SUPPORTING INFORMATION for

Cyclotrimerization Reactions Catalyzed by Rh(I) Half-Sandwich Complexes: a Mechanistic Density Functional Study

Laura Orian*[†], Joost N. P. van Stralen[‡], and F. Matthias Bickelhaupt*[‡]

[†]*Dip. Scienze Chimiche Università degli Studi di Padova, Via Marzolo 1, 35129 Padova, Italy, Fax: +39 – 0498275239, Email: laura.orian@unipd.it*

[‡]*Afdeling Theoretische Chemie, Scheikundig Laboratorium der Vrije Universiteit, De Boelelaan 1083, NL-1081 HV Amsterdam, The Netherlands, Fax: +31 - 20 - 59 87 629, Email: fm.bickelhaupt@few.vu.nl*

Cartesian coordinates (in Å) of equilibrium stuctures and transition states occurring in the acetylene cyclotrimerization catalyzed by CpRh fragment. The indicated energies E are relative to ADF's basic atoms.

A1 E = -4.020146 a.u.

C	1.82787	0.32288	-1.05741
C	1.30763	1.57219	-0.64486
C	1.17950	1.55266	0.79129
C	1.65390	0.29711	1.26948
C	2.00286	-0.48877	0.12055
Rh	-0.23928	-0.09918	-0.01001
C	-2.11756	0.60702	0.74103
C	-2.13371	0.78371	-0.50709
H	2.04613	0.02316	-2.07525
H	1.05148	2.40451	-1.28998
H	0.82538	2.37609	1.40101
H	1.72963	-0.01002	2.30493
H	2.40295	-1.49623	0.13737
H	-2.59661	1.10518	-1.42595
H	-2.55748	0.66800	1.72355
C	-1.02572	-1.86400	-0.93925
C	-0.99152	-2.07489	0.30418
H	-1.14528	-2.69395	1.17384
H	-1.23703	-2.15612	-1.95532

TS(A1,A2) E = -4.000254 a.u.

C	0.86659	-1.11367	1.91836
C	1.47590	0.17300	1.99905
C	0.45239	1.15647	1.84621
C	-0.80577	0.48296	1.68647
C	-0.53527	-0.92607	1.71629
Rh	0.42570	0.00917	-0.16728
C	1.61428	0.67905	-1.86126
C	0.75142	1.56049	-1.47384
C	0.82263	-1.14230	-1.97010
C	-0.42599	-1.14922	-1.63493
H	-1.78046	0.95005	1.61387
H	-1.27541	-1.71239	1.63124
H	1.37643	-2.06695	1.99072
H	2.53155	0.37120	2.14149
H	0.59415	2.23011	1.87423
H	-1.39665	-1.58050	-1.83452
H	2.61944	0.56185	-2.24767
H	1.61174	-1.75676	-2.38613
H	0.41142	2.58025	-1.58634

A2 E = -4.049280 a.u.

C	2.27104	-0.74316	-0.50212
C	2.27588	0.71305	-0.52484
C	1.67216	1.18236	0.64966
C	1.19865	0.01808	1.39668
C	1.66454	-1.17194	0.68602
Rh	-0.02249	-0.00493	-0.32482
C	-2.78767	0.75059	0.15831
C	-1.57281	1.31242	-0.00747
H	2.66806	-1.38046	-1.28405
H	2.67677	1.32323	-1.32593
H	1.53057	2.21582	0.93929
H	0.76663	0.03489	2.39064
H	1.51611	-2.19493	1.00770
H	-1.42054	2.39607	-0.05152
H	-3.71321	1.32377	0.25245
C	-1.58040	-1.30265	0.03349
C	-2.79203	-0.72884	0.18158
H	-3.72085	-1.29334	0.29376

H	-1.43447	-2.38797	0.02335

A2’ E = -4.037656 a.u.

C	-0.54925	-2.09878	0.69976
C	-1.51448	-1.08588	1.14170
C	-2.18979	-0.56312	0.00000
C	-1.51448	-1.08588	-1.14170
C	-0.54926	-2.09878	-0.69976
Rh	0.01948	-0.01940	0.00000
H	-1.72714	-0.83852	2.17605
H	-2.96682	0.19037	0.00000
H	-1.72714	-0.83852	-2.17605
H	0.07874	-2.69395	-1.35142
H	0.07874	-2.69395	1.35142
C	0.04614	2.09802	0.00000
C	2.06502	0.31726	0.00000
C	1.28635	2.61816	0.00000
C	2.39973	1.63088	0.00000
H	-0.84498	2.73373	0.00000
H	1.50147	3.69067	0.00000
H	3.43756	1.98150	0.00000
H	2.84180	-0.45398	0.00000

A3 E = -4.904352 a.u.

C	1.63202	1.27919	0.96621
C	1.28439	0.08166	1.68874
C	1.80962	-1.03398	0.94273
C	2.44646	-0.52689	-0.22045
C	2.33700	0.89884	-0.20598
Rh	0.03807	0.00474	-0.16957
C	-0.60044	-0.65499	-2.11660
C	-1.36998	-1.41239	0.33730
C	-2.57129	-0.93498	0.73631
C	-2.68302	0.51469	0.75126
C	-1.56968	1.17865	0.36405
H	2.92293	-1.11673	-0.99455
H	2.71663	1.56998	-0.96732
H	1.40355	2.29167	1.27549
H	0.80646	0.03518	2.65912
H	1.73886	-2.07549	1.23115
H	-1.49817	2.26727	0.30466
H	-1.13253	-2.47573	0.25570
H	-3.59965	1.02194	1.05956
H	-3.39884	-1.58293	1.03273
C	-0.69700	0.59879	-2.10364
H	-0.73871	-1.64311	-2.51862
H	-0.98589	1.56207	-2.48541

TS(A3,A4) E = -4.896908 a.u.

C	1.71742	1.28416	0.99266
C	1.41991	0.09770	1.75051
C	1.88837	-1.02368	0.98053
C	2.48185	-0.52761	-0.21836
C	2.37665	0.89336	-0.21072
Rh	0.11757	0.01052	-0.07524
C	-0.88604	-0.68848	-1.82675
C	-1.35999	-1.40848	0.19476
C	-2.58466	-0.92542	0.57899
C	-2.69557	0.49701	0.59932
C	-1.56120	1.17468	0.23234
H	2.92390	-1.12769	-1.00492
H	2.72429	1.55997	-0.99102
H	1.50580	2.30062	1.30185
H	0.98427	0.06013	2.74091
H	1.82862	-2.06343	1.27871
H	-1.50379	2.26440	0.20437
H	-1.13425	-2.47486	0.13661
H	-3.63359	1.00526	0.82949
H	-3.43179	-1.57936	0.79326
C	-0.98431	0.59089	-1.81051
H	-0.87546	-1.60555	-2.38954
H	-1.11622	1.51309	-2.34901

A4 E = -4.991018 a.u.

C	-1.49751	0.71205	-1.30352
C	-1.64053	1.31733	0.00677
C	-2.55307	0.67474	0.98315
C	-2.55314	-0.67365	0.98372
C	-1.64065	-1.31721	0.00790
C	-1.49756	-0.71304	-1.30294
Rh	0.15861	-0.00021	-0.13829
C	2.41142	0.70496	-0.62770
C	2.41189	-0.70337	-0.62835
C	1.94319	-1.14748	0.66436
C	1.73142	-0.00036	1.49649
C	1.94255	1.14759	0.66549
H	2.68511	-1.34567	-1.45685
H	1.85863	-2.18072	0.98105
H	1.45728	-0.00091	2.54340
H	1.85733	2.18049	0.98311
H	2.68430	1.34824	-1.45556
H	-1.34983	-1.29370	-2.21020
H	-1.34955	1.29195	-2.21123
H	-1.49234	2.39499	0.07774
H	-1.49279	-2.39484	0.07976
H	-3.19663	-1.27793	1.62014
H	-3.19647	1.27966	1.61906

A5 E = -5.833771 a.u.

