```
13
Cyclopentene
C          1.38203        0.27666        0.09402
C          0.11618        1.13848        0.25036
C         -1.05172        0.23379       -0.18218
H          2.13464        0.47949        0.87356
H          1.88855        0.45673       -0.87339
H         -0.00904        1.40102        1.31293
H          0.16330        2.08282       -0.31147
H         -1.96643        0.40727        0.40812
H         -1.33458        0.39995       -1.23918
C         -0.48672       -1.14964       -0.01003
H         -1.09622       -2.05598       -0.05409
C          0.84127       -1.12625        0.14068
H          1.47629       -2.01067        0.23787
15
Phenylsilane (PhSiH3)
C          0.52046       -0.61257        0.18964
C          1.91418       -0.60916        0.20361
C          2.63404        0.59425        0.15357
C          1.91307        1.79664        0.09326
C          0.51949        1.79757        0.07908
C         -0.17887        0.59179        0.12655
H         -0.02273       -1.55992        0.23128
H          2.44803       -1.56264        0.25930
H          2.44588        2.75185        0.06140
H         -0.02456        2.74427        0.03384
H         -1.27165        0.59095        0.11785
Si         4.51221        0.59423        0.12988
H          5.03869        0.56347       -1.27075
H          5.03020        1.83043        0.79143
H          5.02833       -0.61168        0.84631
15
PhSiH2Cl
C          0.51227       -0.61845        0.11252
C          1.90641       -0.63288        0.11399
C          2.63228        0.56478        0.13762
C          1.92819        1.77896        0.16116
C          0.53563        1.79505        0.15895
C         -0.17391        0.59423        0.13446
H         -0.04097       -1.56058        0.09483
H          2.43987       -1.58709        0.09925
H          2.46887        2.73105        0.18366
H          0.00101        2.74782        0.17811
H         -1.26662        0.60534        0.13383
Si         4.50207        0.59958        0.12730
H          5.03041        1.36692        1.29103
Cl         5.23004       -1.33966        0.24857
H          5.03125        1.20390       -1.12868
71
(NPN)Ni-H
H          7.11913        6.23218        4.94494
C          5.68656        4.08383        5.85620
H          6.77061        3.99050        5.77782
```

C	4.85643	2.95843	5.70683
H	5.31089	1.98217	5.53464
C	3.49291	3.12107	5.75646
H	2.81892	2.27176	5.62058
C	2.95417	4.40666	6.00013
C	1.56218	4.65304	6.10560
H	0.87080	3.81935	5.96246
C	1.08703	5.91050	6.40188
H	0.01303	6.08398	6.49125
C	1.98667	6.97358	6.62281
H	1.60152	7.95156	6.92140
C	3.34784	6.78138	6.49374
C	3.85803	5.49045	6.17385
C	8.11857	8.76743	4.84389
H	8.80402	7.92013	4.88905
C	8.49992	9.96479	4.21166
H	9.50111	10.04575	3.78683
C	7.59195	10.99149	4.12012
H	7.84564	11.92509	3.61197
C	6.31039	10.84032	4.70159
C	5.32807	11.86190	4.67709
H	5.55922	12.79746	4.16240
C	4.11376	11.69163	5.30288
H	3.37005	12.49045	5.28459
C	3.83596	10.49504	5.99441
H	2.89354	10.39085	6.53669
C	4.75571	9.46504	6.01360
C	6.01241	9.61437	5.35865
C	3.90036	7.73161	9.49722
C	4.45356	6.46469	9.58779
H	5.11974	6.10228	8.80077
C	4.16762	5.65501	10.69753
C	3.33991	6.17597	11.68969
H	3.10966	5.56332	12.56027
C	2.78772	7.46708	11.61600
C	3.07474	8.24416	10.49481
H	2.67658	9.25010	10.36825
C	4.75674	4.24448	10.75526
C	4.38507	3.51733	12.04724
H	4.83203	2.51214	12.04984
H	4.75881	4.04807	12.93564
H	3.29638	3.39452	12.15016
C	4.21284	3.43809	9.56646
H	3.11484	3.36987	9.60588
H	4.48577	3.90072	8.60632
H	4.62159	2.41539	9.57485
C	6.28730	4.32529	10.66272
H	6.72704	3.31676	10.70671
H	6.61996	4.79215	9.72291
H	6.70181	4.91442	11.49450
C	1.89443	7.96981	12.75086
C	0.67233	7.04746	12.87238
H	0.01614	7.38948	13.68770
H	0.08584	7.04459	11.94066

H 0.96120 6.00906 13.09170
C 1.40402 9.39663 12.50581
H 2.23968 10.10896 12.42912
H 0.79835 9.47095 11.58948
H 0.77073 9.72088 13.34470
C 2.69192 7.94791 14.06329
H 3.03107 6.93408 14.32164
H 3.58053 8.59368 13.99530
H 2.06753 8.31156 14.89395
N 5.21795 5.30442 6.07005
N 6.92566 8.58459 5.38946
O 4.13111 8.55561 8.40709
P 4.65184 7.94449 6.97124
Ni 6.27376 6.88353 5.94743

Activation of the (NPN)Ni-Cl catalyst by SiH3Ph. Formation of the Ni-H catalyst
71
(NPN)NiCl = Monomer precatalyst with the chloride atom.
Cl 7.96752 5.73811 5.67842
C 5.40732 4.03572 5.99533
H 6.49439 3.92278 6.02065
C 4.55708 2.93470 5.77670
H 4.99978 1.94529 5.65649
C 3.20052 3.13122 5.71192
H 2.51573 2.29815 5.53521
C 2.68171 4.43674 5.89016
C 1.29501 4.72853 5.87674
H 0.59172 3.91226 5.69576
C 0.83316 6.00640 6.10415
H -0.23898 6.21084 6.10274
C 1.74264 7.05112 6.36071
H 1.36619 8.05181 6.58509
C 3.10224 6.80619 6.34579
C 3.60148 5.49570 6.11583
C 8.21184 8.81993 5.65228
H 8.86865 7.97888 5.88694
C 8.71900 10.02621 5.13077
H 9.79683 10.13048 5.00052
C 7.84971 11.02598 4.77087
H 8.21245 11.96019 4.33506
C 6.46058 10.84547 4.98089
C 5.48787 11.82845 4.67069
H 5.81792 12.76501 4.21505
C 4.15376 11.62187 4.94624
H 3.41859 12.39126 4.70360
C 3.73443 10.42983 5.57079
H 2.68212 10.29897 5.83190
C 4.65394 9.44222 5.86156
C 6.03033 9.61930 5.55293
C 3.86203 7.71183 9.36895
C 4.45823 6.46646 9.46208
H 5.11663 6.11365 8.66527
C 4.23500 5.67127 10.59600

```
C          3.42205        6.18810       11.60320
H          3.24291        5.58833       12.49465
C          2.82190        7.45669       11.52080
C          3.04860        8.22070       10.37610
H          2.61561        9.21111       10.24368
C          4.85491        4.27473       10.65702
C          4.68187        3.62934       12.03204
H          5.16498        2.64115       12.04220
H          5.14473        4.23504       12.82570
H          3.62229        3.47707       12.28626
C          4.15214        3.39804        9.60897
H          3.07493        3.31742        9.82033
H          4.26503        3.81684        8.59802
H          4.57899        2.38270        9.60485
C          6.35531        4.35046       10.34018
H          6.80630        3.34839       10.40303
H          6.55429        4.73379        9.32752
H          6.87809        5.00343       11.05514
C          1.94835        7.95416       12.67327
C          0.77780        6.98007       12.87274
H          0.13574        7.32159       13.69926
H          0.15892        6.91496       11.96460
H          1.12388        5.96549       13.11886
C          1.37993        9.34715       12.40218
H          2.17540       10.09721       12.27476
H          0.74009        9.36220       11.50631
H          0.76055        9.66676       13.25305
C          2.79639        8.01392       13.95250
H          3.19710        7.02705       14.22668
H          3.64721        8.70128       13.83024
H          2.18647        8.37175       14.79632
N          4.95954        5.27285        6.15045
N          6.91892        8.60911        5.84187
O          4.06035        8.53225        8.26118
P          4.42488        7.93089        6.79061
Ni         6.15733        6.83846        6.22007
86
Cl  -  (NPN)Ni-Cl catalyst and the phenylsilane interacting
Cl         2.37510       -1.22826       -2.67279
Ni         0.61169       -0.28733       -1.76092
Si         2.33534       -0.93672        1.16574
H          1.13450       -1.27901        0.33536
C          0.00207       -3.13464       -2.06123
H          1.09345       -3.19415       -2.05843
C         -0.79834       -4.26666       -2.31305
H         -0.31228       -5.22936       -2.47558
C         -2.16300       -4.13001       -2.36616
H         -2.80919       -4.98581       -2.57653
C         -2.74208       -2.85920       -2.12835
C         -4.14084       -2.63051       -2.11295
H         -4.81006       -3.46571       -2.33257
C         -4.65454       -1.38929       -1.80768
H         -5.73454       -1.23237       -1.78952
C         -3.78996       -0.32313       -1.48615
```

H	−4.21173	0.63957	−1.18879
C	−2.42121	−0.50264	−1.52451
C	−1.87005	−1.77091	−1.85860
C	2.40252	1.86353	−2.57337
H	3.12857	1.05010	−2.52851
C	2.75567	3.13579	−3.06749
H	3.78635	3.30789	−3.37877
C	1.80147	4.11510	−3.15846
H	2.04070	5.10487	−3.55486
C	0.48297	3.83823	−2.71903
C	−0.56282	4.79289	−2.74644
H	−0.35115	5.78798	−3.14494
C	−1.82056	4.48715	−2.27278
H	−2.61301	5.23736	−2.29581
C	−2.08389	3.21117	−1.73824
H	−3.07146	2.99194	−1.32703
C	−1.09121	2.25034	−1.72065
C	0.20924	2.53972	−2.21378
C	−1.30154	0.21327	1.68734
C	−1.45059	−1.16449	1.62313
H	−1.74195	−1.64147	0.68996
C	−1.22793	−1.94083	2.76462
C	−0.86109	−1.28830	3.94603
H	−0.67798	−1.88232	4.83776
C	−0.71223	0.10245	4.02177
C	−0.94756	0.85414	2.86599
H	−0.85779	1.94143	2.86177
N	−0.50527	−1.93102	−1.85417
N	1.17870	1.56408	−2.17498
O	−1.49567	1.03063	0.57932
P	−1.14017	0.63136	−0.96323
H	3.42146	−1.91173	0.86587
H	1.92497	−1.03808	2.59767
C	−0.27106	0.81763	5.29941
C	−1.35329	−3.46250	2.66044
C	1.07139	1.51558	5.03123
H	0.99405	2.26638	4.23053
H	1.42091	2.03165	5.93881
H	1.84202	0.78805	4.73366
C	−1.32862	1.85886	5.69229
H	−2.30266	1.38170	5.87941
H	−1.02320	2.38182	6.61160
H	−1.47060	2.62042	4.91091
C	−0.08881	−0.15298	6.46625
H	−1.02357	−0.67970	6.71145
H	0.68882	−0.90340	6.25832
H	0.22237	0.40187	7.36343
C	−1.25228	−4.14166	4.02636
H	−0.27273	−3.97403	4.49817
H	−2.03339	−3.78710	4.71570
H	−1.37686	−5.22853	3.91138
C	−2.70616	−3.83159	2.03487
H	−3.54065	−3.44485	2.63916
H	−2.81631	−3.43305	1.01435

```
H         -2.80897       -4.92594        1.97244
C         -0.21732       -3.98304        1.76655
H         -0.25810       -3.53832        0.76071
H          0.76621       -3.74238        2.19848
H         -0.28269       -5.07704        1.65745
C          2.89530        0.80997        0.75700
C          2.04494        1.90204        0.99331
C          4.16326        1.06143        0.21370
C          2.44366        3.20326        0.69485
H          1.05527        1.73331        1.42502
C          4.57197        2.36406       -0.07559
H          4.84502        0.22996        0.01508
C          3.71283        3.43623        0.16407
H          1.76840        4.04018        0.89008
H          5.56956        2.54270       -0.48466
H          4.03558        4.45651       -0.05723
86
TS_Si  -  TS for the coordination of phenylsilane to the Ni-Cl
catalyst
Cl         7.89324        5.44019        5.57914
Ni         6.19798        6.64044        6.30197
Si         7.66518        6.74339        8.69837
H          6.49875        6.09003        7.90076
C          5.04470        3.95997        5.52171
H          6.10942        3.70768        5.53809
C          4.07189        3.02696        5.10429
H          4.38861        2.02438        4.81368
C          2.75168        3.40298        5.06554
H          1.97504        2.70639        4.74010
C          2.39256        4.71566        5.46016
C          1.05870        5.19428        5.47366
H          0.25812        4.52722        5.14509
C          0.76827        6.47186        5.90025
H         -0.26455        6.82498        5.90941
C          1.79966        7.32583        6.34229
H          1.55306        8.32665        6.70480
C          3.11130        6.89441        6.32659
C          3.43545        5.58639        5.87809
C          7.54984        8.23934        4.24079
H          8.11092        7.30429        4.16326
C          7.87666        9.35799        3.44844
H          8.69260        9.27230        2.72964
C          7.18233       10.52988        3.61342
H          7.42850       11.42237        3.03284
C          6.12783       10.57652        4.55650
C          5.36420       11.74080        4.81827
H          5.60138       12.65581        4.27026
C          4.34723       11.73072        5.74794
H          3.77735       12.64023        5.94707
C          4.02893       10.54417        6.43911
H          3.22358       10.53997        7.17697
C          4.75126        9.39407        6.19489
C          5.83433        9.39059        5.28147
C          4.20700        7.34895        9.57536
```

```
C          4.17842        5.97324        9.39980
H          4.08161        5.54543        8.40341
C          4.31086        5.12713       10.50388
C          4.44369        5.71067       11.76773
H          4.54779        5.06359       12.63497
C          4.45306        7.09946       11.95749
C          4.33184        7.92209       10.83239
H          4.34570        9.01009       10.91294
N          4.74329        5.18992        5.89167
N          6.57338        8.24611        5.13152
O          4.15784        8.22356        8.49793
P          4.53307        7.80060        6.96935
H          8.82198        5.82651        8.55324
H          7.10909        6.74929       10.08161
C          4.62031        7.74117       13.33592
C          4.35638        3.61665       10.26742
C          5.91225        8.57263       13.33965
H          5.88841        9.37190       12.58371
H          6.05823        9.04738       14.32217
H          6.78867        7.93942       13.13288
C          3.41659        8.65130       13.61944
H          2.47700        8.07819       13.60746
H          3.51858        9.11796       14.61126
H          3.32717        9.46167       12.88052
C          4.71081        6.69743       14.44959
H          3.80461        6.07520       14.50299
H          5.58043        6.03486       14.32352
H          4.82177        7.20251       15.42033
C          4.35319        2.83102       11.57869
H          5.24103        3.04949       12.19051
H          3.45706        3.04646       12.18012
H          4.36115        1.75160       11.36684
C          3.14062        3.18348        9.43529
H          2.19932        3.43446        9.94725
H          3.12364        3.66267        8.44404
H          3.16159        2.09499        9.27252
C          5.64577        3.28902        9.49714
H          5.68107        3.80267        8.52376
H          6.53518        3.59336       10.07017
H          5.71810        2.20644        9.30902
C          8.01633        8.49362        8.13665
C          7.24148        9.55839        8.62468
C          9.02002        8.76709        7.19434
C          7.44533       10.85748        8.16305
H          6.47011        9.37209        9.37691
C          9.23181       10.06740        6.74167
H          9.62983        7.94963        6.79960
C          8.43903       11.11228        7.21879
H          6.83440       11.67632        8.55023
H         10.02187       10.26864        6.01427
H          8.60702       12.13208        6.86402
86
Si_2  -  Precatalytic structure. Phenylsilane already coordinated to
the Ni-Cl catalyst
```

