141
H	-1.85725	-3.14581	-0.18208
H	-3.23838	-3.10878	0.94960
H	-1.56550	-3.11336	1.56849
H	2.32408	1.27937	-2.74186
H	0.72587	1.21991	-3.50266
H	0.89736	2.34288	1.11701
H	0.18209	3.79012	0.36651
Sn	1.93023	-0.53751	0.31763
C	1.57870	-2.49286	1.19180
H	1.11693	-2.40882	2.18709
H	0.92450	-3.06691	0.51924
H	2.54745	-3.00898	1.29209
C	2.68931	0.72674	1.92325
H	3.53959	0.20809	2.39584
H	3.04435	1.67994	1.50306
H	1.93531	0.93065	2.70132
C	3.60912	-0.81304	-1.01493
H	3.99645	0.15223	-1.37482
H	4.40322	-1.32664	-0.44878
H	3.32772	-1.43882	-1.87486
H	1.51827	-0.31044	-3.03896
O	2.05120	3.22130	-0.36954
H	2.50112	3.79895	0.25758

Z-prod′

Ru	-0.99988	-0.14206	-0.19098
Cl	-0.07483	-2.36320	-0.32931
C	0.90795	0.40362	-1.11110
C	0.20114	1.58324	-0.84133
H	-0.30944	2.07319	-1.69130
C	0.60408	2.55577	0.22799
C	0.95844	-0.12004	-2.52918
C	-2.99451	0.28455	-0.78737
C	-2.61741	1.31707	0.13481
C	-2.23773	0.67964	1.36178
C	-2.50020	-0.74280	1.23409
C	-2.98730	-0.98061	-0.08391
C	-3.42643	0.49731	-2.19364
H	-3.19230	-0.37829	-2.81871
H	-2.92270	1.36970	-2.63895
H	-4.51593	0.67178	-2.25821
C	-2.74805	2.77667	-0.13378
H	-2.22179	3.09345	-1.04831
H	-2.37387	3.38917	0.69917
H	-3.81301	3.03358	-0.27002
C	-1.79813	1.33865	2.62064
H	-1.01142	0.75315	3.12219
H	-2.63988	1.43029	3.33035
H	-1.39982	2.34861	2.44328
C	-2.28008	-1.74093	2.31420
H	-1.33181	-1.54601	2.84084
H	-2.21808	-2.76231	1.91400
H	-3.09345	-1.70722	3.06022
C	-3.39520	-2.28023	-0.67966
H	-4.49520	-2.37210	-0.69625
H	-2.98282	-3.13214	-0.12219
H	-3.03066	-2.37258	-1.71469
H	0.07780	0.19819	-3.11897
H	1.85383	0.27783	-3.04396
H	-0.27830	3.08067	0.64363
H	1.07515	2.00994	1.07576
Sn	2.57480	-0.28948	0.14796
C	3.50375	-1.96748	-0.83744
H	3.77766	-1.69208	-1.86827
H	4.41855	-2.26496	-0.30186
H	2.80002	-2.81159	-0.86577
C	1.98398	-0.75009	2.17910
H	1.50914	0.12421	2.65362
H	1.27072	-1.58801	2.16194
H	2.86659	-1.03009	2.77564
C	4.02716	1.32619	0.24007
H	4.80301	1.18593	-0.52867
H	3.51771	2.28377	0.05372
H	4.51477	1.35069	1.22768
H	1.01278	-1.21879	-2.56646
O	1.48996	3.48454	-0.35552
H	1.73101	4.14157	0.30660