C	-1.51027	-0.68059	-1.60058
C	-1.51016	0.75771	-1.57465
C	-2.66167	1.43961	-1.04590
C	-3.74018	0.73488	-0.55931
C	-3.74069	-0.69471	-0.58619
C	-2.66232	-1.38131	-1.09824
Rh	-0.00320	0.00891	0.00652
C	1.47412	0.65851	-1.38779
C	1.47330	-0.60644	-1.40365
C	-0.32614	-1.19739	2.00036
C	-1.17947	-0.04078	1.97020
C	-0.36546	1.14427	2.04111
C	0.98453	0.72476	1.97394
C	1.00967	-0.72709	1.94444
H	-2.26305	-0.05914	1.98454
H	-0.64588	-2.23147	2.01725
H	1.90534	-1.33747	1.92403
H	-0.85927	1.30879	-2.24745

H	-2.68659	2.52753	-1.07556
H	-4.61258	1.26359	-0.17989
H	-0.72199	2.16522	2.09141
H	1.85816	1.36651	1.97531
H	-0.85893	-1.20669	-2.29262
H	-4.61353	-1.23674	-0.22717
H	-2.68758	-2.46737	-1.16842
H	1.85465	-1.55048	-1.76332
H	1.85615	1.61059	-1.72485

TS(A3,A3') E = -4.895643 a.u.

Rh	0.47090	-0.05300	-0.12960
C	2.37320	0.57410	0.38250
C	0.73470	2.01370	0.37330
C	0.95250	-1.49950	-1.84400
C	0.04820	-2.13570	-0.93440
C	-1.20830	-1.44230	-1.01210
C	-1.07380	-0.39750	-1.97290
C	0.25590	-0.42390	-2.48420
C	-0.20470	1.54980	1.11190
C	0.51590	-0.39790	1.90360
C	1.72950	-0.21340	2.51420
C	2.75460	0.31770	1.67500
H	-1.84120	0.31740	-2.24370
H	0.66570	0.23870	-3.23730
H	1.97620	-1.79980	-2.03150
H	0.26320	-3.00630	-0.32730
H	-2.10730	-1.69350	-0.46190
H	3.05530	0.97690	-0.36880
H	-0.35710	-0.79700	2.42410
H	3.75010	0.55950	2.05160
H	1.88660	-0.40110	3.57790
H	-1.08640	1.71610	1.70560
H	1.19320	2.85590	-0.11500

A3' E = -4.955527 a.u.

H	0.20089	-0.09670	0.85242
C	-0.68774	0.52117	0.80224
C	-1.96905	0.10210	0.25969
C	-2.86742	1.17475	0.38688
C	-2.14352	2.28797	0.96754
C	-0.82329	1.83749	1.30531
Rh	-1.13292	1.90359	-1.00408
C	-1.95934	1.80658	-2.77349
C	-1.75113	2.28916	-4.07048
C	-0.75657	3.13319	-4.59429
C	0.35064	3.74050	-3.99522
C	0.83416	3.70290	-2.67576
C	0.35030	3.06023	-1.53001
H	-2.56543	3.25738	1.20465
H	-0.04966	2.42878	1.77941
H	-3.90019	1.19674	0.06071
H	0.99274	3.27092	-0.66033
H	-2.86289	1.17801	-2.72662
H	1.75473	4.28207	-2.53899
H	0.95287	4.34321	-4.67726
H	-0.86158	3.34612	-5.65953
H	-2.47940	1.96275	-4.82196
H	-2.17879	-0.86838	-0.17387

TS(A3',A4) E = -4.917504 a.u.

C	0.91930	-0.24030	1.49760
C	2.92260	0.04250	1.00650
Rh	1.45240	1.06100	0.00850
C	3.29610	-0.83240	0.03660
C	0.38910	-1.24240	0.74900
H	3.31800	3.46080	-0.32700
C	2.25940	3.24960	-0.40600
C	1.32560	3.16500	0.70210
C	0.00480	2.93220	0.14690
C	0.15600	2.72490	-1.23190
C	1.55840	2.92220	-1.57580
C	0.86420	-1.13890	-0.62440
C	2.24100	-0.94470	-0.96190
H	-0.63350	2.48290	-1.93420
H	1.97520	2.85010	-2.57390
H	-0.91630	2.86460	0.71130
H	3.47870	0.31960	1.90060
H	0.77910	-0.06130	2.56240
H	4.23520	-1.38630	-0.03740
H	2.50190	-1.08790	-2.01080
H	0.20320	-1.41210	-1.44740
H	-0.29990	-2.02570	1.07400
H	1.53810	3.44330	1.72870

C_2H_2 E = -0.810815 a.u.

C	-0.61896	-0.62960	-2.14671
C	-0.71157	0.57148	-2.13425
H	-0.53694	-1.69334	-2.15775
H	-0.79360	1.63521	-2.12321

C_6H_6 E = -2.655799 a.u.

C	0.00000	0.00000	0.00070
H	0.00000	0.00000	1.08880
C	1.21300	0.00000	-0.69970
C	1.21300	0.00000	-2.10030
C	0.00000	0.00000	-2.80070
C	-1.21300	0.00000	-2.10030
C	-1.21300	0.00000	-0.69970
H	2.15530	0.00000	-0.15560
H	2.15530	0.00000	-2.64440
H	0.00000	0.00000	-3.88880
H	-2.15530	0.00000	-2.64440
H	-2.15530	0.00000	-0.15560

A1-CO E = -4.549327 a.u.

H	1.45483	0.00701	-2.10609
C	1.53693	0.67006	-1.25304
C	1.93030	1.97038	-1.26103
H	2.20668	2.55323	-2.13503
C	1.95778	2.47756	0.12282
C	1.58283	1.48303	0.96636
C	1.30030	0.24689	0.16413
Rh	-0.68785	-0.54345	0.41861

C	-1.69451	1.45967	0.42241
C	-1.74765	1.02934	-0.74760
C	-0.77232	-1.90741	-1.22015
C	-0.28924	-2.51532	-0.21067
H	2.24909	3.48533	0.40417
H	1.52531	1.53264	2.04771
H	1.88555	-0.62852	0.46915
H	-1.98399	1.04010	-1.79380
H	-1.83025	2.14822	1.23442
H	0.11752	-3.41807	0.21953
H	-1.06808	-1.93675	-2.25704
C	-0.45495	-0.60901	2.33655
O	-0.44238	-0.72572	3.49041

TS(A1-CO,A2-CO) E = -4.530235 a.u.

C	0.45467	-0.07613	-0.44380
C	2.08237	-1.08152	0.27462
H	1.62833	3.55744	0.40050
C	0.70490	3.37962	0.94060
C	-0.53602	3.85404	0.61918
H	-0.78504	4.46243	-0.24554
C	-1.49164	3.42827	1.64383
C	-0.82813	2.69957	2.58934
C	0.60523	2.59740	2.19760
Rh	1.23206	0.52026	1.71179
C	-0.36903	0.52720	0.31905
C	2.87336	-0.58245	1.15528
H	-2.54994	3.67195	1.64393
H	-1.24754	2.26493	3.48965
H	1.33001	2.85735	2.97214
H	0.67435	-0.26886	-1.48192
H	-1.27318	1.11937	0.33545
H	3.81060	-0.81016	1.63905
H	1.97312	-1.96980	-0.32967
C	1.58988	0.36542	3.51365
O	1.69885	0.23939	4.66639

A2-CO E = -4.654116 a.u.