Cl	3.13920	−1.36177	−1.62571
Si	2.40610	0.13322	0.99053
Ni	1.26937	−0.36934	−1.03218
H	1.35395	−1.06082	0.28350
C	0.34778	−2.73433	−2.79472
H	1.43139	−2.89594	−2.79509
C	−0.53063	−3.60567	−3.47601
H	−0.12293	−4.45984	−4.01862
C	−1.88203	−3.36135	−3.43489
H	−2.58962	−4.01838	−3.94683
C	−2.36554	−2.24233	−2.71158
C	−3.73900	−1.91577	−2.58828
H	−4.47775	−2.54905	−3.08543
C	−4.14290	−0.82595	−1.84775
H	−5.20475	−0.59104	−1.75337
C	−3.19125	−0.01075	−1.19995
H	−3.52462	0.83918	−0.59922
C	−1.84531	−0.29640	−1.31320
C	−1.40471	−1.41754	−2.06455
C	2.26097	1.10198	−3.41402
H	2.83955	0.17865	−3.50767
C	2.50062	2.20869	−4.25350
H	3.25156	2.12363	−5.04002
C	1.81079	3.37765	−4.04199
H	1.99945	4.26356	−4.65337
C	0.83905	3.43116	−3.01398
C	0.08102	4.58691	−2.69989
H	0.25519	5.50058	−3.27306
C	−0.85593	4.56744	−1.68973
H	−1.42459	5.46906	−1.45419
C	−1.09875	3.38356	−0.96098
H	−1.84847	3.37034	−0.16682
C	−0.37207	2.24740	−1.24610
C	0.62836	2.25417	−2.24945
C	−1.21403	0.02571	2.00057
C	−1.12685	−1.33065	1.71734
H	−0.97877	−1.67504	0.69594
C	−1.22505	−2.26233	2.75487
C	−1.42753	−1.77795	4.04962
H	−1.50467	−2.49401	4.86974
C	−1.53274	−0.41095	4.34254
C	−1.41938	0.50010	3.28829
H	−1.47351	1.57640	3.44458
N	−0.07148	−1.68434	−2.12143
N	1.37009	1.12251	−2.44120
O	−1.07048	0.98770	1.00319
P	−0.53250	0.63355	−0.48803
H	1.51862	0.32110	2.17306
H	3.53065	−0.78098	1.30035
C	2.87962	1.82805	0.35790
C	3.90568	2.01990	−0.58077
C	2.14611	2.94103	0.79948
C	4.18655	3.29394	−1.06624
H	4.47174	1.15854	−0.94528

```
C          2.42589        4.21577        0.30941
H          1.34695        2.81144        1.53527
C          3.44420        4.39183       -0.62585
H          4.99236        3.43405       -1.79069
H          1.85163        5.07490        0.66380
H          3.66885        5.39098       -1.00700
C         -1.09793       -3.76346        2.49187
C         -1.75156        0.04026        5.78757
C         -2.36802       -4.47346        2.98024
H         -2.29384       -5.55710        2.80001
H         -2.52997       -4.32687        4.05796
H         -3.25814       -4.09799        2.45257
C          0.12370       -4.29703        3.25430
H          1.04644       -3.79781        2.92026
H          0.02935       -4.13764        4.33835
H          0.23968       -5.37863        3.08391
C         -0.91147       -4.06896        1.00328
H         -1.76877       -3.72449        0.40301
H          0.00428       -3.60910        0.59876
H         -0.82301       -5.15543        0.85741
C         -0.57831       -0.45157        6.64813
H          0.37612       -0.03765        6.28830
H         -0.71518       -0.13498        7.69358
H         -0.49370       -1.54812        6.64164
C         -3.06513       -0.56300        6.30654
H         -3.04845       -1.66262        6.28859
H         -3.24199       -0.25017        7.34714
H         -3.92027       -0.22865        5.69949
C         -1.83523        1.56209        5.90653
H         -0.90785        2.05121        5.57085
H         -2.67610        1.97372        5.32737
H         -1.99161        1.84361        6.95821
86
TS_Cl_H  -  TS of the formation of the (NPN)Ni-H catalyst and
SiH2PhCl
Cl         7.98627        5.50924        6.97853
Si         7.36182        6.89799        8.89932
Ni         6.04157        6.54932        6.86866
H          5.47786        5.68659        7.85385
C          5.54974        4.54010        4.52674
H          6.63152        4.40581        4.63927
C          4.81269        3.74717        3.61970
H          5.32931        3.00733        3.00646
C          3.45074        3.91672        3.54317
H          2.84600        3.31235        2.86235
C          2.81964        4.88334        4.36538
C          1.42121        5.11492        4.37830
H          0.78289        4.52854        3.71300
C          0.87132        6.05583        5.22082
H         -0.20850        6.21633        5.23149
C          1.69463        6.81879        6.07695
H          1.24531        7.55180        6.75182
C          3.06209        6.63099        6.07478
C          3.65029        5.64993        5.22914
```

C	7.67707	8.11923	4.95799
H	8.29489	7.21821	5.00347
C	8.09254	9.24350	4.21747
H	9.02716	9.19774	3.65705
C	7.32333	10.38172	4.24236
H	7.63051	11.28158	3.70368
C	6.11500	10.38774	4.97964
C	5.26532	11.51735	5.08261
H	5.55361	12.43988	4.57332
C	4.09892	11.45890	5.81246
H	3.45771	12.33902	5.89076
C	3.71654	10.26162	6.45464
H	2.78780	10.22248	7.02846
C	4.52450	9.14759	6.37323
C	5.75083	9.19464	5.65915
C	3.46926	7.07416	9.59630
C	3.39168	5.69585	9.44825
H	3.17806	5.26842	8.46956
C	3.60231	4.87272	10.55863
C	3.84314	5.48748	11.79141
H	4.01849	4.85465	12.66326
C	3.87358	6.87828	11.95790
C	3.68110	7.67820	10.82743
H	3.71178	8.76565	10.87891
N	4.99498	5.45488	5.28909
N	6.56013	8.09207	5.65782
O	3.39325	7.90768	8.48183
P	4.22226	7.53882	7.12656
H	6.30177	6.52132	9.87607
H	8.66191	6.42636	9.44703
C	7.47058	8.73961	8.60063
C	8.58939	9.29744	7.96206
C	6.42944	9.59047	9.00177
C	8.65571	10.66654	7.71584
H	9.41954	8.65495	7.65325
C	6.50057	10.96225	8.76706
H	5.55412	9.17678	9.50820
C	7.60951	11.49999	8.11555
H	9.53280	11.08924	7.22003
H	5.68711	11.61443	9.09331
H	7.66574	12.57503	7.92889
C	3.62451	3.34921	10.43440
C	4.16230	7.47445	13.33621
C	2.61190	2.73561	11.41047
H	2.62811	1.63737	11.33668
H	2.83479	3.00051	12.45422
H	1.59019	3.07861	11.18711
C	5.04098	2.85899	10.77193
H	5.78136	3.29498	10.08266
H	5.33448	3.13133	11.79642
H	5.09833	1.76266	10.68692
C	3.27913	2.88679	9.01754
H	2.27129	3.21075	8.71439
H	4.00357	3.26001	8.27600

H 3.30033 1.78810 8.97094
C 5.55170 7.00600 13.79426
H 6.32974 7.33011 13.08575
H 5.79028 7.43017 14.78174
H 5.60865 5.91091 13.87924
C 3.09662 6.99150 14.33031
H 3.08659 5.89542 14.42173
H 3.29349 7.40657 15.33080
H 2.09123 7.31280 14.01854
C 4.15035 9.00311 13.31223
H 4.92314 9.40941 12.64121
H 3.17252 9.40093 13.00003
H 4.35682 9.39124 14.32044
86
H - (NPN)Ni-H catalyst already formed with the SiH2PhCl silane still interacting with the Ni atom.
Cl 3.20614 -1.42727 -0.96174
Si 3.42598 -0.49384 0.97296
Ni 1.10511 -0.45503 -1.14446
H 0.60338 -1.30258 -0.08543
C 0.37800 -2.53808 -3.52030
H 1.46535 -2.66076 -3.56815
C -0.45819 -3.35057 -4.31765
H -0.01570 -4.08762 -4.98954
C -1.81945 -3.19831 -4.21414
H -2.50236 -3.81412 -4.80490
C -2.34688 -2.23031 -3.32389
C -3.73691 -2.01725 -3.14539
H -4.44078 -2.62040 -3.72402
C -4.19465 -1.07241 -2.25515
H -5.26722 -0.92327 -2.11619
C -3.28151 -0.29211 -1.51440
H -3.65419 0.44111 -0.79444
C -1.92107 -0.46102 -1.67541
C -1.42107 -1.44476 -2.57853
C 2.66235 1.18908 -3.03517
H 3.31193 0.31006 -3.04050
C 3.02474 2.34256 -3.75815
H 3.94682 2.34024 -4.34093
C 2.21276 3.44939 -3.69993
H 2.47089 4.36734 -4.23392
C 1.02426 3.39756 -2.93311
C 0.13875 4.49595 -2.79153
H 0.37717 5.43250 -3.30118
C -0.99847 4.38898 -2.02316
H -1.66823 5.24449 -1.91515
C -1.31278 3.17332 -1.37680
H -2.21584 3.09757 -0.76687
C -0.47478 2.08629 -1.50002
C 0.72120 2.18301 -2.26023
C -1.43139 0.03223 1.77527
C -1.52347 -1.34718 1.63951
H -1.64781 -1.78474 0.65099
C -1.45236 -2.16029 2.77470

```
C         -1.31655       -1.53838        4.01939
H         -1.25551       -2.16369        4.91219
C         -1.25286       -0.14664        4.17071
C         -1.31110        0.64199        3.01828
H         -1.25873        1.72910        3.05984
N         -0.07551       -1.62396       -2.69226
N          1.56387        1.10309       -2.30949
O         -1.43469        0.86492        0.66748
P         -0.67808        0.46227       -0.72990
H          2.56857       -1.27931        1.89266
H          4.87909       -0.67684        1.22645
C          2.91768        1.28495        0.83275
C          3.66377        2.19916        0.07304
C          1.74599        1.72437        1.46923
C          3.23217        3.51581       -0.06963
H          4.58755        1.88263       -0.42037
C          1.32173        3.04381        1.33457
H          1.15107        1.02675        2.06528
C          2.05966        3.93744        0.55875
H          3.81694        4.21969       -0.66623
H          0.40660        3.37396        1.83096
H          1.72277        4.97073        0.44754
C         -1.48766       -3.68563        2.67095
C         -1.09950        0.46112        5.56587
C         -2.64488       -4.23149        3.51853
H         -2.67907       -5.33024        3.45626
H         -2.53933       -3.96269        4.57968
H         -3.61097       -3.83851        3.16684
C         -0.15376       -4.24221        3.19104
H          0.68954       -3.85998        2.59463
H          0.02280       -3.96478        4.24071
H         -0.14645       -5.34158        3.12930
C         -1.67728       -4.15477        1.22691
H         -2.62712       -3.79569        0.80095
H         -0.85549       -3.81858        0.57488
H         -1.69589       -5.25415        1.19325
C          0.19840       -0.06177        6.19874
H          1.07359        0.22160        5.59342
H          0.32984        0.36161        7.20659
H          0.19626       -1.15730        6.29530
C         -2.30122        0.04813        6.42809
H         -2.37603       -1.04436        6.53082
H         -2.20972        0.47294        7.43971
H         -3.24365        0.40977        5.98937
C         -1.03401        1.98807        5.52222
H         -0.17264        2.34474        4.93602
H         -1.95023        2.42621        5.09760
H         -0.92219        2.38394        6.54236

Structures of the Cycle with the (NPN)Ni-H catalyst
84
I - Coordination of the cyclopentene
H          5.80803        8.78760        8.35857
Ni         6.20148        7.63611        7.59745
```

C	7.49598	8.94699	10.36659
C	7.20732	7.43827	10.45029
C	7.52613	6.92716	9.07580
C	8.16973	7.87883	8.32577
C	8.39985	9.12945	9.13384
H	7.95355	9.34111	11.28455
H	6.17891	7.20322	10.76407
H	7.87704	6.92677	11.16623
H	7.46395	5.86245	8.83791
H	8.70672	7.68789	7.38987
H	8.19752	10.05610	8.57631
H	9.46892	9.15848	9.41325
H	6.55140	9.49195	10.21800
C	7.37223	5.28908	6.22725
H	8.25719	5.56261	6.80810
C	7.41534	4.15688	5.39192
H	8.33391	3.57218	5.32918
C	6.28966	3.81129	4.68397
H	6.27902	2.93158	4.03562
C	5.12694	4.60993	4.79619
C	3.92351	4.32450	4.10153
H	3.88761	3.44561	3.45360
C	2.82210	5.13765	4.23803
H	1.90038	4.90789	3.69986
C	2.88029	6.27854	5.06833
H	2.00582	6.92789	5.16150
C	4.03325	6.58100	5.76042
C	5.17744	5.74820	5.64910
C	6.66241	9.40186	3.85345
H	7.54732	8.76423	3.74809
C	6.49734	10.52202	3.00494
H	7.25202	10.74319	2.24824
C	5.38416	11.31582	3.15573
H	5.22616	12.19145	2.52084
C	4.43100	10.99009	4.15172
C	3.24866	11.73249	4.40516
H	3.03933	12.61751	3.79930
C	2.37841	11.34802	5.40048
H	1.47401	11.92998	5.58906
C	2.64010	10.20312	6.18940
H	1.95001	9.90737	6.98237
C	3.77668	9.46006	5.95476
C	4.69642	9.83892	4.94244
C	3.30461	7.24004	9.16512
C	3.63564	5.89444	9.13232
H	3.64482	5.37062	8.17514
C	3.91965	5.21532	10.32715
C	3.85037	5.93690	11.51852
H	4.06501	5.42732	12.45718
C	3.51123	7.30143	11.56312
C	3.23932	7.95197	10.35930
H	2.98199	9.00936	10.31746
N	6.30663	6.05598	6.36778
N	5.79939	9.06911	4.78545

```
O          3.04708        7.92366        7.98506
P          4.26126        7.99774        6.87906
C          4.27662        3.72870       10.26946
C          3.46340        8.02447       12.91033
C          4.54306        3.14659       11.65737
H          4.79594        2.07943       11.57146
H          5.38657        3.64681       12.15724
H          3.66007        3.22496       12.30899
C          3.11156        2.95881        9.63036
H          2.18787        3.08964       10.21371
H          2.90992        3.29688        8.60263
H          3.34049        1.88258        9.58922
C          5.54056        3.54557        9.41602
H          5.40819        3.94003        8.39678
H          6.39800        4.06157        9.87541
H          5.79550        2.47772        9.33203
C          2.42356        7.33835       13.80850
H          1.42469        7.36808       13.34748
H          2.67552        6.28480       13.99904
H          2.36593        7.84853       14.78240
C          4.84750        7.95187       13.57200
H          5.60618        8.45988       12.95665
H          4.82499        8.44514       14.55604
H          5.17621        6.91369       13.72755
C          3.07885        9.49605       12.75770
H          3.80350       10.04710       12.13837
H          2.07967        9.61487       12.31188
H          3.05824        9.97789       13.74631
84
TS_I_II - TS for the C-H bond formation
H          5.95043        8.89409        8.14640
Ni         6.32250        7.63889        7.56631
C          7.13628        8.52035       10.62797
C          7.50995        7.07378       10.26006
C          7.93480        7.16946        8.81438
C          8.06695        8.48559        8.43353
C          7.88030        9.40067        9.61631
H          7.38196        8.76982       11.66926
H          6.68258        6.36830       10.43093
H          8.36897        6.70675       10.85120
H          8.41124        6.33246        8.30471
H          8.56639        8.81299        7.51471
H          7.36768       10.34534        9.38475
H          8.88972        9.66569        9.98167
H          6.05041        8.65427       10.50766
C          7.31379        5.14023        6.27140
H          8.23801        5.37471        6.80072
C          7.26325        3.97514        5.48324
H          8.14430        3.33529        5.42125
C          6.09939        3.66901        4.82308
H          6.01350        2.76500        4.21512
C          4.99725        4.54929        4.92789
C          3.76479        4.31655        4.26504
H          3.65954        3.41377        3.65888
```