TS2-3′

Ru	-0.66341	0.25760	-0.07996
Cl	0.06040	0.63830	-2.37917
C	-0.90451	2.08492	0.14733
C	-0.01183	1.89927	1.21960
H	-0.40508	1.67634	2.22679
C	1.25443	2.73453	1.25325
C	-1.51084	3.19600	-0.58344
C	-2.72997	-0.19048	0.67766
C	-1.76948	-0.87043	1.51012
C	-1.12932	-1.88640	0.71917
C	-1.59331	-1.73904	-0.61893
C	-2.60326	-0.69637	-0.64918
C	-3.70629	0.83037	1.15559
H	-4.06854	1.46717	0.33415
H	-3.27104	1.49208	1.92222
H	-4.58849	0.34665	1.60970
C	-1.62654	-0.72552	2.98580
H	-1.93506	0.27208	3.33639
H	-0.58519	-0.88480	3.30880
H	-2.25299	-1.46188	3.52060
C	-0.28176	-2.97556	1.27968
H	0.25357	-3.52841	0.49504
H	-0.91309	-3.70242	1.82181
H	0.46573	-2.60169	1.99744
C	-1.22724	-2.57001	-1.79935
H	-0.93378	-1.93363	-2.65069
H	-2.08044	-3.19297	-2.11963
H	-0.38148	-3.23915	-1.58297
C	-3.39065	-0.32245	-1.85589
H	-4.00696	0.57234	-1.67965
H	-4.07091	-1.13699	-2.16199
H	-2.72398	-0.10476	-2.70714
H	-0.66785	3.81712	-0.94285
H	-2.10487	2.86620	-1.44885
H	2.09313	2.14899	1.69199
Sn	1.94730	-0.47181	0.03040
C	2.35631	-2.25323	-1.15274
H	1.89498	-2.13761	-2.14600
H	3.44852	-2.33215	-1.28120
H	1.99493	-3.18248	-0.68590
C	2.59076	-0.85690	2.09114
H	2.82490	-1.92238	2.24782
H	3.49941	-0.27066	2.30565
H	1.80986	-0.55470	2.80927
C	3.43390	0.89394	-0.79114
H	3.65871	1.76671	-0.15908
H	4.35918	0.30423	-0.90270
H	3.12572	1.23121	-1.79409
H	-2.10930	3.84158	0.08335
O	1.58635	3.28941	0.01585
H	1.77952	2.57288	-0.60672
H	1.09610	3.58495	1.94410

INT3′

Ru	-0.65379	0.28239	-0.08748
Cl	0.26913	0.66606	-2.31226
C	-0.94429	2.01136	0.50358
C	0.33007	1.84965	1.08464
C	1.39818	2.84628	0.66064
C	-1.89168	3.12134	0.37382
C	-2.79406	-0.24896	0.48279
C	-1.84268	-0.87938	1.37238
C	-1.14067	-1.89110	0.62561
C	-1.52437	-1.74862	-0.73432
C	-2.56013	-0.73528	-0.82538
C	-3.88839	0.65824	0.92176
H	-4.27329	1.28097	0.10039
H	-3.57553	1.32772	1.73796
H	-4.73725	0.06330	1.30219
C	-1.79761	-0.72518	2.85382
H	-2.03958	0.30405	3.16534
H	-0.79674	-0.96007	3.24988
H	-2.51578	-1.39852	3.35636
C	-0.33833	-2.98072	1.25003
H	0.10931	-3.64466	0.49805
H	-0.99382	-3.60043	1.88768
H	0.47325	-2.60992	1.89764
C	-1.06662	-2.55952	-1.89645
H	-0.26543	-3.26000	-1.61955
H	-0.67670	-1.91315	-2.70078
H	-1.90279	-3.14557	-2.31558
C	-3.26477	-0.36575	-2.08264
H	-3.84833	0.56037	-1.96510
H	-3.95854	-1.16068	-2.40968
H	-2.54212	-0.19643	-2.89751
H	-1.32127	3.92011	-0.13938
H	-2.77724	2.88879	-0.23549
H	2.41462	2.44510	0.86344
Sn	1.96105	-0.44642	0.15422
C	2.36916	-2.32731	-0.86942
H	3.46691	-2.42007	-0.92369
H	1.96769	-3.22401	-0.37607
H	1.97830	-2.26181	-1.89728
C	2.48953	-0.66217	2.26404
H	2.99346	0.25777	2.60390
H	1.60308	-0.82029	2.89978
H	3.17986	-1.50924	2.40638
C	3.50023	0.78600	-0.76139
H	3.15025	1.77350	-1.09273
H	4.33291	0.91959	-0.05071
H	3.87019	0.23699	-1.64195
H	0.38978	1.61039	2.16377
H	-2.19764	3.53635	1.35112
O	1.25273	3.30036	-0.64835
H	1.10875	2.54225	-1.24430
H	1.29938	3.73408	1.31827