Rh	2.85810	1.43470	-2.83430
C	0.60400	0.71040	-3.23380
C	0.55800	1.89070	-2.43480
C	1.21420	1.59720	-1.19400
C	1.64460	0.23250	-1.23230
C	1.26720	-0.32030	-2.49450
H	2.16380	-0.28810	-0.43790
H	1.43000	-1.33990	-2.82090
H	0.20350	0.60900	-4.23480
H	0.09590	2.83190	-2.70550
H	1.33970	2.27830	-0.36200
C	3.80090	3.21080	-2.28520
C	5.02840	3.06380	-1.74750
C	5.52900	1.69210	-1.67470
C	4.70190	0.74140	-2.15360
H	3.29950	4.16850	-2.43700
H	5.61970	3.90930	-1.38970
H	6.51280	1.46190	-1.26040
H	4.93830	-0.32330	-2.19980
C	3.61830	1.61310	-4.52030
O	4.09050	1.72750	-5.57300

A3-CO E = -5.413925 a.u.

Rh	0.56580	3.71135	0.62985
C	-0.54428	2.63817	1.83109
O	-1.33284	2.11960	2.49703
C	0.81885	1.67221	-0.48490
C	1.43614	2.53633	-1.11513
C	1.30195	5.27860	-0.58481
C	0.72272	6.47188	-0.32054
C	-0.14849	6.52897	0.85287
C	-0.29637	5.37350	1.52849
H	2.03379	3.01248	-1.86470
H	0.39050	0.74809	-0.15685
H	2.00559	5.17556	-1.41594
H	0.89373	7.36046	-0.93355
H	-0.62550	7.45887	1.16811
H	-0.90251	5.27647	2.43036
C	2.25757	3.86115	2.01348
C	1.90052	3.53869	3.42739
C	2.31300	4.55744	4.22618
C	2.96921	5.58619	3.39777
C	2.94508	5.18998	2.10133
H	2.82907	3.08375	1.48931
H	1.43359	2.61448	3.74792
H	2.21021	4.60818	5.30628
H	3.40576	6.50248	3.78340
H	3.35834	5.71438	1.24968

Cartesian coordinates (in Å) of the optimized intermediates and transition state geometries of acetylene and acetonitrile cyclocotrimerization catalyzed by CpRh fragment

B3 E = -5.368167 a.u.

C	2.34853	0.89205	-0.13996
C	1.61112	1.24522	1.01358
C	1.21874	0.02517	1.68843
C	1.78291	-1.07457	0.94224
C	2.44655	-0.54098	-0.18553
Rh	0.03712	0.02004	-0.17597
C	-1.52985	1.19837	0.47575
C	-2.62970	0.53834	0.90132
C	-2.55344	-0.91401	0.78953
C	-1.38662	-1.38495	0.30114
N	-0.43742	-0.59733	-2.24543
C	-0.69148	0.57657	-2.14905
H	2.93000	-1.11357	-0.96842
H	2.76811	1.57723	-0.86708
H	1.37612	2.24941	1.34349
H	0.71610	-0.04252	2.64533
H	1.69114	-2.12294	1.19617
H	-1.43942	2.28789	0.46918
H	-1.17235	-2.43563	0.09608
H	-3.51394	1.04490	1.29453
H	-3.38884	-1.56204	1.06306
C	-1.22334	1.81062	-2.78106
H	-1.48974	1.60649	-3.82497
H	-2.11152	2.15170	-2.23939
H	-0.47500	2.61049	-2.74617

B4 E =-5.367568 a.u.

C	-2.52540	0.78107	-0.04299
C	-2.57839	-0.32443	-0.93474
C	-2.18105	-1.48849	-0.20207
C	-1.91396	-1.12284	1.13940
C	-2.09555	0.29908	1.24964
Rh	-0.30830	0.13102	-0.14607
C	1.52065	0.02596	0.92207
C	2.28075	1.27155	0.72041
C	1.74532	2.16555	-0.17284
C	0.46319	1.80437	-0.67439
N	1.04859	-1.20724	-0.95847
C	1.97987	-1.05071	-0.10945
C	3.31472	-1.75938	-0.08247
H	-2.86744	-0.29664	-1.97835
H	-2.07035	-2.48187	-0.61964
H	-1.61103	-1.78953	1.93755
H	-2.03080	0.88382	2.15917
H	-2.78787	1.80476	-0.27812
H	1.48783	-0.37265	1.94358
H	-0.08588	2.52122	-1.29881
H	3.24608	1.43444	1.20613
H	2.26296	3.07719	-0.47783
H	3.43746	-2.30318	0.86558
H	3.39130	-2.46597	-0.91592
H	4.13648	-1.03362	-0.15337

TS(B3,B4) E = -5.350765 a.u.

Rh	-0.09515	-0.07206	-0.00583
N	1.95981	0.31253	-0.26434
C	-0.06589	2.02300	0.21410
C	1.60293	1.21823	0.51071
C	-0.89836	-1.45090	1.83789
C	-1.95985	-0.77887	1.14801
C	-1.98301	-1.24787	-0.20898
C	-0.90916	-2.20639	-0.35286
C	-0.25572	-2.32048	0.90896
C	-0.11121	2.70714	-0.99137
C	0.10171	1.91802	-2.16296
C	0.15844	0.57018	-1.93738
H	0.61464	-2.93447	1.11471
H	-0.63363	-1.32340	2.88219
H	-2.65161	-0.06504	1.58238
H	-2.71179	-0.98438	-0.96704
H	-0.66988	-2.76452	-1.25133
H	-0.31644	2.52917	1.15003
H	0.38474	-0.15204	-2.72677
H	-0.25457	3.79062	-1.03534
H	0.26129	2.36799	-3.14612
C	2.29007	1.92984	1.65133
H	3.23119	1.42153	1.88792
H	2.49865	2.97128	1.37560
H	1.64894	1.93893	2.54037

TS(B4,B5) E = -5.350775 a.u.

C	0.26155	-0.14485	0.35755
N	2.69734	-0.46099	0.32044
C	0.32812	3.04657	-0.40001
C	1.23552	3.09918	0.72926
C	2.55813	3.27811	0.21531
C	2.49502	3.30914	-1.20277
C	1.11634	3.15666	-1.59087
Rh	1.54546	1.19562	-0.49413
C	1.52718	-0.46369	-1.92973
C	0.37413	-1.25291	-1.70792
C	-0.20254	-1.18702	-0.42469
C	2.77388	-0.65892	-0.93707
C	4.04588	-1.11602	-1.64962
H	0.95267	3.07464	1.77623
H	3.46359	3.32156	0.81098
H	3.33588	3.43073	-1.87767
H	0.73486	3.16985	-2.60639
H	-0.75319	2.98872	-0.34848
H	1.88207	-0.36945	-2.95997
H	-0.04383	-0.03744	1.40329
H	0.00077	-1.92728	-2.48328
H	-0.92176	-1.92931	-0.06984
H	4.29326	-0.42164	-2.46247
H	4.87977	-1.15943	-0.94309
H	3.88665	-2.10870	-2.09248

B5 E = -5.402863 a.u.