C	2.72400	5.20900	4.37654
H	1.77997	5.01990	3.86184
C	2.87727	6.37928	5.15068
H	2.05446	7.09506	5.22542
C	4.06006	6.62789	5.81264
C	5.14351	5.71657	5.72992
C	6.60897	9.21009	3.59205
H	7.44606	8.51859	3.44441
C	6.43491	10.30295	2.71009
H	7.13498	10.44967	1.88579
C	5.38204	11.16436	2.91356
H	5.21871	12.02079	2.25430
C	4.49840	10.93412	3.99665
C	3.38123	11.75095	4.30961
H	3.16978	12.62125	3.68350
C	2.57575	11.45528	5.38644
H	1.72055	12.09293	5.61929
C	2.84069	10.33037	6.20256
H	2.20141	10.10433	7.05837
C	3.91540	9.51732	5.91357
C	4.76710	9.80296	4.81476
C	3.43601	7.35450	9.17815
C	3.76900	6.00937	9.11320
H	3.80175	5.51148	8.14435
C	4.02218	5.29191	10.29144
C	3.91002	5.97181	11.50382
H	4.09799	5.43187	12.43105
C	3.54859	7.32827	11.58393
C	3.31829	8.02102	10.39435
H	3.05313	9.07734	10.38164
N	6.30471	5.97939	6.42091
N	5.80953	8.96533	4.60435
O	3.21805	8.08150	8.01709
P	4.39293	8.06960	6.86442
C	4.36781	3.80430	10.19848
C	3.40725	7.99161	12.95480
C	4.81285	3.23510	11.54572
H	5.08314	2.17490	11.43183
H	5.69309	3.76496	11.94144
H	4.01235	3.28721	12.29824
C	3.11862	3.04449	9.72695
H	2.28720	3.17778	10.43518
H	2.77860	3.39707	8.74116
H	3.33072	1.96672	9.64672
C	5.50159	3.59170	9.18434
H	5.21114	3.90215	8.16977
H	6.40236	4.15800	9.46786
H	5.77093	2.52545	9.13585
C	2.25850	7.30806	13.71242
H	1.31013	7.40592	13.16265
H	2.45080	6.23556	13.86385
H	2.12837	7.76857	14.70406
C	4.71321	7.82955	13.74552
H	5.55415	8.30614	13.21988

```
H          4.61850        8.30278       14.73495
H          4.97116        6.77310       13.90909
C          3.09587        9.48386       12.83904
H          3.89012       10.02739       12.30389
H          2.14138        9.66582       12.32240
H          3.01363        9.92458       13.84346
84
II - Ni-Alkyl post TS. Agostic interaction.
H          6.38112        9.08964        8.35566
Ni         6.39387        7.74111        7.52902
C          7.21390        7.25331       10.51964
C          8.25493        6.74640        9.51979
C          8.11634        7.70373        8.35018
C          7.49430        8.94283        8.84158
C          7.24900        8.77021       10.34137
H          7.40813        6.93641       11.55387
H          8.11070        5.68675        9.25306
H          9.27263        6.82355        9.94576
H          8.92936        7.77354        7.61578
H          7.92356        9.89819        8.50857
H          6.34146        9.27593       10.70217
H          8.10931        9.20627       10.87548
H          6.21353        6.87457       10.24777
C          7.41066        5.28421        6.47148
H          8.29687        5.57786        7.03282
C          7.40427        4.07254        5.75693
H          8.29466        3.44295        5.77163
C          6.27447        3.70968        5.06612
H          6.22986        2.77115        4.50806
C          5.15070        4.56848        5.07902
C          3.94561        4.26513        4.39505
H          3.88362        3.32910        3.83516
C          2.87586        5.12913        4.43379
H          1.95278        4.88526        3.90437
C          2.97001        6.33737        5.15711
H          2.11986        7.02425        5.18348
C          4.12613        6.66080        5.83464
C          5.24029        5.78254        5.81678
C          6.58564        9.31764        3.60675
H          7.47088        8.67914        3.51011
C          6.36622       10.36269        2.67822
H          7.07932       10.52495        1.86812
C          5.25384       11.15938        2.81948
H          5.05487       11.97821        2.12326
C          4.35493       10.91135        3.88598
C          3.17816       11.66361        4.13671
H          2.92962       12.49519        3.47276
C          2.36157       11.35360        5.20107
H          1.46016       11.94144        5.38589
C          2.67312       10.27723        6.06516
H          2.02290       10.03900        6.90954
C          3.80619        9.52611        5.83739
C          4.67168        9.83102        4.75407
C          3.36961        7.42035        9.14533
```

```
C          3.60980        6.05516        9.10408
H          3.58127        5.53731        8.14508
C          3.86141        5.35128       10.29087
C          3.83657        6.06374       11.48914
H          4.02308        5.53340       12.42203
C          3.57968        7.44488       11.54654
C          3.35399        8.12336       10.34798
H          3.15651        9.19430       10.31770
N          6.37895        6.11254        6.51681
N          5.77356        9.05807        4.60537
O          3.14087        8.12503        7.97356
P          4.35672        8.14596        6.85344
C          4.14997        3.85121       10.21445
C          3.55047        8.15105       12.90362
C          4.44592        3.25221       11.58910
H          4.65261        2.17630       11.48982
H          5.32687        3.71700       12.05773
H          3.59245        3.36089       12.27488
C          2.92962        3.13525        9.61753
H          2.03712        3.29225       10.24160
H          2.69811        3.49642        8.60390
H          3.11505        2.05177        9.55267
C          5.37071        3.62091        9.31025
H          5.19463        3.98213        8.28583
H          6.25716        4.14080        9.70558
H          5.60400        2.54655        9.24891
C          2.42286        7.54270       13.75125
H          1.44762        7.66548       13.25636
H          2.57773        6.46809       13.92789
H          2.37342        8.03897       14.73285
C          4.89557        7.95018       13.61623
H          5.72006        8.39491       13.03844
H          4.87717        8.43311       14.60530
H          5.12632        6.88606       13.77093
C          3.29835        9.65202       12.76291
H          4.08380       10.14596       12.16956
H          2.32556        9.86315       12.29366
H          3.29285       10.12304       13.75688

Formation of the C-Si bond = Silane Product
99
III  -  Inclusion of the silane forming the Ni-C-Si-H ordering
Si         0.03121       -0.06749        2.48419
C          1.18976       -2.76135        1.60320
H         -0.46942       -1.19477        1.18100
Ni         0.87441       -1.10278        0.62976
H         -0.26733       -0.97858        3.62419
H          1.85128       -3.22398        0.84115
C          0.72977       -3.40250       -1.54987
H          0.97062       -4.00064       -0.66757
C          0.53080       -4.04478       -2.79024
H          0.62164       -5.13011       -2.85242
C          0.21733       -3.28395       -3.88899
H          0.04572       -3.74316       -4.86574
```

C	0.11430	−1.87915	−3.74893
C	−0.21811	−1.01761	−4.82397
H	−0.40063	−1.45359	−5.80904
C	−0.31851	0.34181	−4.63251
H	−0.58618	0.99572	−5.46468
C	−0.07984	0.89727	−3.35827
H	−0.17821	1.97552	−3.20948
C	0.25763	0.08555	−2.29469
C	0.34926	−1.32133	−2.45843
C	3.86389	−1.35075	0.70397
H	3.60827	−2.36805	1.00268
C	5.20741	−0.93012	0.74459
H	5.97498	−1.63131	1.07456
C	5.51433	0.35924	0.38657
H	6.54138	0.72989	0.43022
C	4.48085	1.21354	−0.06319
C	4.70817	2.54818	−0.48252
H	5.72552	2.94387	−0.43913
C	3.67280	3.33166	−0.93866
H	3.86055	4.35951	−1.25502
C	2.36504	2.80843	−1.00811
H	1.54375	3.43068	−1.37046
C	2.11420	1.51737	−0.59609
C	3.15640	0.69502	−0.09513
N	0.64259	−2.10102	−1.37544
N	2.86375	−0.57538	0.33336
O	−0.51486	1.94864	−0.44655
P	0.52297	0.68670	−0.60608
C	1.77826	−4.37507	3.29990
H	1.70195	−4.53459	4.38533
H	2.68347	−4.90760	2.96990
C	0.53643	−4.88981	2.53576
H	0.82687	−5.66175	1.80567
H	−0.20762	−5.35439	3.19904
C	−0.02929	−3.65833	1.81280
H	−0.57507	−3.90655	0.88983
H	−0.74996	−3.14168	2.46901
C	1.88745	−2.87620	2.95670
H	1.34376	−2.29055	3.71440
H	2.92779	−2.52007	2.96780
H	−1.15600	0.79918	2.23659
C	−1.86845	1.72276	−0.23561
C	−2.60696	2.78736	0.27393
C	−2.44829	0.49232	−0.49353
C	−3.96298	2.61271	0.54685
H	−2.09515	3.73047	0.46002
C	−3.80713	0.28556	−0.21854
H	−1.85376	−0.32604	−0.90030
C	−4.53864	1.35347	0.29520
H	−5.59626	1.21341	0.51510
C	1.48796	1.06916	2.82431
C	2.68128	0.61815	3.41099
C	1.40577	2.41295	2.42713
C	3.76122	1.47904	3.58486

```
H          2.76873       -0.41860        3.74048
C          2.48725        3.27635        2.59899
H          0.48578        2.79150        1.97277
C          3.66790        2.80957        3.17277
H          4.67889        1.11339        4.05185
H          2.40521        4.32024        2.28718
H          4.51433        3.48648        3.31118
C         -4.82953        3.73473        1.12033
C         -4.39976       -1.09772       -0.48997
C         -5.41687        3.27802        2.46406
H         -4.61838        3.03811        3.18282
H         -6.03891        4.07617        2.89782
H         -6.05066        2.38582        2.35440
C         -4.02917        5.01643        1.35237
H         -3.20897        4.86327        2.07064
H         -3.60319        5.40940        0.41645
H         -4.68702        5.79483        1.76626
C         -5.96742        4.04084        0.13521
H         -6.60573        3.16233       -0.03963
H         -6.60788        4.84473        0.53004
H         -5.56964        4.36783       -0.83761
C         -5.87940       -1.17095       -0.11512
H         -6.03960       -0.96740        0.95436
H         -6.48363       -0.45866       -0.69686
H         -6.26696       -2.17938       -0.32251
C         -3.63077       -2.13995        0.33745
H         -2.56446       -2.17566        0.06463
H         -3.69561       -1.91551        1.41332
H         -4.04942       -3.14504        0.17292
C         -4.25302       -1.42213       -1.98431
H         -4.78416       -0.68236       -2.60215
H         -3.19832       -1.42874       -2.30115
H         -4.67410       -2.41593       -2.20278
99
TSA1 - TS for the C-Si bond formation
Si        -5.53475       -3.16349        5.15039
C         -4.09646       -4.97877        4.67103
H         -5.60163       -4.00153        2.98060
Ni        -4.29848       -3.50073        3.29178
H         -6.24519       -4.18618        5.96907
H         -3.14153       -5.03333        4.11266
C         -2.46303       -5.75218        1.70545
H         -2.27566       -6.07519        2.73671
C         -1.94821       -6.51230        0.63310
H         -1.35388       -7.40386        0.83852
C         -2.22721       -6.11436       -0.65216
H         -1.86209       -6.68389       -1.51053
C         -3.00338       -4.94945       -0.86601
C         -3.35530       -4.47031       -2.15268
H         -3.01060       -5.01935       -3.03220
C         -4.12462       -3.33757       -2.29383
H         -4.40258       -2.98431       -3.28876
C         -4.55744       -2.62096       -1.15702
H         -5.17467       -1.72768       -1.27763
```

C	−4.21527	−3.05186	0.10847
C	−3.45157	−4.23742	0.28382
C	−1.80891	−2.58152	4.60586
H	−1.93343	−3.51896	5.14756
C	−0.78056	−1.69234	4.97135
H	−0.11136	−1.95922	5.78969
C	−0.66402	−0.49875	4.30330
H	0.10807	0.22622	4.57217
C	−1.56753	−0.20130	3.25541
C	−1.54334	1.01814	2.53309
H	−0.78025	1.75952	2.78144
C	−2.46957	1.27315	1.54655
H	−2.44776	2.22108	1.00540
C	−3.45074	0.31036	1.22838
H	−4.18744	0.51875	0.44832
C	−3.49223	−0.89087	1.90587
C	−2.56535	−1.16587	2.94341
N	−3.18204	−4.66490	1.54702
N	−2.67348	−2.34112	3.63973
O	−6.06553	−1.46136	1.14790
P	−4.69839	−2.21620	1.63176
C	−3.34933	−6.73297	6.09314
H	−3.28758	−7.17526	7.09847
H	−2.36420	−6.87916	5.61806
C	−4.46087	−7.34648	5.23259
H	−4.11155	−8.22642	4.67323
H	−5.28803	−7.69151	5.87073
C	−4.94304	−6.20825	4.30326
H	−4.84211	−6.45262	3.23570
H	−6.01253	−6.00403	4.46787
C	−3.68146	−5.24133	6.12749
H	−4.52285	−5.07997	6.82060
H	−2.84686	−4.62146	6.48398
H	−6.60975	−2.34036	4.52532
C	−7.07069	−1.21725	2.08300
C	−7.02354	−0.05025	2.83897
C	−8.06268	−2.16605	2.24330
C	−7.99737	0.17002	3.81412
H	−6.22261	0.66501	2.65379
C	−9.04758	−1.97591	3.22309
H	−8.03881	−3.06054	1.61874
C	−8.99036	−0.80838	3.98602
H	−9.74547	−0.64736	4.75454
C	−4.56253	−1.93061	6.19524
C	−3.98787	−2.17740	7.45070
C	−4.41472	−0.64380	5.64806
C	−3.27112	−1.18507	8.12058
H	−4.10877	−3.15073	7.93021
C	−3.69645	0.34864	6.30944
H	−4.88287	−0.41456	4.68595
C	−3.11508	0.07609	7.54808
H	−2.84031	−1.39639	9.10231
H	−3.59972	1.34195	5.86360
H	−2.55556	0.85226	8.07566

```
C         -8.00416        1.41942        4.69534
C        -10.09990       -3.06223        3.44399
C         -7.88156        0.99650        6.16720
H         -6.94520        0.44641        6.34574
H         -7.88732        1.88349        6.81967
H         -8.71614        0.35086        6.47737
C         -6.84611        2.36099        4.36159
H         -5.86823        1.88022        4.51856
H         -6.89511        2.71852        3.32157
H         -6.88573        3.24417        5.01610
C         -9.32242        2.17705        4.48059
H        -10.19497        1.56252        4.74580
H         -9.34917        3.08181        5.10753
H         -9.43450        2.48488        3.42983
C        -11.10375       -2.67804        4.53106
H        -10.61648       -2.53067        5.50681
H        -11.65228       -1.75885        4.27516
H        -11.84487       -3.48193        4.65212
C         -9.38598       -4.35365        3.87421
H         -8.67603       -4.70369        3.10907
H         -8.82524       -4.19937        4.80898
H        -10.11833       -5.15841        4.04295
C        -10.86497       -3.30407        2.13534
H        -11.37468       -2.38748        1.80184
H        -10.19967       -3.63375        1.32353
H        -11.62711       -4.08573        2.27799
99
IV  -  Product post TS. New silane formed: PhSiH2Cyclopentyl, with
still a strong interaction with the Ni atom.
Si        -0.63905       -1.04094        2.31771
C          0.37251       -2.54291        1.65256
H         -0.49151       -1.61453       -0.67790
Ni         0.72311       -1.06443       -0.10683
H         -1.37194       -1.71537        3.43874
H          1.11325       -2.48048        0.79828
C          2.80410       -3.21947       -1.67092
H          3.04971       -3.52310       -0.64666
C          3.32857       -3.94747       -2.76165
H          3.98483       -4.80008       -2.58021
C          2.98286       -3.56512       -4.03542
H          3.35600       -4.10813       -4.90749
C          2.12688       -2.45198       -4.22166
C          1.71002       -1.99710       -5.49803
H          2.06736       -2.52188       -6.38734
C          0.86474       -0.91793       -5.61649
H          0.53775       -0.58258       -6.60267
C          0.41345       -0.23455       -4.46608
H         -0.26821        0.61304       -4.56914
C          0.81509       -0.64071       -3.21005
C          1.66898       -1.77128       -3.05647
C          3.08307       -0.10465        1.36264
H          2.95168       -1.03727        1.91303
C          4.10130        0.79414        1.73417
H          4.75961        0.53976        2.56508
```