TS3-4′

Ru	-0.96387	0.29574	-0.00801
Cl	-0.84607	1.84072	-1.83067
C	0.07986	1.26320	1.20444
C	1.53388	1.25922	0.85011
C	1.90387	2.41450	-0.12219
C	-0.25947	2.05813	2.40662
C	-2.53655	-0.42555	1.22894
C	-1.66897	-1.53460	0.97621
C	-1.77498	-1.87477	-0.43562
C	-2.64372	-0.97151	-1.06008
C	-3.05268	0.00084	-0.05665
C	-2.98340	0.06470	2.55976
H	-3.29727	1.11971	2.52505
H	-2.19397	-0.02841	3.32198
H	-3.85167	-0.52061	2.91281
C	-1.02392	-2.38248	2.01843
H	-0.64414	-1.77679	2.85764
H	-0.17425	-2.95390	1.61697
H	-1.74042	-3.11317	2.43710
C	-1.05275	-3.01617	-1.05817
H	-1.10093	-2.99303	-2.15656
H	-1.48225	-3.97602	-0.72078
H	0.01212	-3.02435	-0.77136
C	-2.99236	-0.88641	-2.50454
H	-2.64935	0.06931	-2.93899
H	-4.08357	-0.94854	-2.65683
H	-2.52971	-1.69866	-3.08492
C	-4.02537	1.10404	-0.28134
H	-3.87024	1.92124	0.44026
H	-5.06480	0.74441	-0.17131
H	-3.91565	1.53204	-1.28853
H	0.32024	1.71755	3.28760
H	0.07915	3.09158	2.19980
H	1.85238	2.06479	-1.17340
H	2.95798	2.68477	0.07201
Sn	2.44618	-0.54179	-0.07229
C	1.71126	-0.98467	-2.05750
H	0.61110	-0.96026	-2.09829
H	2.09515	-0.22146	-2.75254
H	2.07286	-1.97466	-2.37863
C	2.43964	-2.23615	1.27464
H	1.93444	-3.10579	0.82576
H	3.48177	-2.51569	1.49434
H	1.93697	-1.98307	2.22037
C	4.50738	0.09131	-0.28904
H	4.60316	0.81506	-1.11374
H	4.86661	0.56680	0.63775
H	5.15302	-0.77355	-0.50869
H	2.12530	1.37624	1.78495
H	-1.32986	2.07799	2.65226
O	1.12602	3.56195	0.02622
H	0.33160	3.41383	-0.51789