C	2.48572	0.69765	-0.77379
C	2.27929	-0.72746	-0.85361
C	2.06666	-1.23820	0.46986
C	2.00868	-0.09968	1.33871
C	2.31349	1.08584	0.56804
Rh	0.26585	-0.00241	-0.07696
C	-1.34434	-0.88028	-1.28824
N	-1.47026	0.52844	-1.23166
C	-1.59803	-0.02692	1.11862
C	-2.31167	-1.29403	0.84264
C	-2.18069	-1.74136	-0.42125
H	2.36047	-1.32520	-1.75424
H	1.96695	-2.27744	0.75539
H	1.85973	-0.13198	2.41199
H	2.37277	2.09479	0.95818
H	2.68035	1.35562	-1.61188
H	-1.08205	-1.24231	-2.28231
H	-2.67364	-2.62444	-0.82123
H	-2.93108	-1.76624	1.60264
H	-1.56874	0.33613	2.14701
C	-1.62194	0.98439	0.06505
C	-1.88011	2.45300	0.29277
H	-1.51325	2.76850	1.27602
H	-1.40659	3.05919	-0.48590
H	-2.96280	2.64668	0.26425

TS(B5,B6) E = -5.382011 a.u.

Rh	0.19202	0.04300	0.186059
C	2.80890	0.27942	0.059324
C	2.40349	1.57831	-0.218243
C	-2.61414	0.30795	0.622342
C	-1.56308	0.52956	1.649190
C	-0.89187	-0.70620	1.867765
C	-1.26664	-1.54175	0.742888
C	-2.46132	-0.94578	0.105328
C	1.40039	1.78918	-1.222696
N	0.90575	0.83263	-2.032020
C	2.11443	-0.77705	-0.591156
H	-1.52629	1.39101	2.307595
H	-0.27462	-0.98354	2.713575
H	-0.97428	-2.58246	0.627352
H	-3.02782	-1.39360	-0.702934
H	-3.33593	1.05589	0.311009
H	1.06962	2.80489	-1.437123
H	2.81788	2.43273	0.309851
H	3.58537	0.06828	0.788962
H	2.39949	-1.81259	-0.413161
C	1.19488	-0.47585	-1.671583
C	0.72496	-1.55296	-2.623320
H	0.71568	-2.53524	-2.139467
H	-0.27852	-1.32197	-2.992687
H	1.40034	-1.60538	-3.489561

B6 E = -5.421993 a.u.

Rh	0.38150	-0.13380	0.11010
C	-1.56680	-0.85550	-0.43560
C	-1.59510	-0.36320	0.90110
C	-1.25910	1.04590	1.00190
C	-1.80860	1.91510	-0.08150
N	-1.79160	1.47450	-1.29590
C	-1.20480	0.16410	-1.40030
C	2.40160	0.67330	0.79610
C	2.42440	0.53970	-0.62020
C	2.26770	-0.86420	-0.91170
C	2.26100	-1.59040	0.32810
C	2.31310	-0.64740	1.38050
H	2.48920	1.60140	1.34840
H	2.53290	1.33760	-1.34350
H	2.25580	-1.30350	-1.90280
H	2.18210	-2.66510	0.43460
H	2.30840	-0.86770	2.44160
H	-0.97890	-0.13730	-2.42130
H	-1.74950	-1.89680	-0.68780
H	-1.82000	-0.99080	1.75930
H	-1.14890	1.47510	1.99900
H	-2.77590	3.74790	-0.64840
H	-3.30860	3.09390	0.92540
H	-1.73370	3.88110	0.79950
C	-2.44480	3.23840	0.26050

B7 E = -6.251517 a.u.

C	1.00068	-0.72491	1.93561
C	-0.33675	-1.19485	1.98579
C	-1.18887	-0.03904	1.95946
C	-0.37124	1.14622	2.03539
C	0.97756	0.72649	1.97745
Rh	-0.00942	0.01644	0.00041
C	1.48667	-0.59763	-1.39751
C	1.48092	0.66611	-1.38547
C	-1.47578	-0.70053	-1.61552
C	-1.49083	0.73453	-1.56501
C	-2.66190	1.35163	-0.99616
N	-3.70580	0.70281	-0.52408
C	-3.70050	-0.68523	-0.59536
C	-2.63738	-1.38739	-1.11715
H	-2.27246	-0.05118	1.97693
H	-0.65612	-2.22916	1.99670
H	1.89590	-1.33600	1.91828
H	-0.87902	1.33025	-2.23752
H	-2.71796	2.44246	-0.97298
H	-0.72871	2.16657	2.09233
H	1.85181	1.36711	1.98418
H	-0.83405	-1.21820	-2.32219
C	-4.95860	-1.35852	-0.09568
H	-2.68719	-2.47247	-1.19593
H	1.86877	-1.54520	-1.74520
H	1.85348	1.62270	-1.71894
H	-4.90286	-2.44737	-0.19821
H	-5.13715	-1.11366	0.95976
H	-5.83105	-0.99583	-0.65475

B8 E = -6.191650 a.u.

C	-2.03614	2.94625	-0.03279
C	-0.97044	2.54273	0.85487
C	-1.18020	1.18534	1.19977
C	-2.40235	0.74499	0.57215
C	-2.93869	1.82702	-0.15536

Rh	-0.82876	1.44294	-1.16885
N	-1.59604	1.44335	-3.09574
C	-1.92001	2.46310	-3.79808
C	-2.66643	2.17590	-5.11614
C	0.67272	2.66855	-1.83849
C	0.58915	3.84620	-2.49539
C	-0.59486	4.49920	-3.04454
C	-1.69788	3.91462	-3.56607
H	-0.54191	0.57858	1.83150
H	-2.19940	3.94300	-0.42272
H	-0.15146	3.16966	1.18383
H	-3.84150	1.80890	-0.75333
H	1.67720	2.37077	-1.51675
H	1.51530	4.42251	-2.60375
H	-0.54759	5.58983	-3.09107
H	-2.46170	4.56845	-3.99190
H	-2.82812	-0.24869	0.64751
H	-2.08573	2.54409	-5.97342
H	-2.83467	1.10163	-5.22935
H	-3.63408	2.69794	-5.12746
C	0.73844	-0.12225	-1.39927
C	-0.28480	-0.61371	-1.89988
H	-0.98364	-1.21115	-2.45036
H	1.77301	-0.03137	-1.12621

B3’ E = -5.381639 a.u.

C	2.40284	0.72042	-0.13321
C	1.58700	1.16878	0.92765
C	1.02923	0.01039	1.58762
C	1.58822	-1.15781	0.94611
C	2.40305	-0.72496	-0.12178
Rh	0.08860	-0.00463	-0.42749
C	-1.48309	1.30692	-0.18106
C	-2.69304	0.74167	0.02275
C	-2.69792	-0.72172	0.04086
C	-1.49167	-1.29991	-0.14781
H	2.94380	-1.36122	-0.81262
H	2.94428	1.34619	-0.83300
H	1.38321	2.19933	1.18938
H	0.42208	0.01725	2.48474
H	1.38525	-2.18444	1.22354
H	-1.32108	2.38694	-0.24994
H	-1.33686	-2.38232	-0.19094
H	-3.60827	1.32267	0.16181
H	-3.61719	-1.29294	0.19319
N	-0.32162	-0.03555	-2.38018
C	-0.66033	-0.05952	-3.49247
C	-1.10791	-0.09348	-4.88250
H	-2.16936	-0.36798	-4.92448
H	-0.98440	0.88876	-5.35558
H	-0.53532	-0.83256	-5.45657

TS(B3’,B4) E = -5.352652 a.u.