C	4.22084	1.98234	1.05659
H	4.98564	2.71316	1.33038
C	3.32970	2.26822	−0.00558
C	3.35269	3.48250	−0.73684
H	4.10295	4.23466	−0.48183
C	2.44193	3.71857	−1.74265
H	2.46378	4.66240	−2.29101
C	1.48035	2.74051	−2.07583
H	0.76314	2.93174	−2.87817
C	1.43940	1.54456	−1.38954
C	2.34711	1.29320	−0.32812
N	2.01272	−2.17959	−1.80535
N	2.23653	0.12203	0.37726
O	−1.12397	0.84339	−2.13927
P	0.29096	0.16757	−1.68401
C	1.19237	−4.63363	2.57401
H	1.52253	−5.20749	3.45252
H	1.84252	−4.92365	1.72926
C	−0.27187	−4.85681	2.21395
H	−0.46775	−5.83856	1.75906
H	−0.88404	−4.79700	3.12849
C	−0.61079	−3.69430	1.27392
H	−0.45702	−3.97785	0.22283
H	−1.66704	−3.39230	1.35578
C	1.25554	−3.12523	2.79050
H	0.81954	−2.88780	3.77537
H	2.28003	−2.72425	2.79723
H	−1.63799	−0.49121	1.36343
C	−2.10010	1.07548	−1.17068
C	−2.05827	2.25563	−0.43407
C	−3.07620	0.11570	−0.97551
C	−3.02699	2.48547	0.54451
H	−1.27354	2.98093	−0.64730
C	−4.05862	0.31741	0.00525
H	−3.05215	−0.78726	−1.58742
C	−4.00695	1.49970	0.74538
H	−4.76331	1.67287	1.51002
C	0.38175	0.36674	3.03038
C	1.15403	0.21460	4.19271
C	0.38194	1.61898	2.39559
C	1.91385	1.27097	4.69453
H	1.15674	−0.73835	4.72935
C	1.13920	2.67765	2.89346
H	−0.22419	1.76591	1.49683
C	1.90992	2.50372	4.04294
H	2.50176	1.13532	5.60557
H	1.12358	3.64574	2.38640
H	2.49891	3.33433	4.43942
C	−3.06010	3.76832	1.37651
C	−5.12372	−0.75643	0.23153
C	−2.97496	3.41432	2.86865
H	−2.03648	2.88911	3.10165
H	−3.01355	4.33051	3.47814
H	−3.80914	2.77140	3.18524

```
C         -1.90058        4.70355        1.03047
H         -0.92362        4.23075        1.21404
H         -1.93573        5.02900       -0.02049
H         -1.95195        5.60641        1.65664
C         -4.37773        4.50637        1.09593
H         -5.25213        3.89761        1.36840
H         -4.42427        5.43843        1.68024
H         -4.46661        4.76480        0.02977
C         -6.11831       -0.35896        1.32237
H         -5.62417       -0.21154        2.29474
H         -6.66075        0.56362        1.06598
H         -6.86576       -1.15584        1.45070
C         -4.43462       -2.06239        0.65509
H         -3.72012       -2.41417       -0.10462
H         -3.88587       -1.92677        1.59973
H         -5.18142       -2.85737        0.80562
C         -5.89680       -0.98108       -1.07593
H         -6.38688       -0.05325       -1.40771
H         -5.24000       -1.32429       -1.88907
H         -6.67561       -1.74598       -0.93205
28
PhSiH2Cyclopentyl product
Si         4.43426       -0.67994       -0.92250
C          3.52520        0.44315        0.28927
H          3.64897       -1.93424       -1.15312
C          3.50448        2.26684        1.83835
H          2.53506        2.69329        1.53027
H          4.04677        3.05696        2.38018
C          3.28420        1.00381        2.68184
H          4.10492        0.88262        3.40606
H          2.35589        1.05748        3.27005
C          3.27816       -0.17822        1.68063
H          4.07512       -0.89533        1.94063
H          2.33613       -0.74619        1.70253
C          4.24127        1.76401        0.59913
H          4.22427        2.47188       -0.24364
H          5.30289        1.57629        0.84584
H          2.55019        0.69090       -0.16998
H          5.76276       -1.03857       -0.32712
C          4.70091        0.18049       -2.57254
C          5.77049        1.07196       -2.75303
C          3.80613       -0.00067       -3.63810
C          5.93859        1.76099       -3.95268
H          6.49003        1.22983       -1.94364
C          3.96964        0.68596       -4.84039
H          2.96683       -0.69470       -3.53083
C          5.03663        1.56897       -4.99880
H          6.77920        2.44885       -4.07395
H          3.26277        0.52897       -5.65906
H          5.16803        2.10653       -5.94120

Formation of the second C-C bond = Alkane Product
99
V - Insertion of the silane (PhSiH3) forming the Ni-C-H-Si sequence.
```

Si	−0.26512	−0.24617	2.55760
C	0.43763	−3.29161	1.62810
H	0.96891	−1.11882	2.02237
Ni	0.48096	−1.59914	0.67142
H	−1.60805	−0.27088	1.91727
H	0.64242	−4.00939	0.81829
C	−0.67814	−3.55360	−1.18858
H	−1.00753	−4.01981	−0.26072
C	−0.93443	−4.19212	−2.41549
H	−1.47427	−5.13966	−2.41757
C	−0.47968	−3.61602	−3.57595
H	−0.63551	−4.09535	−4.54558
C	0.18323	−2.36878	−3.51059
C	0.64282	−1.68144	−4.66229
H	0.51405	−2.15340	−5.63913
C	1.22297	−0.43816	−4.55724
H	1.56814	0.08485	−5.45112
C	1.34478	0.17822	−3.29435
H	1.76110	1.18611	−3.21803
C	0.92800	−0.47415	−2.15265
C	0.36315	−1.77024	−2.23092
C	3.91040	−2.24010	0.54127
H	3.53830	−3.26848	0.58223
C	5.26536	−1.96300	0.83475
H	5.93928	−2.78154	1.09264
C	5.70491	−0.65980	0.79805
H	6.74353	−0.41000	1.02981
C	4.79646	0.37031	0.45187
C	5.13238	1.74763	0.38050
H	6.15664	2.05431	0.60620
C	4.18384	2.68389	0.03533
H	4.45228	3.74140	−0.00725
C	2.85680	2.29633	−0.26371
H	2.10302	3.04451	−0.51586
C	2.50927	0.96557	−0.20989
C	3.46182	−0.01977	0.15995
N	−0.03338	−2.40371	−1.07730
N	3.03993	−1.30907	0.22072
O	0.03108	1.67344	−0.74729
P	0.87626	0.27931	−0.50382
C	0.72001	−4.01326	3.97139
H	0.46696	−3.16285	4.62588
H	1.29494	−4.72512	4.58163
C	−0.56322	−4.60450	3.39514
H	−0.36467	−5.60094	2.96443
H	−1.36504	−4.72189	4.13966
C	−0.91440	−3.61779	2.28181
H	−1.66782	−4.00738	1.57855
H	−1.37540	−2.72502	2.73987
C	1.49675	−3.52066	2.73984
H	2.10816	−2.63475	2.97424
H	2.21094	−4.29256	2.40989
H	−0.31295	−0.89363	3.89998
C	−1.34606	1.69699	−0.80248

```
C         -1.94843        2.95385       -0.75958
C         -2.10075        0.53857       -0.88397
C         -3.33797        3.05409       -0.78073
H         -1.30410        3.82956       -0.69765
C         -3.50115        0.60911       -0.90895
H         -1.60884       -0.43359       -0.91412
C         -4.09295        1.86850       -0.85451
H         -5.17948        1.94501       -0.87101
C         -4.29615       -0.69470       -0.99869
C         -5.80428       -0.44849       -1.01056
H         -6.11275        0.15815       -1.87521
H         -6.33849       -1.40825       -1.07207
H         -6.14157        0.05926       -0.09445
C         -3.90803       -1.42749       -2.29214
H         -4.12895       -0.81062       -3.17619
H         -2.83563       -1.67499       -2.31669
H         -4.47135       -2.36955       -2.38212
C         -3.95389       -1.57764        0.21092
H         -2.88023       -1.81745        0.25431
H         -4.22237       -1.07667        1.15354
H         -4.50848       -2.52791        0.16142
C         -4.05686        4.40244       -0.71611
C         -4.95544        4.43168        0.52906
H         -5.48704        5.39367        0.59375
H         -5.71191        3.63383        0.50816
H         -4.36089        4.30844        1.44761
C         -3.07567        5.57187       -0.63235
H         -2.44758        5.51558        0.27050
H         -2.41561        5.61765       -1.51192
H         -3.63095        6.52029       -0.58679
C         -4.91452        4.57576       -1.97818
H         -4.29150        4.54905       -2.88515
H         -5.67549        3.78676       -2.06884
H         -5.43936        5.54327       -1.95242
C          0.47621        1.46258        2.62956
C          1.80962        1.63190        3.03826
C         -0.27429        2.59635        2.28769
C          2.37867        2.90014        3.09957
H          2.41755        0.76275        3.31018
C          0.29686        3.86668        2.34266
H         -1.31297        2.49090        1.96325
C          1.62214        4.01892        2.74758
H          3.41628        3.01802        3.41961
H         -0.29884        4.74230        2.07305
H          2.06716        5.01573        2.79601
99
TSA2 - TS to form the second C-H bond = Alkane generation
Si        -4.84544       -1.86883        5.29195
C         -4.13309       -4.98306        4.68035
H         -4.05036       -3.34524        5.01153
Ni        -4.12486       -3.33140        3.55314
H         -6.17921       -1.52479        4.72590
H         -3.75153       -5.62770        3.87458
C         -4.91585       -5.50552        1.68291
```

H	−5.16018	−6.01033	2.61818
C	−5.10329	−6.18194	0.46244
H	−5.50022	−7.19775	0.47304
C	−4.77165	−5.54815	−0.70975
H	−4.88978	−6.04502	−1.67586
C	−4.28202	−4.22220	−0.65927
C	−3.94928	−3.47786	−1.81898
H	−4.04789	−3.95758	−2.79556
C	−3.52412	−2.17260	−1.72091
H	−3.27680	−1.60614	−2.62074
C	−3.42605	−1.55456	−0.45675
H	−3.12010	−0.50763	−0.38529
C	−3.72691	−2.25829	0.69049
C	−4.14648	−3.60777	0.61785
C	−0.78395	−4.03775	3.60799
H	−1.18287	−5.04796	3.74420
C	0.58210	−3.77632	3.85696
H	1.23702	−4.58772	4.17840
C	1.05703	−2.49528	3.69345
H	2.10642	−2.25620	3.88430
C	0.17153	−1.47400	3.27257
C	0.54602	−0.11854	3.08176
H	1.58360	0.17362	3.26069
C	−0.38329	0.81620	2.68699
H	−0.08647	1.85883	2.55716
C	−1.72801	0.44708	2.44935
H	−2.46350	1.19674	2.15182
C	−2.11250	−0.86392	2.61413
C	−1.18003	−1.84621	3.04031
N	−4.44341	−4.27555	1.77923
N	−1.63408	−3.11392	3.21781
O	−4.61981	−0.14671	2.16076
P	−3.76014	−1.53538	2.35468
C	−4.16552	−5.65524	7.05080
H	−4.54741	−4.78530	7.61036
H	−3.66599	−6.31162	7.77805
C	−5.31869	−6.32788	6.31317
H	−5.01194	−7.32676	5.95829
H	−6.21759	−6.46142	6.93307
C	−5.54460	−5.39565	5.12342
H	−6.14631	−5.85024	4.32143
H	−6.12138	−4.51760	5.46377
C	−3.22726	−5.19167	5.92915
H	−2.64375	−4.30179	6.21742
H	−2.48489	−5.97626	5.71106
H	−5.06518	−2.47554	6.64541
C	−5.99966	−0.16059	2.08093
C	−6.64512	1.06904	2.19565
C	−6.71063	−1.33713	1.91358
C	−8.03796	1.12157	2.15399
H	−6.03542	1.96292	2.32022
C	−8.11103	−1.31561	1.87921
H	−6.18743	−2.29030	1.83765
C	−8.74842	−0.08278	1.99688

H -9.83672 -0.04393 1.96959
C -8.85272 -2.64526 1.73644
C -10.36767 -2.45465 1.67926
H -10.66864 -1.83544 0.82075
H -10.86365 -3.43109 1.57464
H -10.75456 -1.98503 2.59605
C -8.39658 -3.34537 0.44724
H -8.60771 -2.72337 -0.43573
H -7.31653 -3.55996 0.45529
H -8.92534 -4.30365 0.32536
C -8.51219 -3.53010 2.94610
H -7.43079 -3.72560 3.01730
H -8.82649 -3.05030 3.88559
H -9.02686 -4.50092 2.86971
C -8.80657 2.43796 2.27889
C -9.75165 2.35686 3.48675
H -10.31170 3.29851 3.59531
H -10.48601 1.54473 3.38237
H -9.18905 2.18514 4.41731
C -7.87255 3.63188 2.47593
H -7.27328 3.53550 3.39460
H -7.18662 3.76182 1.62488
H -8.46397 4.55502 2.56514
C -9.62273 2.66291 0.99738
H -8.96543 2.72052 0.11637
H -10.34694 1.85315 0.82503
H -10.18677 3.60608 1.06540
C -3.71205 -0.39383 5.44661
C -2.38813 -0.55952 5.88602
C -4.16229 0.89658 5.13488
C -1.53764 0.53478 6.00975
H -2.01283 -1.55738 6.13531
C -3.31048 1.99365 5.25744
H -5.18864 1.04995 4.78995
C -1.99900 1.81333 5.69347
H -0.51101 0.39265 6.35478
H -3.67500 2.99549 5.01773
H -1.33288 2.67371 5.79308
99
VI - Direct product post the alkane generation where the alkane group is still interaction with Ni and the catalyst already has the (NPN)Ni-Silyl form.
Si -0.06134 -0.01138 2.42170
C 0.52981 -3.44724 1.96261
H -0.07639 -2.48496 1.95810
Ni 0.41534 -1.39945 0.66064
H -1.46076 0.50367 2.28708
H 1.11904 -3.57441 1.04265
C -0.32946 -3.60474 -1.28049
H -0.45847 -4.19001 -0.36761
C -0.58568 -4.20283 -2.53076
H -0.91073 -5.24392 -2.56786
C -0.41643 -3.45899 -3.67431
H -0.59963 -3.89062 -4.66192

C	−0.01192	−2.10661	−3.56507
C	0.15344	−1.25140	−4.68432
H	−0.01341	−1.65741	−5.68511
C	0.50479	0.06949	−4.51531
H	0.62235	0.72166	−5.38356
C	0.69793	0.59342	−3.21885
H	0.94671	1.65069	−3.09181
C	0.55960	−0.21853	−2.11190
C	0.21243	−1.58363	−2.26062
C	3.75414	−2.16261	0.78478
H	3.37854	−3.17884	0.94762
C	5.12608	−1.88587	0.97597
H	5.80329	−2.68768	1.27653
C	5.57599	−0.59938	0.78564
H	6.62878	−0.34320	0.93393
C	4.65963	0.40721	0.39598
C	5.01827	1.76577	0.19776
H	6.06071	2.06265	0.34018
C	4.06869	2.69863	−0.15188
H	4.35089	3.74587	−0.28022
C	2.72080	2.31771	−0.34218
H	1.96714	3.06535	−0.59860
C	2.34964	1.00111	−0.17619
C	3.30217	0.01999	0.21457
N	0.06752	−2.35232	−1.13515
N	2.87358	−1.25440	0.42202
O	−0.18293	1.75267	−0.39502
P	0.68384	0.36195	−0.39078
C	0.45365	−3.88349	4.31855
H	−0.23776	−3.06502	4.58774
H	0.97182	−4.18915	5.23970
C	−0.30838	−5.02613	3.64691
H	0.30938	−5.93936	3.66562
H	−1.25489	−5.27068	4.15074
C	−0.51697	−4.56808	2.19002
H	−0.38725	−5.40410	1.48406
H	−1.53750	−4.18083	2.03722
C	1.40075	−3.41097	3.22123
H	1.84256	−2.41983	3.40532
H	2.23311	−4.12727	3.10986
H	−0.00717	−0.88670	3.64160
C	−1.55325	1.75868	−0.60698
C	−2.16120	3.00820	−0.71312
C	−2.28210	0.58517	−0.70421
C	−3.53868	3.08561	−0.92362
H	−1.53684	3.89717	−0.62675
C	−3.66751	0.63343	−0.91286
H	−1.78368	−0.37954	−0.58757
C	−4.26927	1.88615	−1.02016
H	−5.34561	1.94543	−1.18322
C	−4.43085	−0.68844	−1.01585
C	−5.93349	−0.47150	−1.19745
H	−6.15823	0.08137	−2.12274
H	−6.44723	−1.44302	−1.25951

```
H         -6.36949        0.08066       -0.35054
C         -3.89537       -1.47641       -2.22271
H         -4.03179       -0.90910       -3.15669
H         -2.82089       -1.69790       -2.11947
H         -4.42856       -2.43564       -2.32262
C         -4.20311       -1.50399        0.26741
H         -3.13620       -1.73393        0.42322
H         -4.55878       -0.95523        1.15329
H         -4.74881       -2.45979        0.21452
C         -4.26966        4.42427       -1.05358
C         -5.33986        4.52118        0.04498
H         -5.87907        5.47928       -0.03143
H         -6.08348        3.71381       -0.03333
H         -4.88405        4.46411        1.04648
C         -3.31925        5.61406       -0.91040
H         -2.82031        5.62430        0.07165
H         -2.54570        5.61750       -1.69470
H         -3.88462        6.55409       -1.00232
C         -4.93749        4.49792       -2.43592
H         -4.18841        4.42514       -3.24055
H         -5.66975        3.68944       -2.58268
H         -5.47039        5.45553       -2.55113
C          1.07693        1.45299        2.72876
C          2.40921        1.25011        3.12773
C          0.63384        2.77024        2.53304
C          3.27192        2.32652        3.32272
H          2.78144        0.23262        3.29199
C          1.49490        3.85078        2.72753
H         -0.39928        2.95642        2.22477
C          2.81515        3.63060        3.12040
H          4.30377        2.15015        3.63851
H          1.13084        4.87159        2.58057
H          3.48863        4.47744        3.27822
15
Cyclopentane
C          1.12478       -0.10463        0.18025
C          2.60155       -0.09204       -0.21555
C          3.04914        1.30901        0.18997
C          1.88769        2.19635       -0.26837
C          0.62042        1.32193       -0.12143
H          0.54452       -0.88358       -0.33706
H          1.04200       -0.31340        1.25979
H          2.70361       -0.21225       -1.30860
H          3.18592       -0.89717        0.25597
H          3.15420        1.35618        1.28797
H          4.01760        1.60675       -0.24049
H          1.82472        3.13835        0.29689
H          2.03369        2.47469       -1.32465
H         -0.03914        1.68794        0.67993
H          0.02235        1.34518       -1.04529

Structures for the (NPN)Ni-Silyl cycle
84
NPNNi-SiPh  - (NPN)Ni-Silyl catalyst alone
```