INT4′

Ru	-1.26174	-0.06186	-0.23221
Cl	0.01562	-2.01399	-0.69157
C	0.30273	1.10969	-0.36522
C	1.35243	1.28774	0.59804
H	1.89898	2.24852	0.48362
C	1.11650	0.97732	2.06772
C	0.45628	1.90559	-1.62816
C	-3.16758	0.63345	-0.90011
C	-2.80881	1.37191	0.27755
C	-2.63083	0.41727	1.33497
C	-2.99961	-0.89965	0.82553
C	-3.34605	-0.76407	-0.53605
C	-3.43016	1.18948	-2.25464
H	-3.07103	0.50450	-3.03935
H	-2.93011	2.15839	-2.40487
H	-4.51173	1.34286	-2.42168
C	-2.64562	2.84857	0.39091
H	-2.40125	3.30677	-0.58049
H	-1.83564	3.11339	1.09005
H	-3.57005	3.33188	0.75320
C	-2.32639	0.70870	2.76341
H	-1.52578	0.05869	3.15236
H	-3.22169	0.55234	3.39163
H	-2.00284	1.75153	2.90364
C	-2.95845	-2.14643	1.63656
H	-2.90339	-3.04291	1.00181
H	-3.85161	-2.23830	2.27964
H	-2.07488	-2.16156	2.29531
C	-3.71703	-1.84599	-1.48870
H	-3.19379	-1.72508	-2.45140
H	-4.80140	-1.85377	-1.69754
H	-3.44026	-2.83685	-1.09960
H	-0.23605	2.76615	-1.56463
H	1.47239	2.32269	-1.77629
H	0.32567	1.66611	2.44404
Sn	3.01941	-0.09437	-0.16814
C	2.89086	-0.46309	-2.28525
H	1.93609	-0.96376	-2.50355
H	2.97009	0.47379	-2.85733
H	3.71919	-1.12590	-2.58017
C	3.26399	-1.83688	1.05991
H	4.24654	-2.29266	0.86133
H	3.18731	-1.54974	2.11794
H	2.45944	-2.54775	0.82514
C	4.64670	1.29301	0.20701
H	4.62010	1.62960	1.25614
H	5.62428	0.82275	0.01796
H	4.55026	2.17525	-0.44644
H	0.16351	1.34299	-2.53100
H	2.03143	1.22903	2.63777
O	0.80837	-0.35194	2.36390
H	0.18557	-0.68493	1.69174

INT0-Si

Ru	0.61505	0.20573	-0.07142
Cl	1.91324	2.14495	-0.76024
C	-0.90771	1.57129	-0.02611
C	-1.44817	0.40112	-0.09522
Si	-3.21034	-0.22735	-0.10353
C	-1.02205	3.05122	-0.04639
C	2.54876	-0.75339	0.41173
C	2.08119	-1.17606	-0.87182
C	0.81167	-1.84906	-0.68023
C	0.49820	-1.81186	0.71839
C	1.54792	-1.07877	1.38298
C	3.82542	-0.05208	0.71174
H	3.66188	0.82691	1.35436
H	4.31703	0.30689	-0.20246
H	4.52011	-0.73335	1.23336
C	2.79113	-1.00864	-2.16747
H	3.27443	-0.02139	-2.22399
H	2.09236	-1.07842	-3.01464
H	3.56618	-1.78288	-2.30550
C	0.04913	-2.52919	-1.76025
H	-0.95541	-2.82388	-1.42766
H	0.57465	-3.43994	-2.09714
H	-0.07140	-1.87244	-2.63688
C	-0.63571	-2.47454	1.41580
H	-1.02976	-1.84389	2.22822
H	-0.31038	-3.42867	1.86653
H	-1.46743	-2.69946	0.73210
C	1.62626	-0.79985	2.84067
H	2.22724	0.09928	3.04137
H	2.09264	-1.64373	3.38059
H	0.62752	-0.63541	3.27262
H	-2.06324	3.31567	0.21736
O	-0.18112	3.70676	0.84075
C	-3.48499	-1.75420	-1.16425
C	-4.22290	1.17826	-0.83117
C	-3.78306	-0.54591	1.65679
H	-0.87458	3.37794	-1.09928
H	-3.56811	0.32653	2.29589
H	-3.30186	-1.42701	2.10945
H	-4.87343	-0.71490	1.67132
H	-4.17117	2.07354	-0.18906
H	-5.28447	0.89318	-0.92722
H	-3.85409	1.46017	-1.83154
H	-3.05640	-2.67469	-0.73523
H	-3.06899	-1.62013	-2.17674
H	-4.57076	-1.92124	-1.27127
H	0.72332	3.48375	0.55433