C	0.10690	-0.10560	0.10370
C	2.21040	0.06100	-0.11650
C	0.44160	4.04510	0.18310
C	-0.66550	3.36260	-0.37030
C	-1.47230	2.88240	0.72140
C	-0.86080	3.34830	1.94900
C	0.32290	4.06190	1.61510
Rh	0.42010	1.73580	1.02700
C	0.00780	-1.16670	0.99290
C	0.18150	-0.82440	2.36760
C	0.35680	0.52180	2.59880
H	1.00020	4.54830	2.30650
H	1.26570	4.46980	-0.37840
H	-0.85940	3.20130	-1.42370
H	-2.42510	2.37370	0.63820
H	-1.25710	3.19710	2.94480
H	-0.13950	-0.20410	-0.95700
H	0.43950	0.91700	3.61790
H	-0.18950	-2.19350	0.67220
H	0.18390	-1.57620	3.15900
N	2.34240	1.15330	0.37680
C	2.89150	-1.11670	-0.70860
H	2.77850	-1.98110	-0.04430
H	2.45630	-1.37280	-1.68140
H	3.96030	-0.89810	-0.83480

TS(B4,B5’) E = -5.354244 a.u.

Rh	0.00860	0.13550	0.10880
C	2.84330	-0.34710	-0.18320
C	-1.97920	1.20890	-0.13570
C	-2.07180	-0.08640	0.53250
C	-1.52130	0.07980	1.87090
C	-0.99110	1.37040	1.95890
C	-1.26910	2.07280	0.71180
C	2.61140	0.22340	-1.39540
C	1.52800	-0.16790	-2.31800
C	0.28530	-0.36190	-1.84010
N	0.87160	-1.67460	0.47360
C	2.14040	-1.56770	0.35530
C	3.06140	-2.70630	0.78870
H	-2.62760	-0.94840	0.17890
H	-1.45060	-0.70070	2.61780
H	-0.45170	1.78450	2.80270
H	-0.97980	3.09310	0.48880
H	-2.34780	1.43610	-1.12780
H	3.68100	0.02200	0.41320
H	-0.53400	-0.68800	-2.48740
H	3.29290	1.01250	-1.72280
H	1.77010	-0.24560	-3.38230
H	3.76650	-2.36160	1.55900
H	2.46990	-3.53550	1.18740
H	3.65820	-3.06070	-0.06420

B5’ E = -5.385601 a.u.

C	-0.68620	2.02630	1.07390
C	-0.89600	0.62940	0.97050
C	-2.28120	0.41640	0.59590
C	-2.91840	1.66290	0.47820
C	-1.92320	2.68540	0.69650
Rh	-1.08440	1.67730	-1.08310
C	0.54050	2.67200	-1.69480
C	0.72780	3.65140	-2.63350
C	-0.21320	4.25310	-3.55850
C	-1.31990	3.72260	-4.15390
C	-1.73270	2.32130	-3.99940
N	-1.69950	1.73620	-2.86440

H	-0.16980	-0.14870	1.17090
H	-2.10140	3.75420	0.71010
H	0.22850	2.52290	1.37310
H	-3.94690	1.83400	0.18550
H	1.40860	2.48700	-1.04820
H	1.71180	4.13320	-2.64370
H	0.04840	5.26680	-3.87170
H	-1.88120	4.33570	-4.86140
C	-2.20430	1.57020	-5.24280
H	-2.73750	-0.55140	0.42220
H	-1.41760	1.56670	-6.00930
H	-2.47420	0.54020	-4.99250
H	-3.08100	2.07440	-5.67390

TS(B5',B6) E = -5.361953 a.u.

C	0.03717	0.13350	0.16268
N	2.01083	0.29723	0.42105
Rh	1.09949	1.91852	0.08529
C	1.71498	-0.72047	2.54441
C	-0.37809	3.61742	-0.11216
C	0.73500	3.95926	-0.91184
C	1.89092	4.12418	-0.04215
C	1.49150	3.87130	1.28289
C	0.09704	3.47532	1.24713
C	-0.41019	-0.50987	1.29854
C	0.32548	-0.70911	2.49939
C	2.50670	-0.43992	1.38970
H	0.73360	4.09905	-1.98610
H	-0.51386	3.23164	2.10923
H	-1.38942	3.43876	-0.45518
H	2.11966	3.90095	2.16415
H	-0.37222	-0.17335	-0.80621
H	-1.35819	-1.05350	1.22618
H	-0.21114	-1.09863	3.36384
H	2.21214	-1.12196	3.42784
C	3.87470	-1.09267	1.20602
H	2.88782	4.39326	-0.37152
H	3.77862	-2.17450	1.03616
H	4.40180	-0.65118	0.35568
H	4.48258	-0.95320	2.10932

B8' E = -6.268744 a.u.

C	2.19020	-0.44920	0.14750
C	1.95970	0.43750	-0.97160
C	1.30040	1.61390	-0.51310
C	0.98710	1.39650	0.86940
C	1.57090	0.13600	1.27510
Rh	-0.15320	-0.19620	-0.22650
C	-1.76360	-0.87060	0.94650
C	-2.13060	0.21110	0.37930
N	-0.93330	-1.26990	-1.89910
C	-0.65970	-2.57950	-2.19220
C	-1.18200	-3.18370	-3.34640
C	-1.99810	-2.46560	-4.22120
C	-2.28880	-1.13580	-3.90830
C	-1.74820	-0.58550	-2.74950
C	0.21270	-3.36290	-1.24520
H	1.05130	2.48710	-1.10200
H	0.48110	2.09650	1.52510
H	1.53850	-0.27900	2.27540
H	2.74180	-1.38060	0.12370
H	2.30740	0.26570	-1.98460
H	-2.87890	0.98710	0.28290
H	-1.99020	-1.65730	1.65430
H	-1.95340	0.44020	-2.46600
H	-2.92750	-0.52750	-4.54320
H	-2.40130	-2.93450	-5.11570
H	-0.94770	-4.22740	-3.54310
H	0.19720	-4.42830	-1.49760
H	1.24810	-3.00600	-1.28990
H	-0.12240	-3.21730	-0.21340

CH_3CN E = -1.294027 a.u.

C	0.41032	0.00001	0.33094
N	-0.38875	-0.00000	1.17238
C	1.41798	-0.00000	-0.73006
H	0.93369	0.00004	-1.71323
H	2.05207	0.89041	-0.65113
H	2.05199	-0.89048	-0.65118

2-methyl-pyridine E = -3.071083 a.u.

C	0.02507	-0.00000	0.023502
H	0.03618	0.00000	1.111372
C	1.21738	0.00001	-0.704183
C	1.13538	0.00000	-2.100821
N	-0.02228	-0.00001	-2.782681
C	-1.17554	-0.00001	-2.077865
C	-1.18632	-0.00001	-0.672329
H	2.18528	0.00003	-0.208240
H	2.04343	0.00001	-2.703887
C	-2.45744	0.00001	-2.883460
H	-2.13277	-0.00001	-0.134917
H	-3.34217	0.00002	-2.238760
H	-2.49513	0.88176	-3.534698
H	-2.49515	-0.88172	-3.534726

Cartesian coordinates (in Å) of equilibrium stuctures and transition states occurring in the acetylene cyclotrimerization catalyzed by IndRh fragment

C1 E = -5.529857 a.u.