Ni	0.74493	1.24542	0.70891
Si	3.00041	1.64300	0.77306
H	3.26812	2.58142	−0.36655
C	1.62713	−1.35028	1.55599
H	1.75779	−0.87784	2.53201
C	2.08770	−2.65891	1.33352
H	2.55131	−3.20583	2.15427
C	2.00214	−3.18883	0.06880
H	2.40271	−4.18067	−0.15288
C	1.37112	−2.44540	−0.95744
C	1.19307	−2.93115	−2.27602
H	1.59079	−3.91593	−2.53183
C	0.51010	−2.18752	−3.21291
H	0.36821	−2.57669	−4.22295
C	−0.05514	−0.94391	−2.86098
H	−0.67535	−0.41104	−3.58560
C	0.12985	−0.41830	−1.59682
C	0.87137	−1.15646	−0.63530
C	0.94939	4.02958	1.37625
H	1.24392	3.66026	2.36095
C	1.03018	5.40063	1.07835
H	1.35681	6.09521	1.85294
C	0.73713	5.82406	−0.19635
H	0.83429	6.87594	−0.47601
C	0.28472	4.88675	−1.15531
C	−0.08898	5.24921	−2.47388
H	0.01783	6.29170	−2.78242
C	−0.60195	4.31154	−3.34095
H	−0.89841	4.60267	−4.35047
C	−0.79180	2.97985	−2.91613
H	−1.28332	2.26562	−3.58006
C	−0.40264	2.57893	−1.65252
C	0.16832	3.52670	−0.75937
N	1.06276	−0.61423	0.61109
N	0.56568	3.11940	0.49249
O	−2.29078	0.76959	−1.57172
P	−0.79327	0.98527	−0.88395
C	−3.04021	−0.35625	−1.29139
C	−4.11133	−0.61935	−2.14354
C	−2.74146	−1.19247	−0.22656
C	−4.90127	−1.74791	−1.93129
H	−4.30373	0.07572	−2.95961
C	−3.51141	−2.34245	0.00182
H	−1.91178	−0.94817	0.44149
C	−4.57777	−2.59667	−0.85786
H	−5.18792	−3.48436	−0.69651
C	−3.14024	−3.26007	1.16832
C	−6.09565	−2.08553	−2.82582
C	−4.07220	−4.46690	1.27091
H	−4.03719	−5.09051	0.36483
H	−3.77104	−5.09875	2.11976
H	−5.11585	−4.16252	1.44037
C	−3.22117	−2.46805	2.48140
H	−2.53272	−1.60896	2.48662

```
H         -4.23841       -2.08238        2.64624
H         -2.95797       -3.11290        3.33445
C         -1.70483       -3.76692        0.96394
H         -1.61308       -4.32175        0.01751
H         -0.98134       -2.93835        0.93744
H         -1.41348       -4.43898        1.78643
C         -7.36959       -2.11346       -1.96819
H         -8.24436       -2.35294       -2.59255
H         -7.31117       -2.86999       -1.17206
H         -7.54608       -1.13675       -1.49256
C         -5.87267       -3.46387       -3.46534
H         -6.72302       -3.72455       -4.11438
H         -4.95956       -3.47037       -4.08035
H         -5.77613       -4.25723       -2.70979
C         -6.28516       -1.05902       -3.94247
H         -6.47570       -0.05068       -3.54442
H         -5.40898       -1.01085       -4.60730
H         -7.15160       -1.33813       -4.56013
H          3.36490        2.34655        2.05093
C          4.10027        0.13312        0.59313
C          4.77130       -0.41954        1.69636
C          4.22376       -0.50908       -0.64967
C          5.53815       -1.57627        1.56350
H          4.70576        0.06744        2.67421
C          4.98913       -1.66562       -0.78574
H          3.72136       -0.09584       -1.53022
C          5.64559       -2.20276        0.32222
H          6.06416       -1.98468        2.42987
H          5.08293       -2.14537       -1.76326
H          6.25334       -3.10444        0.21495

Formation of the Calkene-Si bond
97
VII - Entrance of the cyclopentene
Ni        -0.15714       -0.24547        1.33509
C         -0.50709       -1.73632        2.70561
Si         0.47822        1.10405        3.07230
C         -1.66840       -1.00126        2.43219
C          0.15973       -2.31979       -0.84404
H          0.90761       -2.69132       -0.13959
C         -0.14454       -3.05542       -2.00663
H          0.38774       -3.98629       -2.20656
C         -1.14032       -2.60305       -2.84137
H         -1.43497       -3.17323       -3.72601
C         -1.77255       -1.36803       -2.56226
C         -2.77681       -0.78476       -3.37823
H         -3.12881       -1.33278       -4.25528
C         -3.29188        0.45517       -3.07482
H         -4.06936        0.89144       -3.70528
C         -2.79578        1.19454       -1.97521
H         -3.16505        2.20273       -1.77382
C         -1.82899        0.64698       -1.16073
C         -1.34793       -0.66476       -1.40277
C          2.73833       -0.48971        0.94910
```

H	2.61317	−1.28061	1.69278
C	4.00131	−0.23878	0.37737
H	4.84743	−0.86817	0.65484
C	4.14013	0.82147	−0.48387
H	5.10989	1.06564	−0.92477
C	3.01148	1.61700	−0.80267
C	3.07360	2.73136	−1.67564
H	4.03664	3.00197	−2.11493
C	1.94097	3.45644	−1.97135
H	1.99892	4.31378	−2.64495
C	0.69708	3.08542	−1.41890
H	−0.20194	3.65483	−1.66980
C	0.59661	2.00722	−0.56286
C	1.76037	1.26342	−0.22218
N	−0.44620	−1.19370	−0.52406
N	1.66336	0.21835	0.65828
O	−1.86098	2.82077	0.36412
P	−0.96318	1.44836	0.20899
C	−1.97948	−3.18367	1.41527
C	−0.66143	−3.16079	2.21824
C	−2.68995	−1.84794	1.71132
H	−2.60337	−4.04183	1.70222
H	0.20006	−3.54761	1.65051
H	−0.73215	−3.80991	3.10820
H	0.13070	−1.54772	3.57298
H	−2.01191	−0.17389	3.05701
H	−3.10252	−1.36962	0.80870
H	−3.54657	−1.99222	2.39172
H	−1.79324	−3.29851	0.33974
H	0.63432	2.51427	2.60600
H	−0.54239	1.00257	4.15813
C	−1.70183	3.53875	1.54823
C	−2.39031	3.12065	2.68326
C	−0.82691	4.60957	1.56927
C	−2.18544	3.78530	3.89278
H	−3.07293	2.27516	2.59757
C	−0.58904	5.28599	2.77421
H	−0.30708	4.88535	0.65142
C	−1.27707	4.85691	3.90985
H	−1.10404	5.37139	4.85415
C	2.16071	0.64189	3.77571
C	2.35822	−0.40962	4.68506
C	3.28479	1.38370	3.37402
C	3.63155	−0.72511	5.15631
H	1.50492	−0.98664	5.05369
C	4.55938	1.07643	3.84576
H	3.16056	2.22227	2.68091
C	4.73569	0.01474	4.73272
H	3.76249	−1.54476	5.86682
H	5.41845	1.67145	3.52617
H	5.73319	−0.22818	5.10652
C	−2.91721	3.39177	5.17674
C	0.44231	6.41437	2.80252
C	−3.84600	4.54573	5.58374

```
H         -4.38858        4.29291        6.50805
H         -3.28349        5.47312        5.76726
H         -4.58722        4.75205        4.79674
C         -1.89756        3.13175        6.29486
H         -1.20681        2.32007        6.01995
H         -1.29563        4.02353        6.52170
H         -2.41685        2.84043        7.22076
C         -3.75913        2.12896        4.98996
H         -4.54818        2.26571        4.23494
H         -3.13956        1.26741        4.69448
H         -4.25434        1.86892        5.93709
C          0.55375        7.05857        4.18433
H          0.87591        6.33576        4.94916
H          1.30152        7.86496        4.15834
H         -0.40027        7.50227        4.50689
C          1.81333        5.82883        2.42708
H          2.11168        5.04367        3.13935
H          1.80753        5.38594        1.41915
H          2.58316        6.61618        2.44304
C          0.04598        7.49658        1.78886
H         -0.00489        7.10239        0.76288
H         -0.93805        7.92416        2.03364
H          0.78401        8.31358        1.79455
97
TS_VII_VIII  -  TS for the initial C-Si bond formation
C         -2.01641       -9.15309        5.59603
Si         0.66367       -7.78536        7.04746
C         -1.57086       -8.32247        6.65173
Ni        -0.19061       -8.68647        5.06051
C         -3.09416       -7.03578        5.26003
C         -3.16650       -8.51306        4.85861
C         -2.34582       -7.00867        6.60012
H         -4.08567       -6.56791        5.33054
H         -3.15311       -8.67304        3.76920
H         -4.10018       -8.97546        5.22616
H         -1.97108      -10.24661        5.68072
H         -1.38628       -8.76833        7.63868
H         -1.72253       -6.10945        6.71426
H         -3.05061       -7.01290        7.44869
H         -2.53995       -6.45928        4.50597
H          0.02486       -6.84837        8.01663
H          1.83014       -7.00745        6.51343
C          1.39133       -9.28806        7.92336
C          2.73854       -9.23944        8.31633
C          0.69262      -10.49051        8.12099
C          3.36434      -10.34652        8.88755
H          3.31613       -8.32237        8.16556
C          1.31483      -11.60212        8.68779
H         -0.35624      -10.57890        7.82178
C          2.65423      -11.53231        9.07067
H          4.41255      -10.28401        9.18968
H          0.75128      -12.52663        8.83500
H          3.14309      -12.40202        9.51587
O         -0.25798       -5.02310        3.63193
```

P	0.01305	−6.64645	3.91101
C	−0.58261	−4.25051	4.73706
C	0.32902	−4.12005	5.78481
C	−1.82770	−3.64649	4.77348
C	−0.01538	−3.36816	6.90912
H	1.30329	−4.60237	5.70040
C	−2.20343	−2.89013	5.89372
H	−2.50045	−3.78731	3.92597
C	−1.28593	−2.77128	6.93900
H	−1.56159	−2.18788	7.81654
C	−3.59288	−2.25188	5.93602
C	−3.82110	−1.45355	7.21983
H	−3.09963	−0.62890	7.32266
H	−4.82816	−1.01099	7.20674
H	−3.75183	−2.08774	8.11672
C	−3.75086	−1.30441	4.73848
H	−2.99504	−0.50507	4.76750
H	−3.64592	−1.83249	3.77913
H	−4.74635	−0.83422	4.75246
C	−4.65169	−3.36218	5.85891
H	−4.56659	−3.94410	4.92874
H	−4.55295	−4.05880	6.70616
H	−5.66372	−2.92943	5.89000
C	0.93761	−3.17186	8.08927
C	0.28445	−3.73077	9.36177
H	0.95406	−3.59719	10.22562
H	−0.66291	−3.22247	9.59357
H	0.07384	−4.80610	9.25567
C	2.27219	−3.88604	7.87395
H	2.14253	−4.97291	7.76053
H	2.79976	−3.50638	6.98545
H	2.92643	−3.71892	8.74242
C	1.21467	−1.67180	8.26692
H	1.67689	−1.24665	7.36304
H	0.29482	−1.10521	8.47251
H	1.90192	−1.50902	9.11174
C	−0.67676	−10.81799	3.21187
H	−0.49397	−11.40444	4.11627
C	−1.02144	−11.46224	2.01076
H	−1.08115	−12.55088	1.98294
C	−1.30712	−10.69340	0.90753
H	−1.61061	−11.15413	−0.03583
C	−1.20847	−9.28522	0.99189
C	−1.50228	−8.43029	−0.10016
H	−1.82398	−8.87445	−1.04477
C	−1.38767	−7.06713	0.03455
H	−1.62590	−6.41077	−0.80496
C	−0.94007	−6.50449	1.24986
H	−0.82645	−5.42229	1.34392
C	−0.63279	−7.30514	2.33145
C	−0.80144	−8.71309	2.23344
C	2.35762	−10.02795	5.07209
H	1.76518	−10.74029	5.65033
C	3.71073	−10.29823	4.79513

H 4.14384 −11.24194 5.12796
C 4.45889 −9.34309 4.15186
H 5.52134 −9.50118 3.95007
C 3.84816 −8.13151 3.74743
C 4.55751 −7.09486 3.09213
H 5.62229 −7.23188 2.89023
C 3.91498 −5.93619 2.72085
H 4.46885 −5.13579 2.22604
C 2.53307 −5.78154 2.95858
H 2.02145 −4.86667 2.64914
C 1.80569 −6.77694 3.58037
C 2.45984 −7.95903 4.01705
N −0.57740 −9.50591 3.32735
N 1.75415 −8.91112 4.70432
97
VIII – Silylalkyl already formed with an interaction between Ni and the C–Si bond.
Ni 0.59365 −0.58047 0.85912
C −0.27242 −1.73416 2.02782
Si 1.54714 0.63911 3.02703
C 0.12739 −0.74165 3.06630
C 0.76741 −2.78850 −0.92440
H 1.56293 −3.08183 −0.23403
C 0.43674 −3.61044 −2.01634
H 0.99612 −4.53136 −2.18512
C −0.60831 −3.23907 −2.82768
H −0.91342 −3.86263 −3.67171
C −1.30442 −2.03500 −2.56926
C −2.39854 −1.60437 −3.35989
H −2.71914 −2.22602 −4.19888
C −3.04295 −0.42541 −3.06976
H −3.89211 −0.10022 −3.67430
C −2.60342 0.38282 −1.99977
H −3.11249 1.32397 −1.78170
C −1.53203 0.00748 −1.21248
C −0.87953 −1.23233 −1.46893
C 3.17771 0.00947 −0.30003
H 3.40710 −0.92912 0.21072
C 4.18424 0.67870 −1.02197
H 5.17891 0.23610 −1.08208
C 3.89237 1.88904 −1.60211
H 4.65454 2.45104 −2.14795
C 2.58216 2.41459 −1.49809
C 2.19656 3.64943 −2.07651
H 2.94481 4.23641 −2.61397
C 0.90027 4.09669 −1.96313
H 0.60889 5.05152 −2.40552
C −0.06730 3.31810 −1.29222
H −1.09990 3.66840 −1.21943
C 0.27197 2.10813 −0.72045
C 1.61291 1.65082 −0.78641
N 0.14409 −1.65392 −0.66180
N 1.94817 0.47501 −0.17209
O −2.23661 2.07991 0.26872

P	−0.92180	1.04456	0.17060
C	−2.31946	−0.66777	2.73252
C	−1.76660	−1.94208	2.09482
C	−1.17738	−0.08236	3.57896
H	−3.21932	−0.85655	3.33563
H	−2.21505	−2.16685	1.11325
H	−1.97244	−2.81884	2.73439
H	0.32469	−2.66003	1.97257
H	0.68338	−1.26359	3.87139
H	−1.16662	1.01723	3.51514
H	−1.29719	−0.32924	4.64508
H	−2.62230	0.05034	1.95924
H	1.44135	1.85449	2.16777
H	1.35771	1.12219	4.42834
C	−2.47989	2.69681	1.48269
C	−3.74122	2.54104	2.04499
C	−1.47934	3.42660	2.11835
C	−4.01792	3.10546	3.29297
H	−4.48031	1.95718	1.49805
C	−1.73256	4.01180	3.36433
H	−0.51110	3.53891	1.63044
C	−2.99952	3.82852	3.92706
H	−3.20657	4.27072	4.90339
C	−0.67633	4.82580	4.11421
C	−1.21707	6.23967	4.37127
H	−2.13444	6.22490	4.97744
H	−0.47028	6.84192	4.91161
H	−1.44901	6.75060	3.42438
C	−0.37222	4.13652	5.45250
H	−1.26834	4.06020	6.08565
H	0.01433	3.11792	5.29239
H	0.38595	4.70491	6.01361
C	0.62589	4.94429	3.32147
H	1.08219	3.96048	3.13438
H	0.47116	5.44283	2.35227
H	1.35303	5.54342	3.88942
C	−5.37171	2.93519	3.98414
C	−5.99165	4.31864	4.22844
H	−6.96764	4.21735	4.72794
H	−5.35407	4.94738	4.86707
H	−6.14786	4.85315	3.27908
C	−6.34478	2.10868	3.14303
H	−6.55187	2.58286	2.17157
H	−5.96552	1.09158	2.95859
H	−7.30378	2.01123	3.67307
C	−5.15846	2.21756	5.32522
H	−6.12030	2.08085	5.84355
H	−4.70888	1.22392	5.17214
H	−4.49667	2.78596	5.99513
C	3.23795	−0.15044	2.82263
C	4.36262	0.66288	2.61501
C	3.41556	−1.54307	2.80833
C	5.62012	0.10580	2.38996
H	4.25712	1.75215	2.61509