INT0′-Si

Ru	0.38449	-0.14631	-0.04375
Cl	-0.70155	-2.19899	-0.74046
C	-1.56812	0.53478	0.06082
C	-0.76779	1.54342	0.02046
C	-0.68789	3.02157	0.04508
Si	-3.31225	-0.14558	0.07954
C	2.12587	-1.38612	0.47945
C	1.95594	-0.31029	1.41454
C	2.13114	0.93275	0.70693
C	2.31279	0.61812	-0.68042
C	2.30325	-0.82153	-0.82148
C	2.08947	-2.83253	0.81988
H	1.80439	-3.44435	-0.04671
H	1.35340	-3.04076	1.61137
H	3.07929	-3.16704	1.17723
C	1.74331	-0.45627	2.87839
H	1.18131	-1.37337	3.10931
H	1.17815	0.39340	3.29002
H	2.70805	-0.50980	3.41444
C	2.22617	2.27248	1.34844
H	1.97932	3.08136	0.64604
H	3.25019	2.44346	1.72488
H	1.54811	2.35178	2.21330
C	2.59810	1.57057	-1.78709
H	1.99328	1.33598	-2.67851
H	3.65835	1.50487	-2.08884
H	2.38758	2.60724	-1.49262
C	2.49332	-1.57731	-2.08790
H	1.80178	-2.43258	-2.13760
H	3.52564	-1.95835	-2.17778
H	2.29239	-0.94307	-2.96437
C	-4.39168	1.32266	0.56790
C	-3.46964	-1.48688	1.37407
H	-0.41318	3.35298	1.06256
O	0.25124	3.58288	-0.83269
H	0.10266	3.19988	-1.70575
H	-1.70477	3.42540	-0.14170
H	-4.51309	-1.83692	1.44892
H	-3.16547	-1.10962	2.36466
H	-2.82395	-2.33939	1.11396
H	-5.45073	1.02335	0.65111
H	-4.33125	2.12945	-0.18247
H	-4.08469	1.74108	1.54149
C	-3.80477	-0.72855	-1.63003
H	-4.85577	-1.06446	-1.63306
H	-3.70675	0.08655	-2.36605
H	-3.16086	-1.56275	-1.94727

[Cp*Ru(Cl)(*E*-2-butene)]

Ru	-0.255113	-0.187359	0.260486
Cl	-0.419223	-2.404209	1.063219
C	-2.463385	-0.420553	0.105735
C	-2.088460	0.565411	-0.787561
H	-2.636222	-1.422261	-0.282253
H	-2.234948	1.602806	-0.488507
C	-2.032202	0.304730	-2.261505
C	-3.059281	-0.132862	1.448894
C	1.898016	-0.187418	0.155213
C	1.476766	0.366598	1.388859
C	0.668213	1.532378	1.104745
C	0.658697	1.731482	-0.306701
C	1.351932	0.633766	-0.899717
C	2.741544	-1.387577	-0.062950
H	2.361942	-1.984300	-0.894758
H	2.753608	-2.034232	0.813506
H	3.772731	-1.102535	-0.295240
C	1.761221	-0.149257	2.750688
H	2.087682	-1.187985	2.724994
H	0.868356	-0.109574	3.378008
H	2.540505	0.446935	3.235921
C	0.058558	2.420454	2.124546
H	-0.824839	2.929294	1.734263
H	0.766203	3.188386	2.455460
H	-0.248052	1.853732	3.005462
C	0.105082	2.913055	-1.014621
H	-0.266766	2.665708	-2.009856
H	0.881064	3.674782	-1.138166
H	-0.713097	3.374374	-0.459695
C	1.611927	0.415938	-2.344643
H	1.423525	-0.622354	-2.626281
H	2.657661	0.635164	-2.584411
H	0.987330	1.051366	-2.972563
H	-2.735367	-0.861550	2.194041
H	-4.153276	-0.179293	1.398439
H	-2.785749	0.866141	1.799617
H	-1.763494	-0.735227	-2.463819
H	-1.313630	0.942743	-2.779208
H	-3.010538	0.488746	-2.719662

[Cp*Ru(Cl)($CH_3C{\equiv}CCH_3$)]