C	1.93270	-0.46270	0.05180
C	1.86950	0.34980	-1.15560
C	1.31790	1.62910	-0.78050
C	1.05340	1.58220	0.65120
C	1.57100	0.35500	1.16810
Rh	-0.32210	-0.13900	0.03990
C	-1.20790	-1.88610	-0.88280
C	-0.83550	-2.19620	0.27700
C	-2.06490	0.64000	1.00470
C	-2.32350	0.64650	-0.22550
H	0.69300	2.41440	1.24580
H	1.64840	0.08250	2.21350
H	2.36010	-1.45790	0.11210
H	-2.93790	0.79870	-1.09600
H	-2.28100	0.84360	2.04070
H	-0.68080	-2.88470	1.09230
H	-1.66710	-2.06250	-1.84090
C	1.12640	2.63040	-1.75600
C	2.21890	0.09790	-2.49940
C	1.50260	2.36570	-3.07050
C	2.04380	1.11110	-3.43870
H	2.62920	-0.86650	-2.79140
H	2.32790	0.93840	-4.47420
H	1.38040	3.13520	-3.82930
H	0.70470	3.59490	-1.48120

TS(C1,C2) E = -5.505822 a.u.

C	0.47730	-0.29120	-0.05980
C	2.40490	-0.27680	-0.10940
C	0.26010	3.65930	-0.00550
C	0.71710	3.52350	1.35580
C	2.16990	3.53210	1.32980
C	2.57610	3.67280	-0.04670
C	1.40250	3.83640	-0.85100
Rh	1.42340	1.67240	-0.22180
C	-0.08660	0.47520	-0.93710
C	2.91090	0.49750	-1.01460
H	3.59620	3.75850	-0.40120
H	1.38240	4.07760	-1.90730
H	-0.77320	3.73360	-0.32230
H	2.69210	-0.99940	0.64510
H	3.70860	0.63650	-1.72920
H	-0.92350	0.60190	-1.60770
H	0.24090	-1.01760	0.70850
C	2.89770	3.41940	2.54250
C	0.03440	3.40300	2.59380
C	2.19980	3.32280	3.73540
C	0.77570	3.31470	3.76100
H	-1.05330	3.39560	2.62210
H	0.26530	3.24040	4.71850
H	2.74520	3.25450	4.67390
H	3.98580	3.42430	2.53160

C2 E = -5.564590 a.u.

C	1.14310	0.70830	0.74210
C	0.84150	-0.67740	1.11420
C	1.94660	-1.50500	0.61050
C	2.76200	-0.65980	-0.22190
C	2.22360	0.69930	-0.14650
Rh	0.22770	-0.52470	-0.88940
C	-1.56140	0.44750	-0.85880
C	-2.63700	-0.30820	-1.16470
C	-2.35440	-1.74070	-1.37710
C	-1.05550	-2.08280	-1.23280
H	2.64360	1.56410	-0.64770
H	0.58700	1.57670	1.07140
H	0.14060	-0.97750	1.88610
H	-1.60440	1.52550	-0.67260
H	-0.69040	-3.11150	-1.33500
H	-3.64490	0.10180	-1.26180
H	-3.14780	-2.44740	-1.63080
C	2.24890	-2.87100	0.74900
C	3.84510	-1.20890	-0.93090
C	3.35000	-3.38910	0.06200
C	4.13330	-2.56810	-0.77390
H	1.63770	-3.50980	1.38270
H	3.60430	-4.44070	0.16830
H	4.97810	-3.00050	-1.30460
H	4.45800	-0.58410	-1.57710

C3 E = -6.411786 a.u.

C	4.14080	-2.60410	-0.63170
C	3.86320	-1.26260	-0.86220
C	2.74530	-0.67750	-0.22510
C	1.89470	-1.48180	0.62530
C	2.19560	-2.84910	0.83160
C	3.31440	-3.39060	0.21180
C	2.20750	0.66710	-0.23580
C	1.09840	0.71070	0.63700
C	0.81900	-0.62520	1.10590
Rh	0.23510	-0.61210	-1.03550
C	-1.09740	-2.18220	-0.96120
C	-2.40570	-1.83880	-0.92260
C	-2.65640	-0.40600	-0.94410
C	-1.54990	0.37090	-0.98760
H	2.63440	1.51280	-0.76260
H	0.53140	1.59530	0.89970
H	0.08820	-0.88700	1.86120
H	-1.55530	1.46260	-1.03600
H	-0.72820	-3.21180	-0.97040
H	-3.66530	0.01120	-0.92690
H	-3.21670	-2.56810	-0.87300
H	1.56420	-3.45910	1.47400
H	3.56500	-4.43640	0.37340
H	5.00630	-3.06320	-1.10360
H	4.49990	-0.66640	-1.51230
C	0.28400	-1.23500	-3.10670
C	0.27210	0.01770	-3.11530

H	0.22570	-2.22990	-3.51020
H	0.21750	1.00420	-3.53920

TS(C3,C4) E = -6.401086 a.u.

C	0.27560	0.34750	-0.22570
C	2.43790	-0.18040	-0.10940
C	0.23840	1.62200	-0.10430
C	2.23710	2.39350	0.16860
C	-1.07000	2.43010	4.50560
C	-0.80780	1.11870	4.14110
C	0.50770	0.76320	3.75180
C	1.54720	1.77660	3.71400
C	1.24000	3.11480	4.07770
C	-0.05130	3.42270	4.47510
C	1.09990	-0.48550	3.34150
C	2.49030	-0.26650	3.12920
C	2.77460	1.13210	3.28690
Rh	1.56940	0.87990	1.40670
C	3.02580	1.97700	-0.87690
C	3.13350	0.56270	-1.02840
H	0.59510	-1.44370	3.29560
H	3.22080	-1.02930	2.88820
H	3.75640	1.58780	3.25020
H	2.42900	-1.27170	-0.09340
H	2.06880	3.44720	0.40240
H	3.67460	0.10280	-1.85700
H	3.49060	2.67240	-1.57780
H	2.01470	3.87870	4.05810
H	-0.29510	4.44020	4.77180
H	-2.07180	2.71050	4.82300
H	-1.59340	0.36640	4.16620
H	-0.30100	2.54640	-0.21440
H	-0.19500	-0.56830	-0.53670

C4 E = -6.507687 a.u.

C	1.92896	0.51418	-0.73173
C	1.92974	0.54762	0.70528
C	0.85651	1.45670	1.11539
C	0.35238	2.11951	-0.04945
C	0.85547	1.40344	-1.18260
Rh	-0.56488	0.11544	-0.00224
C	-1.66409	-1.59068	0.75402
C	-1.66369	-1.62679	-0.67350
C	-2.35405	-0.56212	-1.34214
C	-3.47103	0.10758	-0.68536
C	-3.47148	0.14216	0.67660
C	-2.35468	-0.49304	1.36723
H	0.66082	1.76000	2.13847
H	-0.30382	2.98057	-0.06918
H	0.65879	1.65883	-2.21849
H	-1.14269	-2.33883	1.34477
H	-1.14152	-2.40363	-1.22528
H	-2.27539	-0.50373	-2.42680
H	-2.27689	-0.37982	2.44759
H	-4.25088	0.64175	1.24747
H	-4.25007	0.57748	-1.28137
C	2.84795	-0.29317	-1.42061
C	2.84956	-0.22694	1.42979
C	3.77197	-1.04134	-0.68263
C	3.77277	-1.00860	0.72625
H	2.85302	-0.21099	2.51808
H	4.50824	-1.59393	1.27342
H	4.50688	-1.65139	-1.20293
H	2.85012	-0.32759	-2.50848

C5 E = -7.330428 a.u.