C	4.67101	−2.10555	2.57735
H	2.56523	−2.21041	2.97605
C	5.77501	−1.28036	2.36314
H	6.48414	0.75592	2.23303
H	4.79050	−3.19166	2.57237
H	6.75984	−1.71867	2.18525

Formation of the C–H bond = Silane product
112
IX – Entrance of the second silane forming the Ni–C–H–Si interaction

Si	−1.30949	−0.29662	1.93634
C	0.11202	−3.00600	1.24731
H	0.29807	−0.69977	1.64287
Ni	0.02643	−1.29390	0.31505
H	−2.54775	−0.65423	1.18229
H	0.40943	−3.60980	0.37117
C	0.54147	−4.06684	3.44031
H	0.16450	−3.44185	4.26968
H	1.25153	−4.77966	3.88322
C	−0.64359	−4.72776	2.74516
H	−0.30040	−5.57544	2.12754
H	−1.40112	−5.11202	3.44480
C	−1.16229	−3.60609	1.84929
H	−1.89752	−3.94758	1.10470
H	−1.69301	−2.87789	2.48493
C	1.20016	−3.18931	2.34264
H	2.03750	−3.76038	1.90409
H	−1.36764	−0.93777	3.27933
Si	2.07189	−1.71973	3.17532
H	2.73431	−0.80650	2.19278
H	1.07654	−0.91959	3.95730
C	−1.18259	−3.22423	−1.60337
H	−1.41811	−3.75028	−0.67839
C	−1.50760	−3.81137	−2.84084
H	−2.00653	−4.78110	−2.85515
C	−1.17403	−3.15267	−3.99841
H	−1.39514	−3.58222	−4.97864
C	−0.54683	−1.88787	−3.91462
C	−0.20741	−1.12253	−5.05882
H	−0.41318	−1.53994	−6.04725
C	0.35345	0.12709	−4.93034
H	0.60329	0.71178	−5.81771
C	0.58434	0.66789	−3.64803
H	0.99055	1.67775	−3.54763
C	0.28168	−0.05908	−2.51624
C	−0.27909	−1.35631	−2.62073
C	3.04304	−2.43105	−0.36191
H	2.51389	−3.38806	−0.40783
C	4.44661	−2.40280	−0.20627
H	4.99989	−3.34112	−0.14274
C	5.08594	−1.18679	−0.12091
H	6.16789	−1.12967	0.02328
C	4.32964	0.00524	−0.22867

C	4.87514	1.31378	−0.16022
H	5.95041	1.43159	−0.00667
C	4.06281	2.41902	−0.28089
H	4.49441	3.42012	−0.21909
C	2.67084	2.27824	−0.49584
H	2.03060	3.15671	−0.59963
C	2.11926	1.01902	−0.56613
C	2.92865	−0.13508	−0.40805
N	−0.58149	−2.05461	−1.47857
N	2.30818	−1.34439	−0.44069
O	−0.25597	2.09933	−0.94941
P	0.39029	0.59520	−0.82667
C	3.37989	−2.39328	4.33418
C	3.11343	−2.61098	5.69450
C	4.64441	−2.75027	3.83940
C	4.07652	−3.17116	6.53230
H	2.14016	−2.33531	6.11129
C	5.60966	−3.31117	4.67294
H	4.88277	−2.58077	2.78425
C	5.32498	−3.52325	6.02173
H	3.85316	−3.33119	7.58978
H	6.59005	−3.58104	4.27269
H	6.08096	−3.96066	6.67817
C	−1.57527	2.31344	−1.29294
C	−1.95948	3.63557	−1.47003
C	−2.47513	1.26915	−1.46524
C	−3.27550	3.93615	−1.82957
H	−1.21336	4.41487	−1.30979
C	−3.79612	1.53926	−1.84049
H	−2.15738	0.23648	−1.30952
C	−4.17363	2.87434	−2.01045
H	−5.19665	3.09780	−2.30211
C	−1.08840	1.55232	2.05915
C	−2.18142	2.41484	1.89487
C	0.17392	2.10611	2.32941
C	−2.01865	3.79454	2.00110
H	−3.17116	2.01067	1.66430
C	0.33897	3.48486	2.42742
H	1.04473	1.45539	2.45957
C	−0.75904	4.33027	2.26234
H	−2.87739	4.45482	1.86634
H	1.32650	3.90230	2.63831
H	−0.63224	5.41279	2.34152
C	−4.74742	0.36702	−2.09261
C	−3.68422	5.39934	−2.01673
C	−4.21092	−0.44742	−3.28046
H	−4.14905	0.17240	−4.18781
H	−3.20403	−0.84331	−3.07730
H	−4.87371	−1.30140	−3.49178
C	−6.16458	0.83624	−2.42113
H	−6.59847	1.42744	−1.60062
H	−6.19400	1.44450	−3.33738
H	−6.81637	−0.03507	−2.58339
C	−4.80830	−0.53220	−0.85068

H -3.82730 -0.96923 -0.61037
H -5.15149 0.03008 0.03121
H -5.50904 -1.36513 -1.01682
C -5.13986 5.54015 -2.46311
H -5.32313 5.04204 -3.42727
H -5.84004 5.12711 -1.72124
H -5.38613 6.60473 -2.58980
C -3.51097 6.14191 -0.68394
H -4.16228 5.71033 0.09172
H -2.47336 6.09496 -0.32068
H -3.77905 7.20360 -0.79892
C -2.78631 6.04209 -3.08387
H -1.72514 6.02374 -2.79470
H -2.88335 5.51854 -4.04720
H -3.07036 7.09468 -3.23765
112
TSB2 - TS of the formation of the C-H bond for the Ni-Si catalyst= Formation of the PhSiH2Cyclopentyl product
Si -5.11131 -1.92702 5.14305
C -4.09434 -4.96504 4.67654
H -4.07473 -3.35371 5.00585
Ni -4.11372 -3.30653 3.55239
H -6.42715 -1.83307 4.44696
H -3.77252 -5.55191 3.80289
C -3.94266 -6.02237 6.89982
H -4.30733 -5.31820 7.66891
H -3.36235 -6.79364 7.42633
C -5.13927 -6.57315 6.13162
H -4.84680 -7.47519 5.56729
H -5.98435 -6.84810 6.78019
C -5.46540 -5.43491 5.16811
H -6.15023 -5.72232 4.35540
H -5.97650 -4.63184 5.72655
C -3.09826 -5.28092 5.83462
H -2.34159 -5.98312 5.44291
H -5.37368 -2.53135 6.48822
Si -2.07072 -3.91005 6.65883
H -1.31335 -3.10001 5.65585
H -2.99852 -2.99562 7.39670
C -5.03567 -5.42359 1.63432
H -5.31153 -5.92223 2.56573
C -5.25474 -6.07524 0.40516
H -5.71044 -7.06619 0.39976
C -4.87888 -5.44716 -0.75734
H -5.02189 -5.92459 -1.72993
C -4.30792 -4.15463 -0.68973
C -3.92065 -3.41845 -1.83812
H -4.04468 -3.87717 -2.82188
C -3.41235 -2.14530 -1.71944
H -3.12460 -1.58369 -2.61028
C -3.28075 -1.55052 -0.44616
H -2.91141 -0.52539 -0.35938
C -3.63176 -2.24804 0.68976
C -4.14276 -3.56544 0.59535

C	−0.92729	−4.45283	3.14127
H	−1.42043	−5.42972	3.09497
C	0.45482	−4.36931	3.42226
H	1.02954	−5.28359	3.57898
C	1.04627	−3.12884	3.50505
H	2.10905	−3.02776	3.73953
C	0.26605	−1.96961	3.27632
C	0.76083	−0.63977	3.32558
H	1.81388	−0.47512	3.56611
C	−0.07226	0.42761	3.07572
H	0.31898	1.44587	3.12384
C	−1.43646	0.22782	2.75551
H	−2.09441	1.07921	2.57131
C	−1.93873	−1.05168	2.70316
C	−1.10778	−2.16832	2.97793
N	−4.49368	−4.22502	1.74337
N	−1.68297	−3.39740	2.93965
O	−4.33070	−0.06706	2.15090
P	−3.63539	−1.53959	2.36267
C	−0.85618	−4.69700	7.84399
C	−1.22015	−5.00587	9.16404
C	0.43130	−5.04959	7.40984
C	−0.32965	−5.65147	10.01971
H	−2.21250	−4.73403	9.53594
C	1.32466	−5.69524	8.26244
H	0.74574	−4.80855	6.38946
C	0.94345	−5.99821	9.56902
H	−0.62842	−5.88160	11.04513
H	2.32448	−5.95990	7.90972
H	1.64299	−6.50189	10.24031
C	−5.68522	0.06488	1.91422
C	−6.19842	1.35503	1.89626
C	−6.50354	−1.03838	1.70984
C	−7.56567	1.55557	1.68255
H	−5.51412	2.18690	2.06827
C	−7.87240	−0.86887	1.48662
H	−6.08749	−2.04551	1.73976
C	−8.38154	0.43280	1.47912
H	−9.44511	0.58119	1.30988
C	−4.32800	−0.24166	5.34260
C	−5.11743	0.90229	5.14421
C	−2.98827	−0.07497	5.72561
C	−4.58086	2.17592	5.31949
H	−6.16273	0.80245	4.83878
C	−2.45242	1.19819	5.90495
H	−2.34722	−0.94654	5.87965
C	−3.24733	2.32549	5.69952
H	−5.21025	3.05554	5.16453
H	−1.40831	1.30995	6.20669
H	−2.82859	3.32446	5.84338
C	−8.73200	−2.11367	1.25588
C	−8.11738	2.98300	1.68521
C	−8.22116	−2.84549	0.00479
H	−8.28328	−2.19878	−0.88351

H -7.17215 -3.16110 0.11621
H -8.82426 -3.74736 -0.18506
C -10.20495 -1.76289 1.05015
H -10.62777 -1.24947 1.92674
H -10.35210 -1.11953 0.16974
H -10.78953 -2.68098 0.88987
C -8.61389 -3.04537 2.47177
H -7.57638 -3.37545 2.63814
H -8.95627 -2.54461 3.39013
H -9.23130 -3.94514 2.32368
C -9.63168 3.01699 1.47574
H -9.92155 2.58683 0.50517
H -10.16851 2.47489 2.26896
H -9.98359 4.05903 1.49144
C -7.79954 3.64128 3.03620
H -8.24959 3.07567 3.86680
H -6.71577 3.70439 3.21532
H -8.20040 4.66620 3.06557
C -7.45054 3.77989 0.55457
H -6.35823 3.82851 0.67692
H -7.66029 3.32333 -0.42471
H -7.83158 4.81288 0.53831
112
X - Direct product post the formation of the PhSiH2Cyclopentyl silane by the Ni-Si catalyst. Adduct between the catalyst and substrate still formed.
Si -0.91701 0.70037 1.75286
C -0.72183 -2.79465 1.68016
H -1.04073 -1.70339 1.58772
Ni -0.37567 -0.90558 0.20980
H -2.31580 1.09435 1.38277
H -0.01709 -3.09522 0.89207
C -1.36444 -2.85797 3.97731
H -1.69289 -1.81081 4.08060
H -1.17840 -3.23404 4.99369
C -2.41816 -3.67890 3.22092
H -2.40123 -4.72398 3.56387
H -3.43672 -3.30637 3.39983
C -2.02640 -3.61036 1.72637
H -1.84987 -4.62242 1.32945
H -2.81596 -3.15759 1.10777
C -0.12018 -2.92521 3.08331
H 0.27968 -3.95468 3.15005
H -0.98356 0.01532 3.08840
Si 1.33113 -1.77865 3.52008
H 1.48517 -0.75528 2.43755
H 1.07571 -1.05407 4.80097
C -0.99419 -3.24933 -1.58532
H -1.44431 -3.65765 -0.67964
C -1.03889 -3.99660 -2.77773
H -1.52440 -4.97323 -2.77737
C -0.46415 -3.47684 -3.91256
H -0.47162 -4.03080 -4.85453
C 0.13211 -2.19523 -3.85912

C	0.71649	−1.56259	−4.98592
H	0.73372	−2.09741	−5.93839
C	1.23991	−0.29397	−4.88655
H	1.68184	0.18719	−5.76121
C	1.19348	0.40007	−3.65777
H	1.58714	1.41756	−3.59143
C	0.64790	−0.19687	−2.54189
C	0.11701	−1.50595	−2.61447
C	3.27313	−2.03857	0.27752
H	2.87348	−3.05696	0.22295
C	4.58655	−1.82675	0.75645
H	5.18325	−2.67861	1.08595
C	5.07151	−0.54227	0.82308
H	6.07922	−0.34185	1.19573
C	4.24955	0.53438	0.40656
C	4.63904	1.89874	0.41637
H	5.64080	2.16010	0.76622
C	3.77045	2.88079	−0.00476
H	4.07784	3.92797	0.01659
C	2.46812	2.55697	−0.44924
H	1.77207	3.34360	−0.74475
C	2.06983	1.23953	−0.46952
C	2.94554	0.20578	−0.04937
N	−0.42949	−2.05848	−1.48618
N	2.47878	−1.06567	−0.10485
O	−0.29310	2.04267	−1.32845
P	0.44791	0.63255	−0.93573
C	2.95473	−2.71957	3.64278
C	3.13210	−4.01031	3.12424
C	4.06592	−2.08142	4.21694
C	4.37532	−4.64206	3.17037
H	2.28893	−4.54555	2.67677
C	5.30988	−2.70588	4.26642
H	3.96006	−1.07684	4.63860
C	5.46728	−3.98899	3.74047
H	4.49053	−5.65155	2.76819
H	6.15972	−2.19504	4.72559
H	6.43999	−4.48463	3.78541
C	−1.64996	2.11710	−1.57720
C	−2.20561	3.38732	−1.65470
C	−2.43297	0.97981	−1.71819
C	−3.58281	3.53342	−1.84761
H	−1.54638	4.24967	−1.54665
C	−3.81369	1.09401	−1.89723
H	−1.97881	−0.00935	−1.65642
C	−4.36687	2.37576	−1.96042
H	−5.44029	2.48028	−2.09834
C	0.06860	2.28269	1.99750
C	−0.42184	3.49701	1.49256
C	1.28819	2.29745	2.69355
C	0.28915	4.68397	1.66225
H	−1.37882	3.51788	0.96440
C	1.99852	3.48215	2.86891
H	1.69263	1.37003	3.10565

```
C          1.50311        4.67801        2.34867
H         -0.11380        5.62095        1.26906
H          2.94395        3.47381        3.41644
H          2.05764        5.60898        2.49001
C         -4.63907       -0.19073       -1.98664
C         -4.17901        4.94145       -1.90481
C         -4.13624       -1.03624       -3.16658
H         -4.23336       -0.48668       -4.11499
H         -3.07785       -1.31658       -3.04948
H         -4.72132       -1.96573       -3.24819
C         -6.12709        0.09364       -2.18693
H         -6.54686        0.67413       -1.35186
H         -6.31400        0.64663       -3.11969
H         -6.68447       -0.85315       -2.24493
C         -4.46197       -0.98109       -0.67983
H         -3.40455       -1.23392       -0.50046
H         -4.81295       -0.39804        0.18516
H         -5.03529       -1.92105       -0.71705
C         -5.69472        4.91804       -2.10500
H         -5.97616        4.42719       -3.04899
H         -6.21085        4.40438       -1.27977
H         -6.07866        5.94814       -2.14298
C         -3.87386        5.66570       -0.58470
H         -4.30279        5.12288        0.27150
H         -2.79153        5.76680       -0.41245
H         -4.30347        6.67929       -0.59661
C         -3.54524        5.70947       -3.07374
H         -2.45431        5.79940       -2.96294
H         -3.74646        5.20546       -4.03129
H         -3.95954        6.72807       -3.13031

Formation of the second C-Si bond = Double-silylated products
112
XI -  Entrance of the second silane forming the Ni-C-Si-H
interactions.
Si        -0.65450        0.25367        2.00613
C          0.50578       -2.51180        1.40587
H         -0.96113       -0.84239        0.63372
Ni         0.47438       -0.84725        0.37718
H         -1.24694       -0.65384        3.02761
H          0.54961        0.96177        2.54382
H          1.13408       -3.02927        0.64986
C          0.97719       -4.30059        2.87105
H          1.14679       -4.69062        3.88652
H          1.70029       -4.81804        2.21762
C         -0.45716       -4.53640        2.36383
H         -0.52245       -5.46067        1.77109
H         -1.16039       -4.65472        3.20133
C         -0.80844       -3.28327        1.53103
H         -1.25890       -3.52370        0.55493
H         -1.55427       -2.67567        2.06692
C          1.19879       -2.77313        2.75156
H          2.27837       -2.55284        2.71001
Si         0.71739       -1.97041        4.41518
```