Ru	0.27020	0.25837	0.00007
Cl	-0.13770	2.62420	0.00023
C	2.22563	0.89802	0.00012
C	2.20967	-0.37199	0.00014
C	2.99272	-1.61515	0.00024
C	2.93518	2.17773	0.00013
C	-1.97504	0.07307	0.00031
C	-1.39486	-0.52297	1.15030
C	-0.53780	-1.59913	0.71300
C	-0.53795	-1.59853	-0.71410
C	-1.39512	-0.52201	-1.15032
C	-2.97366	1.16780	0.00096
H	-2.87240	1.80747	-0.87499
H	-2.87149	1.80722	0.87700
H	-3.98251	0.74243	0.00143
C	-1.68625	-0.17394	2.56194
H	-1.87359	0.89504	2.67003
H	-0.84761	-0.42972	3.21101
H	-2.56815	-0.71100	2.92738
C	0.09987	-2.58051	1.62665
H	0.78732	-3.24139	1.09854
H	-0.65866	-3.20784	2.10503
H	0.65994	-2.08010	2.42021
C	0.09953	-2.57910	-1.62874
H	0.66005	-2.07800	-2.42155
H	-0.65916	-3.20551	-2.10808
H	0.78650	-3.24095	-1.10122
C	-1.68679	-0.17186	-2.56163
H	-1.87406	0.89722	-2.66886
H	-2.56879	-0.70858	-2.92731
H	-0.84829	-0.42719	-3.21105
H	2.76885	-2.22470	0.87884
H	4.06517	-1.40561	-0.00075
H	2.76741	-2.22593	-0.87712
H	2.65668	2.77327	0.87111
H	2.65663	2.77331	-0.87081
H	4.01744	2.02257	0.00009

Cp*RuCl

Ru	-0.67207	-0.00194	-0.00040
Cl	-2.91564	-0.00762	-0.00104
C	1.05600	1.22070	-0.03164
C	1.05913	0.34874	-1.16738
C	1.06296	-1.00075	-0.68910
C	1.06209	-0.96302	0.74208
C	1.05774	0.40984	1.14850
C	1.04345	2.70307	-0.07082
H	0.53020	3.11777	0.79774
H	0.53178	3.07120	-0.96104
H	2.06205	3.10503	-0.08054
C	1.05109	0.76924	-2.58946
H	0.54200	1.72543	-2.71700
H	0.53811	0.03800	-3.21556
H	2.07100	0.88008	-2.97250
C	1.06058	-2.22358	-1.52806
H	0.54382	-3.04464	-1.02944
H	2.08206	-2.55392	-1.74411
H	0.55863	-2.04976	-2.48072
C	1.05867	-2.13997	1.64434
H	0.55554	-1.91607	2.58585
H	2.07989	-2.45832	1.87881
H	0.54259	-2.98634	1.18912
C	1.04807	0.90499	2.54632
H	0.53905	1.86669	2.62225
H	2.06755	1.03580	2.92421
H	0.53410	0.20819	3.20974

$CH_3C{\equiv}CCH_3$

C	-0.59954	-0.00003	0.00002
C	0.59954	-0.00003	0.00001
C	2.04832	0.00002	-0.00001
C	-2.04832	0.00002	-0.00001
H	2.44542	-0.23512	-0.99010
H	2.44547	-0.73985	0.69867
H	2.44540	0.97505	0.29139
H	-2.44542	-0.23401	-0.99037
H	-2.44540	0.97472	0.29248
H	-2.44548	-0.74063	0.69784

E-2-butene

C	0.53316	-0.39284	-0.00006
C	-0.53315	0.39278	-0.00008
H	0.37909	-1.47203	-0.00008
H	-0.37906	1.47198	-0.00006
C	-1.94286	-0.07785	0.00005
C	1.94285	0.07788	0.00005
H	2.48705	-0.28645	-0.87621
H	2.48699	-0.28661	0.87627
H	1.99584	1.16854	0.00012
H	-1.99596	-1.16850	-0.00036
H	-2.48716	0.28691	-0.87596
H	-2.48681	0.28629	0.87653

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