C	1.09140	-0.72923	1.97382
C	-0.25087	-1.21844	1.93179
C	-1.11665	-0.07631	1.89727
C	-0.33326	1.12790	1.97242
C	1.03772	0.74114	2.00894
Rh	0.00007	-0.00549	-0.07794
C	1.41222	-0.64598	-1.52787
C	1.41721	0.62065	-1.52516
C	-1.54373	-0.67218	-1.57058
C	-1.52748	0.77375	-1.53547
C	-2.65992	1.46272	-0.96175
C	-3.73006	0.76530	-0.45526
C	-3.74732	-0.66890	-0.49385
C	-2.69326	-1.36397	-1.03560
H	-2.19929	-0.11403	1.89908
H	-0.55874	-2.25627	1.94693
C	2.36268	-1.38553	2.03617
H	-0.92668	1.31960	-2.25845
H	-2.67499	2.55111	-0.98220
H	-4.58821	1.29826	-0.05031
H	-0.71855	2.13883	2.01798
C	2.25697	1.48599	2.09850
H	-0.95086	-1.19435	-2.31692
H	-4.61863	-1.20199	-0.11813
H	-2.73307	-2.44922	-1.11228
H	1.78548	-1.59686	-1.87820
H	1.79107	1.57128	-1.87572
C	3.45328	0.81011	2.15612
C	3.50542	-0.62619	2.12547
H	2.22627	2.57333	2.13114
H	4.38543	1.36563	2.23058
H	4.47570	-1.11502	2.17836
H	2.41258	-2.47251	2.02130

C1-CO E = -6.075260 a.u.

C	1.72710	1.07490	-3.70360
C	1.42390	0.27150	-2.58880
C	1.51010	0.81990	-1.31060
C	1.92130	2.17240	-1.14430
C	2.22090	2.96850	-2.25270
C	2.11380	2.41070	-3.53740
C	2.01310	2.44570	0.29430
C	1.68960	1.32500	0.98650
C	1.32590	0.21270	0.05600
Rh	-0.67800	-0.55920	0.40360
C	-1.70650	1.46060	0.34880
C	-1.83120	0.96290	-0.78400
C	-0.88630	-2.02010	-1.13370
C	-0.32700	-2.56110	-0.12350
H	2.32110	3.39540	0.72210
H	1.70460	1.21850	2.06510

H	1.87550	-0.71880	0.21840
H	-2.12250	0.88760	-1.81290
H	-1.78190	2.17990	1.14090
H	0.10610	-3.43980	0.33120
H	-1.26810	-2.13260	-2.13630
H	1.11920	-0.76330	-2.72940
H	1.66220	0.65360	-4.70410
H	2.34440	3.01820	-4.40970
H	2.55270	3.99750	-2.12550
C	-0.43070	-0.52440	2.31510
O	-0.44730	-0.60580	3.47310

TS(C1-CO,C2-CO) E = -6.054821 a.u.

C	0.30210	-0.19050	-0.21880
C	2.32390	-0.35480	-0.00450
C	-0.10770	4.66730	0.09630
C	0.44810	3.79420	1.04530
C	-0.39300	2.92370	1.74190
C	-1.79840	2.93990	1.50650
C	-2.34530	3.81030	0.55570
C	-1.48940	4.66970	-0.14940
C	-2.41990	1.98950	2.43300
C	-1.45420	1.41530	3.20190
C	-0.10600	1.91240	2.80760
Rh	1.20520	0.39580	1.87140
C	-0.49530	-0.26700	0.77600
C	2.99590	0.32540	0.85460
H	-3.48770	1.80150	2.50040
H	-1.61520	0.69180	3.99410
H	0.50950	2.27250	3.63390
H	0.31680	-0.04180	-1.28740
H	-1.54960	-0.24720	1.01100
H	4.02500	0.49470	1.13210
H	2.48100	-1.07600	-0.79290
H	1.52090	3.79680	1.23000
H	0.53810	5.35030	-0.45090
H	-1.90210	5.35430	-0.88730
H	-3.41880	3.83640	0.37620
C	1.93120	0.16000	3.54590
O	2.32280	-0.06140	4.62160

C2-CO E = -6.153021 a.u.

C	1.97910	-0.45490	0.01110
C	1.50080	0.17380	-1.19650
C	1.12350	1.54110	-0.86460
C	1.38390	1.73800	0.54490
C	1.95410	0.53070	1.04620
C	0.66020	2.41320	-1.89050
C	0.59340	1.94400	-3.18690
C	0.95960	0.60320	-3.51120
C	1.39660	-0.27790	-2.54260
Rh	-0.27480	0.06470	0.53670
C	-0.90200	-0.60960	2.12170
O	-1.29590	-1.03210	3.12840
C	-2.07390	1.11850	0.36120
C	-3.03780	0.46300	-0.31270
H	1.27190	2.66780	1.08860
H	2.29680	0.37640	2.06170
H	2.39230	-1.45290	0.08950
H	-4.00980	0.90890	-0.53470
H	-2.17950	2.12110	0.77960
H	1.67910	-1.29620	-2.79990
H	0.89140	0.27510	-4.54570
H	0.25590	2.60440	-3.98200
H	0.38410	3.43790	-1.65220
C	-2.71040	-0.89920	-0.74610
C	-1.48470	-1.34830	-0.41760
H	-3.42630	-1.50240	-1.30860
H	-1.10330	-2.34650	-0.63950

C3-CO E = -6.938616 a.u.

C	0.56870	3.71370	0.63150
C	-0.23050	2.94280	1.47210
C	-1.63290	3.17400	1.52190
C	-2.23160	4.13200	0.70030
C	-1.41870	4.88310	-0.16560
C	-0.03300	4.68520	-0.18960
C	-2.18810	2.34030	2.59280
C	-1.18450	1.64570	3.18920
C	0.11350	1.90960	2.51020
Rh	1.05700	0.00760	1.88170
C	2.85160	-0.22310	3.38510
C	3.24410	0.40730	2.39950
C	0.13640	-1.10400	3.20070
O	-0.41290	-1.91810	3.81140
C	-0.57110	-0.34730	0.63510
C	-0.34570	-0.14480	-0.67710
C	0.96440	0.40730	-1.01420
C	1.78100	0.69980	0.02410
H	-3.23500	2.32390	2.88180
H	-1.29250	0.99320	4.04780
H	0.95540	2.16530	3.16230
H	-1.09530	-0.35190	-1.44310
H	-1.51180	-0.73410	1.03060
H	2.76400	1.14540	-0.15620
H	1.24710	0.58340	-2.05500
H	1.64480	3.56270	0.59150
H	0.58520	5.28520	-0.85320
H	-1.86790	5.63480	-0.81100
H	-3.30380	4.31470	0.74630
H	3.88170	0.93500	1.72100
H	2.78150	-0.73170	4.32390

Selected structural parameters of the computed CpRh complexes

	A1	**TS(A1,A2)**	**A2**	**A2'**	**A3**	**TS(A3,A4)**	**A4**
Rh-Q (Å)	1.98	2.01	1.96	1.88	2.03	2.00	1.98
Δ (Å)	0.060	0.096	0.064	0.036	0.13	0.12	0.11
FA (º)	4	1	-6	9	1	1	5
	A5	**TS(A3,A3')**	**TS(A3',A4)**	**A3'**			
Rh-Q (Å)	1.98	2.01	2.04	1.97			
Δ (Å)	-0.044	0.089	0.077	0.0005			
FA (º)	-6	0	-7	-6			
	B3	**TS(B3,B4)**	**B4**	**B3'**	**TS(B3',B4)**	**TS(B4,B5)**	**B5**
Rh-Q (Å)	2.03	1.99	2.05	2.02	2.01	1.97	1.98
Δ (Å)	0.14	0.12	0.10	0.11	0.1	0.14	0.16
FA (º)	-2	1	2	-3	-2	2	6
	TS(B5,B6)	**B6**	**B7**	**B8**	**TS(B4,B5')**	**B5'**	**TS(B5',B6)**
Rh-Q (Å)	2.18	1.97	1.98	2.02	1.97	1.97	1.93
Δ	0.56	0.10	-0.040	0.088	0.12	0.15	0.032
FA (º)	16	4	-6	-3	-6	4	-6
	B8'	**A1-CO**	**TS(A1-CO,A2-CO)**	**A2-CO**	**A3-CO**		
Rh-Q (Å)	1.98	-	-	2.03	-		
Δ (Å)	-0.033	-	-	-0.051	-		
FA (º)	0	-	-	-1	-		

The slippage parameter Δ is defined as Δ = 1/2[(M–C1a + M–C3a) – (M–C1+ M–C3)] where M-C1a and M-C3a are the longest distances between M and two adjacent C atoms of the Cp ring and M-C1 and M-C3 are the distances between M and the C atoms adjacent to C1a and C3a respectively; the folding angle FA is the dihedral angle between the planes C1,C2,C3 and C1,C3,C3a,C7a: Marder, T. B.; Calabrese, J. C.; Roe, D. C.; Tulip, T. H. *Organometallics* **1987**, *6*, 2012.