H	0.95588	−0.49685	4.39708
H	−0.69468	−2.26693	4.80506
C	0.50434	−3.08583	−1.84582
H	0.16094	−3.68830	−1.00033
C	0.75120	−3.70167	−3.09054
H	0.58628	−4.77427	−3.20143
C	1.20256	−2.93037	−4.13356
H	1.41545	−3.37030	−5.11108
C	1.38228	−1.53962	−3.93951
C	1.81457	−0.66361	−4.96651
H	2.04367	−1.08001	−5.95037
C	1.93205	0.68838	−4.73617
H	2.25869	1.35552	−5.53616
C	1.61011	1.22184	−3.47044
H	1.66985	2.30080	−3.30557
C	1.20178	0.39396	−2.44520
C	1.08842	−1.00618	−2.65150
C	3.40296	−1.37675	0.86864
H	3.07838	−2.41734	0.80855
C	4.70209	−1.06520	1.31762
H	5.37633	−1.87493	1.59984
C	5.07658	0.25359	1.42459
H	6.06023	0.53057	1.81202
C	4.18225	1.26312	0.99493
C	4.48506	2.65001	1.00592
H	5.44541	2.97530	1.41255
C	3.59132	3.56995	0.50617
H	3.83483	4.63405	0.52715
C	2.37150	3.14744	−0.07149
H	1.68698	3.87288	−0.51694
C	2.04837	1.80903	−0.07888
C	2.91642	0.84937	0.50387
N	0.67393	−1.79963	−1.62128
N	2.51695	−0.46119	0.52657
O	−0.33774	2.26531	−1.19891
P	0.63286	1.00074	−0.83020
C	1.86941	−2.72569	5.69089
C	1.42434	−3.69072	6.60650
C	3.22317	−2.35481	5.72516
C	2.30210	−4.27086	7.52181
H	0.37261	−3.99247	6.61083
C	4.10441	−2.93163	6.63688
H	3.59792	−1.59188	5.03383
C	3.64340	−3.89280	7.53670
H	1.93661	−5.01865	8.22969
H	5.15385	−2.62711	6.65339
H	4.33137	−4.34419	8.25554
C	−1.57238	2.04629	−1.79112
C	−2.32536	3.17285	−2.10401
C	−2.03137	0.76760	−2.06155
C	−3.57531	3.01745	−2.70095
H	−1.91690	4.15108	−1.85738
C	−3.28200	0.58176	−2.66399
H	−1.43441	−0.10433	−1.78813

```
C         -4.03119        1.71481       -2.97282
H         -5.00487        1.59305       -3.44598
C         -3.74312       -0.84696       -2.95671
C         -4.44968        4.21430       -3.07944
C         -4.61890        4.23964       -4.60588
H         -5.10051        3.32309       -4.97756
H         -5.24520        5.09355       -4.90788
H         -3.64432        4.33562       -5.10846
C         -3.82930        5.53923       -2.63518
H         -3.68094        5.57517       -1.54500
H         -2.85927        5.72227       -3.12204
H         -4.49470        6.37157       -2.90815
C         -5.82569        4.07556       -2.41268
H         -6.46135        4.93694       -2.66934
H         -6.35304        3.16715       -2.73811
H         -5.73083        4.03596       -1.31738
C         -5.12620       -0.88159       -3.60553
H         -5.89245       -0.43226       -2.95594
H         -5.13790       -0.35177       -4.56988
H         -5.42413       -1.92327       -3.79689
C         -2.73638       -1.50869       -3.91058
H         -2.66031       -0.94722       -4.85407
H         -1.72930       -1.55981       -3.46934
H         -3.05098       -2.53726       -4.14723
C         -3.79758       -1.64244       -1.64361
H         -2.81570       -1.68268       -1.14611
H         -4.51538       -1.19309       -0.94055
H         -4.11676       -2.67853       -1.83646
C         -1.90080        1.56644        1.53781
C         -3.18071        1.23157        1.06807
C         -1.58635        2.92165        1.71595
C         -4.12304        2.21898        0.79685
H         -3.45093        0.18282        0.91334
C         -2.52804        3.91357        1.44676
H         -0.59426        3.20762        2.07807
C         -3.79744        3.56115        0.99289
H         -5.11382        1.94270        0.42959
H         -2.27342        4.96506        1.59988
H         -4.53826        4.33823        0.78979
112
TSB1 -  TS of the formation of the second C-Si bond for the Ni-Si
catalyst. = Double-silylated products.
Si        -5.28495       -2.84863        5.63222
C         -4.34413       -4.80748        5.00511
H         -5.63470       -3.45268        3.40524
Ni        -4.25236       -3.22415        3.69481
H         -6.47637       -3.61896        6.08871
H         -4.28979       -2.60571        6.72120
H         -3.37561       -4.94055        4.48163
C         -3.75283       -6.81276        6.08007
H         -3.71305       -7.47414        6.95783
H         -2.76433       -6.87950        5.59210
C         -4.86483       -7.19034        5.08890
H         -4.50910       -7.91003        4.33666
```

H	−5.70259	−7.67679	5.61067
C	−5.31690	−5.85667	4.45383
H	−5.31335	−5.88199	3.35538
H	−6.34563	−5.60668	4.75655
C	−4.03648	−5.33742	6.43484
H	−3.14616	−4.85861	6.87816
Si	−5.35159	−5.32745	7.85038
H	−5.51599	−3.97723	8.46032
H	−6.66809	−5.82646	7.34904
C	−2.86162	−5.67929	1.95558
H	−2.68292	−6.07117	2.96401
C	−2.55361	−6.47601	0.83156
H	−2.12207	−7.46792	0.97385
C	−2.82450	−5.98284	−0.42246
H	−2.61650	−6.57440	−1.31765
C	−3.38339	−4.68841	−0.55474
C	−3.70496	−4.09795	−1.80281
H	−3.51722	−4.66416	−2.71825
C	−4.24928	−2.83501	−1.86220
H	−4.50526	−2.39330	−2.82717
C	−4.47891	−2.09936	−0.67937
H	−4.91911	−1.10096	−0.73846
C	−4.16517	−2.64103	0.55031
C	−3.62991	−3.95421	0.64099
C	−1.66982	−2.82104	5.06498
H	−1.98613	−3.72407	5.59084
C	−0.46542	−2.18371	5.41954
H	0.15219	−2.61103	6.21035
C	−0.10734	−1.02771	4.76937
H	0.81203	−0.49679	5.02841
C	−0.94867	−0.51329	3.75419
C	−0.67490	0.68995	3.05621
H	0.23281	1.24531	3.30355
C	−1.53973	1.15818	2.09301
H	−1.32478	2.09256	1.57092
C	−2.70680	0.43305	1.77201
H	−3.39352	0.81021	1.01105
C	−2.99429	−0.74648	2.42561
C	−2.13450	−1.23526	3.44241
N	−3.37738	−4.47407	1.87222
N	−2.47670	−2.37830	4.11853
O	−5.55201	−0.65682	1.76993
P	−4.43682	−1.79052	2.12674
C	−4.72261	−6.50068	9.17198
C	−5.24901	−7.79439	9.30940
C	−3.68538	−6.11138	10.03411
C	−4.75156	−8.67334	10.27043
H	−6.06673	−8.12187	8.66007
C	−3.18385	−6.98695	10.99494
H	−3.26591	−5.10234	9.96460
C	−3.71637	−8.27064	11.11267
H	−5.17691	−9.67522	10.36628
H	−2.37937	−6.66566	11.66098
H	−3.32748	−8.95693	11.86869

C	-6.87494	-0.92399	1.46356
C	-7.66775	0.18691	1.18821
C	-7.38737	-2.20811	1.44449
C	-9.02078	0.01315	0.90995
H	-7.20307	1.17058	1.22858
C	-8.75004	-2.41144	1.17901
H	-6.74224	-3.06164	1.65351
C	-9.54004	-1.29504	0.91590
H	-10.59987	-1.43495	0.70581
C	-9.29146	-3.84091	1.21182
C	-9.94892	1.19330	0.61873
C	-10.53848	1.03157	-0.78991
H	-11.11525	0.10020	-0.88819
H	-11.21522	1.86923	-1.01961
H	-9.74263	1.01683	-1.55021
C	-9.21165	2.53084	0.68753
H	-8.78128	2.70934	1.68517
H	-8.40114	2.59085	-0.05476
H	-9.91175	3.35295	0.47802
C	-11.08273	1.21126	1.65443
H	-11.76186	2.05598	1.46142
H	-11.68201	0.28959	1.62676
H	-10.68454	1.32321	2.67491
C	-10.78118	-3.89881	0.87592
H	-11.38531	-3.32775	1.59685
H	-10.98730	-3.50970	-0.13270
H	-11.13016	-4.94161	0.90621
C	-8.52529	-4.69517	0.19098
H	-8.64654	-4.29466	-0.82702
H	-7.44732	-4.73150	0.41193
H	-8.90175	-5.72986	0.19876
C	-9.08331	-4.41502	2.62232
H	-8.01936	-4.43438	2.90555
H	-9.62011	-3.81555	3.37363
H	-9.46204	-5.44760	2.67686
C	-5.92316	-1.13844	5.15949
C	-7.25977	-0.95206	4.77752
C	-5.07588	-0.01975	5.20265
C	-7.73896	0.31627	4.45849
H	-7.94037	-1.80743	4.73328
C	-5.54870	1.24732	4.86836
H	-4.03404	-0.13659	5.51777
C	-6.88309	1.41606	4.49789
H	-8.78383	0.44405	4.16756
H	-4.87878	2.10970	4.91075
H	-7.25914	2.41072	4.24575

112

XII - Direct products of the double-silylation. Adducts between the catalyst and the double silane still formed.

Si	-2.81796	-0.79502	2.12116
C	-1.76924	-2.15463	1.31676
H	0.05296	-2.08054	-1.59972
Ni	1.11035	-1.78288	-0.65332
H	-3.56099	-1.26713	3.32791

H	−1.60429	−1.79080	0.28118
C	0.12028	−3.60009	1.11640
H	0.96276	−4.14884	1.56701
H	0.46580	−3.32832	0.07528
C	−1.13104	−4.47934	0.90954
H	−1.17139	−4.86688	−0.11857
H	−1.09912	−5.35556	1.57356
C	−2.34233	−3.57445	1.23205
H	−3.14433	−3.66458	0.48579
H	−2.78258	−3.86439	2.20110
C	−0.37481	−2.39261	1.92540
H	0.26341	−1.50439	1.80698
Si	−0.33848	−2.77535	3.80035
H	−1.54530	−2.19976	4.46371
H	−0.32428	−4.25765	4.00880
C	3.21958	−3.96631	−1.86891
H	2.99084	−4.52424	−0.95448
C	4.06616	−4.53487	−2.84466
H	4.50056	−5.52166	−2.67763
C	4.30907	−3.82693	−3.99644
H	4.94734	−4.23460	−4.78445
C	3.72046	−2.55020	−4.16969
C	3.91282	−1.76633	−5.33480
H	4.54705	−2.15783	−6.13378
C	3.30748	−0.53761	−5.46148
H	3.44952	0.05473	−6.36747
C	2.49921	−0.03271	−4.42062
H	2.01152	0.93818	−4.53507
C	2.30456	−0.76057	−3.26386
C	2.89919	−2.04988	−3.11727
C	2.99385	−1.56008	1.60434
H	2.67194	−2.58468	1.80356
C	3.91043	−0.93500	2.46961
H	4.28195	−1.48485	3.33433
C	4.26887	0.36884	2.23048
H	4.95216	0.89474	2.90160
C	3.73635	1.04203	1.10443
C	4.02919	2.39254	0.78546
H	4.70056	2.95344	1.43981
C	3.47449	2.99126	−0.32421
H	3.70044	4.03456	−0.55342
C	2.62355	2.25897	−1.18154
H	2.20239	2.73551	−2.07030
C	2.32184	0.94299	−0.89999
C	2.84572	0.32227	0.26387
N	2.66316	−2.78189	−1.99267
N	2.46839	−0.96405	0.55001
O	0.23242	0.79947	−2.68207
P	1.28062	−0.16761	−1.89342
C	1.20435	−2.05190	4.59534
C	2.21491	−2.86402	5.13346
C	1.33079	−0.65860	4.72643
C	3.30972	−2.30452	5.79513
H	2.13598	−3.95289	5.06021

C	2.41897	−0.09725	5.39048
H	0.55986	0.00248	4.32196
C	3.40823	−0.91954	5.93167
H	4.07775	−2.95314	6.22382
H	2.48632	0.98849	5.49613
H	4.25366	−0.48214	6.46877
C	−1.03113	1.08475	−2.16620
C	−1.21788	2.26993	−1.46247
C	−2.06619	0.20062	−2.41636
C	−2.49100	2.59038	−0.98855
H	−0.36561	2.92896	−1.30411
C	−3.35598	0.49741	−1.95280
H	−1.85945	−0.70179	−2.99371
C	−3.53474	1.68576	−1.24214
H	−4.53053	1.93338	−0.87668
C	−4.50731	−0.45359	−2.28619
C	−2.78284	3.89475	−0.24412
C	−3.78472	4.71662	−1.06922
H	−4.73719	4.18332	−1.20443
H	−4.00466	5.66908	−0.56229
H	−3.38207	4.94478	−2.06795
C	−1.51919	4.73079	−0.04010
H	−0.77027	4.19034	0.55832
H	−1.06210	5.02553	−0.99739
H	−1.77046	5.65475	0.50158
C	−3.38215	3.58111	1.13375
H	−3.61783	4.51652	1.66462
H	−4.31330	3.00106	1.05471
H	−2.67716	3.00534	1.74970
C	−5.81847	−0.02269	−1.62848
H	−5.73286	0.01343	−0.53167
H	−6.15156	0.96439	−1.98266
H	−6.61151	−0.74363	−1.87645
C	−4.70247	−0.46508	−3.80994
H	−4.93477	0.54334	−4.18438
H	−3.80197	−0.81914	−4.33393
H	−5.53454	−1.13233	−4.08395
C	−4.16740	−1.86955	−1.80191
H	−3.23827	−2.25200	−2.25082
H	−4.04953	−1.88705	−0.70906
H	−4.97633	−2.56720	−2.06826
H	−3.81983	−0.30164	1.12928
C	−1.65649	0.60145	2.62090
C	−1.78646	1.26054	3.85231
C	−0.62929	1.01420	1.75570
C	−0.92387	2.29854	4.20831
C	0.24188	2.04173	2.11069
C	0.09407	2.68825	3.33877
H	−2.57319	0.95912	4.54965
H	−0.51348	0.53491	0.77875
H	−1.04499	2.80157	5.17051
H	1.03236	2.34924	1.42190
H	0.77035	3.50061	3.61586

41

PhSiH2AlkSiH2Ph - Double sylilated product
C   1.56060   0.57109   1.97674
C   0.81883   2.90877   1.97247
C   0.51077   1.52188   2.57588
C   2.79859   1.46799   1.78185
C   2.17311   2.77350   1.25012
Si   1.73538   -1.07032   2.89613
H   2.03954   -0.83372   4.34302
H   2.83267   -1.89108   2.29312
Si   3.91281   1.77618   3.29178
H   0.86274   3.66992   2.76509
H   -0.51417   1.18110   2.36681
H   0.61253   1.56376   3.67283
H   1.21167   0.28015   0.96535
H   3.48585   1.02709   1.03753
H   2.01255   2.67313   0.16381
H   2.81718   3.65819   1.38547
H   0.03343   3.22825   1.27136
C   0.11462   -2.01414   2.77084
C   -0.94035   -1.74241   3.65634
C   -0.10209   -2.95769   1.75546
C   -2.16999   -2.38592   3.52963
H   -0.80051   -1.01590   4.46291
C   -1.32988   -3.60530   1.62497
H   0.70335   -3.19648   1.05413
C   -2.36644   -3.31895   2.51199
H   -2.97848   -2.16086   4.22975
H   -1.47787   -4.33905   0.82859
H   -3.32917   -3.82644   2.41221
H   4.45741   0.47900   3.80374
H   5.05122   2.62278   2.81111
C   3.06257   2.68472   4.70301
C   2.92964   4.08211   4.67164
C   2.50675   1.99426   5.79129
C   2.25014   4.76436   5.67933
H   3.36845   4.65235   3.84702
C   1.82812   2.67186   6.80287
H   2.60319   0.90641   5.85034
C   1.69437   4.05852   6.74571
H   2.15752   5.85241   5.63493
H   1.40325   2.11495   7.64178
H   1.16217   4.59140   7.53761