Selected structural parameters of the computed IndRh complexes

	C1	TS(C1,C2)	C2	C3	TS(C3,C4)	C4	C5
Rh-Q (Å)	2.05	2.06	2.05	2.10	2.06	2.06	2.04
Δ (Å)	0.26	0.22	0.28	0.22	0.20	0.19	0.077
FA (º)	10	6	10	7	5	14	2
	C1-CO	**TS(C1-CO,C2-CO)**	**C2-CO**	**C3-CO**			
Rh-Q (Å)	-	-	2.07	-			
Δ (Å)	-	-	0.11	-			
FA (º)	-	-0-	4	-			

The slippage parameter Δ is defined as Δ = 1/2[(M–C1a + M–C3a) – (M–C1+ M–C3)] where M-C1a and M-C3a are the longest distances between M and two adjacent C atoms of the Cp ring and M-C1 and M-C3 are the distances between M and the C atoms adjacent to C1a and C3a respectively; the folding angle FA is the dihedral angle between the planes C1,C2,C3 and C1,C3,C3a,C7a: Marder, T. B.; Calabrese, J. C.; Roe, D. C.; Tulip, T. H. *Organometallics* **1987**, *6*, 2012.

Hirshfeld and Voronoi charges on rhodium nucleus

	A1	TS(A1,A2)	A2	A3	TS(A3,A4)
H	0.2619	0.2830	0.3161	0.3366	0.3164
V	0.219	0.242	0.277	0.300	0.274
	A4	**A5**	**A3’**	**TS(A3,A3’)**	**TS(A3’,A4)**
H	0.2760	0.2650	0.2551	0.3137	0.2812
V	0.199	0.200	0.240	0.270	0.222

	B3	TS(B3,B4)	B4	TS(B4,B5)	B5	TS(B5,B6)	B6	B7
H	0.3360	0.3082	0.3268	0.2874	0.2607	0.2092	0.2498	0.2673
V	0.291	0.258	0.299	0.237	0.182	0.122	0.172	0.202
	B8	**B8’**	**B3’**	**TS(B3’,B4)**	**TS(B4,B5’)**	**B5’**	**TS(B5’,B6)**	
H	0.3364	0.2160	0.2984	0.3079	0.3145	0.2802	0.2461	
V	0.294	0.161	0.261	0.273	0.269	0.257	0.203	

	A1-CO	TS(A1-CO,A2-CO)	A2-CO	A3-CO
H	0.2683	0.2559	0.3112	0.3161
V	0.267	0.246	0.294	0.301

	C1	TS(C1,C2)	C2	C3	TS(C3,C4)	C4	C5
H	0.2619	0.2843	0.3187	0.3421	0.3198	0.2136	0.2866
V	0.210	0.237	0.277	0.300	0.272	0.121	0.224

	C1-CO	TS(C1-CO,C2-CO)	C2-CO	C3-CO
H	0.2583	0.2561	0.3273	0.3052
V	0.255	0.250	0.311	0.291

Selected structural parameters of the crystallographic structures of several CpRh complexes taken from CSD

	AFUBAE RCpRh(CO)$_2$[a]	BEKFON CpRhCOD	COXGUR Cp*Rh(CO$_2$)[b]	FAZFAN (C$_5$Ph$_5$)Rh(CO)$_2$
Rh-Q	1.927	1.906	1.909	1.934
Rh-C1	2.258	2.224	2.223	2.245
Rh-C2	2.292	2.266	2.281	2.327
Rh-C3	2.245	2.234	2.234	2.292
Rh-C1a	2.298	2.273	2.276	2.308
Rh-C3a	2.285	2.278	2.278	2.303
Delta	0.04	0.047	0.049	0.037
HA	4.4	3.0	5.2	3.4
	IXOHOS Cp*Rh(Et)$_2$[b]		**NOCPRH R'CpRh(CO)$_2$[c]**	**PANMOG R''CpRh(Et)$_2$[d]**
Rh-Q	1.882	1.883	1.925	1.908
Rh-C1	2.224	2.233	2.252	2.201
Rh-C2	2.247	2.248	2.289	2.300
Rh-C3	2.204	2.196	2.244	2.220
Rh-C1a	2.264	2.266	2.280	2.263
Rh-C3a	2.271	2.269	2.271	2.290
Delta	0.054	0.053	0.028	0.066
HA	3.9	4.1	4.4	5.8

[a] R=COOCH$_2$CH$_2$OH [b] Cp*=C$_5$(CH$_3$)$_5$ [c] R'=NO$_2$ [d] R''=Ph

Single imaginary frequencies of the transition states (in cm^{-1})

TS(A1,A2)	**TS(A3,A4)**	**TS(A3,A3')**	**TS(A3',A4)**
-406	-351	-352	-357
TS(B3,B4)	**TS(B4,B5)**	**TS(B5,B6)**	**TS(B3',B4)**
-306	-124	-148	-328
TS(B4,B5')	**TS(B5',B6)**	**TS(A1-CO,A2-CO)**	**A2'**
-64	-439	-332	-238
TS(C1,C2)	**TS(C3,C4)**	**TS(C1-CO,C2-CO)**	
-436	-368	-326	

Complete ref. 15b

Computer code ADF2006.01: Baerends, E. J.; Autschbach, J.; Bérces, A.; Bickelhaupt, F. M.; Bo, C.; de Boeij, P. L.; Boerrigter, P. M.; Cavallo, L.; Chong, D. P.; Deng, L.; Dickson, R. M.; Ellis, D. E.; Fan, L.; Fischer, T. H.; Fonseca Guerra, C.; van Gisbergen, S. J. A.; Groeneveld, J. A.; Gritsenko, O. V.; Grüning, M.; Harris, F. E.; van den Hoek, P.; Jacob, C. R.; Jacobsen, H.; Jensen, L.; van Kessel, G.; Kootstra, F.; van Lenthe, E.; McCormack, D. A.; Michalak, A.; Neugebauer, J.; Osinga, V. P.; Patchkovskii, S.; Philipsen, P. H. T.; Post, D.; Pye, C. C.; Ravenek, W.; Ros, P.; Schipper, P. R. T.; Schreckenbach, G.; Snijders, J. G.; Solà, M.; Swart, M.; Swerhone, D.; te Velde, G.; Vernooijs, P.; Versluis, L.; Visscher, L.; Visser, O.; Wang, F.; Wesolowski, T. A.; van Wezenbeek, E.; Wiesenekker, G.; Wolff, S. K.; Woo, T. K.; Yakovlev, A. L.; Ziegler, T. (SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, 2006).