(NPN)Ni-H - (NPN)Ni-Silyl interconversion mediated by a silane moiety
86
NPNNi-H_PhSiH3 - Ni-H catalyst interacting with the SiH3Ph silane
Ni   0.66832   0.05310   -1.22243
H   2.11208   -0.41876   -1.28588
Si   1.98662   -1.05173   0.29594
H   1.00142   0.99282   -0.18796
H   0.83224   -1.45242   1.15573
H   2.60929   -2.33961   -0.16396
C   0.57404   -2.35211   -2.88433

H	1.66028	−2.25968	−2.81028
C	0.00053	−3.42241	−3.59829
H	0.65220	−4.15054	−4.08274
C	−1.36782	−3.52728	−3.65854
H	−1.84698	−4.34879	−4.19688
C	−2.16860	−2.55866	−3.00623
C	−3.58553	−2.60292	−2.99532
H	−4.08951	−3.41743	−3.52077
C	−4.31589	−1.64452	−2.32871
H	−5.40651	−1.69346	−2.32114
C	−3.66032	−0.59509	−1.65025
H	−4.24766	0.15440	−1.11351
C	−2.28238	−0.51884	−1.64733
C	−1.50896	−1.50402	−2.31609
C	1.53400	1.79104	−3.66828
H	2.34136	1.05381	−3.70195
C	1.55122	2.89726	−4.54428
H	2.36468	3.00112	−5.26380
C	0.54730	3.83127	−4.45481
H	0.53596	4.71013	−5.10439
C	−0.48569	3.65370	−3.50269
C	−1.55119	4.57268	−3.32687
H	−1.58678	5.46433	−3.95737
C	−2.52036	4.35311	−2.37441
H	−3.32764	5.07521	−2.23739
C	−2.48287	3.19237	−1.57108
H	−3.25351	3.02841	−0.81398
C	−1.46904	2.27058	−1.73051
C	−0.43393	2.49190	−2.68312
C	−1.59305	0.25667	1.69213
C	−1.98395	−1.07115	1.73786
H	−2.65323	−1.45880	0.96894
C	−1.49382	−1.89937	2.75538
C	−0.64526	−1.33185	3.70933
H	−0.25938	−1.96333	4.50643
C	−0.26198	0.01861	3.68163
C	−0.74491	0.81476	2.63868
H	−0.46936	1.86407	2.53848
N	−0.13950	−1.42590	−2.26939
N	0.58646	1.58923	−2.77563
O	−2.01145	1.05889	0.62262
P	−1.28048	0.74023	−0.80173
C	−1.88117	−3.37872	2.75681
C	0.60870	0.61719	4.78834
C	1.56491	−0.42696	5.37449
H	2.20208	−0.86645	4.59273
H	2.22213	0.04976	6.11684
H	1.03527	−1.23991	5.89177
C	1.44755	1.78898	4.26766
H	2.09204	1.48447	3.42978
H	0.82662	2.63560	3.93949
H	2.09711	2.16494	5.07200
C	−0.33187	1.11828	5.89616
H	−1.01901	1.88901	5.51501

H -0.94036 0.29587 6.30199
H 0.24894 1.55554 6.72358
C -1.23920 -4.13977 3.91641
H -0.14013 -4.10441 3.87049
H -1.55723 -3.74173 4.89165
H -1.53834 -5.19771 3.87837
C -3.40699 -3.50219 2.87283
H -3.76889 -3.04723 3.80714
H -3.92325 -3.00743 2.03635
H -3.70675 -4.56175 2.86997
C -1.41095 -4.01358 1.43806
H -1.87607 -3.53332 0.56317
H -0.31874 -3.92777 1.32802
H -1.67508 -5.08226 1.41251
C 3.25444 -0.05296 1.24167
C 3.93568 -0.66648 2.30540
C 3.53543 1.29047 0.95720
C 4.85930 0.04442 3.06779
H 3.74384 -1.71664 2.54718
C 4.46267 2.00421 1.71578
H 3.02033 1.79104 0.13169
C 5.12249 1.38254 2.77414
H 5.37706 -0.44689 3.89487
H 4.66972 3.05086 1.48086
H 5.84699 1.94096 3.37141
86
TS_H_PhSiH3 - TS of the reaction of the SiH3Ph silane with the Ni-H catalyst to form the Ni-Silyl catalyst
Ni 7.16785 7.90347 6.78432
H 8.14939 7.11767 6.05020
Si 8.67989 8.94959 8.36737
H 8.60819 8.26900 6.83880
H 8.23043 10.36905 8.43647
H 8.17043 8.11619 9.49134
C 5.96874 5.52147 5.69718
H 7.01646 5.25145 5.56327
C 4.94963 4.64851 5.27347
H 5.22306 3.69841 4.81304
C 3.63686 5.01487 5.44592
H 2.82138 4.36252 5.12395
C 3.33983 6.25347 6.06113
C 2.01626 6.69684 6.30947
H 1.18390 6.06395 5.99301
C 1.78070 7.89373 6.94677
H 0.75727 8.22148 7.13866
C 2.86153 8.69712 7.36713
H 2.66864 9.63479 7.89459
C 4.16060 8.29977 7.12860
C 4.42763 7.07477 6.46813
C 7.16970 9.71510 3.92563
H 7.56909 8.76761 3.54926
C 7.23090 10.87982 3.12706
H 7.66696 10.82681 2.12820
C 6.74788 12.06322 3.63462

H	6.78898	12.98533	3.04924
C	6.19239	12.08566	4.93751
C	5.67836	13.24967	5.56495
H	5.70090	14.19707	5.02094
C	5.16578	13.19135	6.84143
H	4.78406	14.09636	7.31824
C	5.12659	11.96745	7.54875
H	4.72832	11.92948	8.56491
C	5.60650	10.81929	6.95691
C	6.16214	10.85557	5.64944
C	5.22935	8.58178	10.24195
C	5.44262	7.23917	9.95943
H	5.72318	6.92613	8.95264
C	5.32957	6.28200	10.97130
C	4.99671	6.71891	12.25648
H	4.90419	5.98568	13.05370
C	4.78053	8.07196	12.55446
C	4.89987	9.00737	11.52115
H	4.74695	10.07395	11.69219
N	5.73227	6.69576	6.26539
N	6.65531	9.69923	5.13538
O	5.33730	9.56047	9.26565
P	5.64051	9.18144	7.69799
C	5.57733	4.81469	10.61643
C	4.42415	8.55577	13.96197
C	4.35180	7.40446	14.96559
H	5.31325	6.87632	15.05440
H	4.09929	7.79784	15.96133
H	3.57678	6.67142	14.69516
C	5.49601	9.54758	14.43753
H	6.48854	9.07251	14.46445
H	5.56220	10.42835	13.78183
H	5.26101	9.90508	15.45202
C	3.05593	9.25209	13.92214
H	3.05644	10.12348	13.25028
H	2.27200	8.56025	13.57792
H	2.77985	9.60737	14.92705
C	5.41704	3.89605	11.82721
H	6.13139	4.14536	12.62608
H	4.40056	3.94599	12.24558
H	5.60262	2.85284	11.53121
C	4.57123	4.38402	9.53776
H	3.53679	4.49402	9.89715
H	4.67312	4.98497	8.62090
H	4.72925	3.32865	9.26545
C	7.00599	4.66523	10.07087
H	7.16349	5.26829	9.16267
H	7.74828	4.98451	10.81821
H	7.20991	3.61387	9.81434
C	10.54415	8.88507	8.27805
C	11.28308	10.00442	7.86663
C	11.22868	7.70123	8.59496
C	12.67247	9.94301	7.77767
H	10.77182	10.93979	7.62014

C 12.61700 7.63965 8.50622
H 10.67427 6.81640 8.92311
C 13.33907 8.76081 8.09652
H 13.23829 10.82260 7.46205
H 13.13979 6.71505 8.76156
H 14.42847 8.71335 8.02918
86
NPNNiPhSiH2_H2 - Ni-Silyl catalyst already formed by a silane moiety. The H2 molecule which has been originated is still interacting with the catalyst
Ni 0.78732 -0.73914 -1.00614
H 2.03237 -1.72514 -1.12406
Si 1.70781 0.22241 0.84720
H 1.56056 -1.98246 -0.44820
H 0.93071 1.34101 1.46418
H 1.95391 -0.82576 1.88306
C 0.05509 -2.68748 -3.12764
H 1.12249 -2.91845 -3.07508
C -0.77379 -3.39749 -4.01884
H -0.33846 -4.16994 -4.65414
C -2.11651 -3.10600 -4.05713
H -2.79120 -3.64423 -4.72748
C -2.63118 -2.09608 -3.20928
C -4.00392 -1.74391 -3.15736
H -4.70671 -2.26923 -3.80823
C -4.44746 -0.76823 -2.29327
H -5.50874 -0.51553 -2.25090
C -3.53625 -0.08767 -1.45639
H -3.89726 0.67904 -0.76642
C -2.19229 -0.39492 -1.49716
C -1.71717 -1.41761 -2.35650
C 2.36478 0.90976 -3.04101
H 2.93805 -0.01655 -3.12626
C 2.79382 2.06462 -3.72572
H 3.68675 2.01669 -4.34986
C 2.08702 3.23158 -3.56798
H 2.39826 4.15166 -4.06888
C 0.94427 3.24506 -2.73229
C 0.17276 4.40907 -2.48742
H 0.45931 5.34256 -2.97763
C -0.91115 4.36998 -1.64001
H -1.48945 5.27573 -1.44738
C -1.28308 3.16121 -1.01232
H -2.13430 3.14129 -0.32790
C -0.56574 2.00643 -1.24564
C 0.57329 2.02576 -2.10001
C -1.56556 -0.01381 1.99934
C -1.53297 -1.39396 1.84964
H -1.65358 -1.83499 0.85842
C -1.34134 -2.21111 2.96844
C -1.21984 -1.59537 4.21773
H -1.07048 -2.21863 5.09589
C -1.27906 -0.20415 4.38173
C -1.44907 0.58963 3.24277

```
H         -1.47149        1.67897        3.29732
N         -0.38622       -1.73703       -2.32491
N          1.29906        0.88018       -2.26566
O         -1.67575        0.81579        0.88906
P         -0.90122        0.39834       -0.49315
C         -1.25793       -3.72521        2.76893
C         -1.13139        0.46914        5.74763
C         -0.96348       -0.54791        6.87671
H         -0.05835       -1.16039        6.74720
H         -0.86849       -0.02059        7.83736
H         -1.83034       -1.22153        6.95416
C          0.10690        1.37793        5.72253
H          1.01738        0.79677        5.51004
H          0.02298        2.16436        4.95785
H          0.23717        1.87315        6.69728
C         -2.38450        1.30973        6.03204
H         -2.53287        2.09612        5.27708
H         -3.28711        0.68001        6.04509
H         -2.29809        1.80278        7.01270
C         -1.01784       -4.46656        4.08369
H         -0.07375       -4.16045        4.55890
H         -1.83536       -4.30049        4.80114
H         -0.95866       -5.54874        3.89511
C         -2.57267       -4.22799        2.15524
H         -3.42469       -4.00913        2.81639
H         -2.77560       -3.75969        1.17996
H         -2.53155       -5.31751        2.00045
C         -0.09378       -4.03446        1.81420
H         -0.23627       -3.55951        0.83057
H          0.86010       -3.67225        2.22833
H         -0.00758       -5.12047        1.65350
C          3.29574        0.96510        0.17766
C          3.37526        2.34941       -0.04228
C          4.37729        0.16446       -0.22276
C          4.49471        2.91426       -0.65132
H          2.55090        2.99811        0.26927
C          5.49946        0.72628       -0.82857
H          4.35190       -0.91680       -0.05197
C          5.55665        2.10304       -1.04945
H          4.54292        3.99459       -0.80870
H          6.33779        0.09008       -1.12287
H          6.43710        2.54512       -1.52187
84
EXTRA ESI - Conformer A
1        5.819988000      7.080293000      8.198037000
6        7.288904000      5.655858000      5.481828000
1        8.239838000      6.114613000      5.766861000
6        7.275233000      4.461350000      4.731180000
1        8.218893000      4.009968000      4.421560000
6        6.067131000      3.884531000      4.423057000
1        6.016248000      2.951603000      3.856064000
6        4.868878000      4.506298000      4.851928000
6        3.581319000      3.971862000      4.594844000
1        3.501576000      3.037657000      4.033880000
```

6	2.450425000	4.613398000	5.047797000
1	1.463943000	4.187835000	4.853342000
6	2.557495000	5.825472000	5.763078000
1	1.654363000	6.321005000	6.129063000
6	3.794187000	6.381703000	6.019315000
6	4.978537000	5.723963000	5.581663000
6	7.222872000	9.814853000	5.065302000
1	8.178493000	9.422406000	5.421757000
6	7.201815000	10.804395000	4.062531000
1	8.142855000	11.160354000	3.641265000
6	5.991710000	11.308248000	3.651569000
1	5.935753000	12.088186000	2.888093000
6	4.799367000	10.811128000	4.230520000
6	3.510875000	11.292272000	3.885015000
1	3.429341000	12.081922000	3.134486000
6	2.383859000	10.784302000	4.489898000
1	1.398167000	11.172477000	4.225950000
6	2.492227000	9.752543000	5.447530000
1	1.592408000	9.349172000	5.918116000
6	3.730085000	9.254024000	5.795757000
6	4.912751000	9.791903000	5.217119000
6	3.117616000	7.460711000	9.307935000
6	3.396753000	6.109877000	9.434125000
1	3.366272000	5.472319000	8.549760000
6	3.721138000	5.579252000	10.691156000
6	3.732813000	6.449524000	11.780337000
1	3.982273000	6.057203000	12.765391000
6	3.438269000	7.819438000	11.664415000
6	3.128595000	8.322384000	10.400182000
1	2.906890000	9.375557000	10.232512000
6	4.061954000	4.092483000	10.801027000
6	4.372834000	3.679074000	12.239358000
1	4.613402000	2.606220000	12.274120000
1	5.238267000	4.224726000	12.644999000
1	3.514498000	3.847220000	12.907140000
6	2.871027000	3.262565000	10.300166000
1	1.968288000	3.469978000	10.894322000
1	2.636522000	3.473997000	9.245985000
1	3.094069000	2.187439000	10.381947000
6	5.294843000	3.798204000	9.931682000
1	5.546745000	2.727188000	9.976419000
1	5.125243000	4.058418000	8.875214000
1	6.169350000	4.367331000	10.282788000
6	3.483685000	8.706448000	12.909195000
6	2.436149000	8.207625000	13.915519000
1	2.449471000	8.833262000	14.821442000
1	1.424206000	8.250663000	13.485010000
1	2.626862000	7.169215000	14.224214000
6	3.185889000	10.169823000	12.581017000
1	3.919466000	10.589377000	11.874887000
1	2.179946000	10.298557000	12.153433000
1	3.232008000	10.772794000	13.499816000
6	4.883261000	8.625198000	13.536957000
1	5.139282000	7.600582000	13.843950000

1 5.654304000 8.968212000 12.829927000
1 4.935636000 9.262363000 14.433275000
7 6.195341000 6.267186000 5.887178000
7 6.136051000 9.323637000 5.628052000
8 2.863524000 8.003220000 8.049116000
15 4.080715000 7.914122000 6.953814000
28 6.182801000 7.943133000 7.132403000
6 7.385020000 7.380902000 10.115244000
6 8.398447000 7.101895000 8.991616000
6 8.046383000 8.110302000 7.918934000
6 7.205064000 9.093743000 8.445452000
6 6.942998000 8.836140000 9.906821000
1 7.801543000 7.202734000 11.116695000
1 8.379701000 6.055319000 8.648210000
1 9.430804000 7.301243000 9.331922000
1 8.723460000 8.276588000 7.073542000
1 7.109632000 10.102005000 8.031165000
1 5.901696000 9.017349000 10.211844000
1 7.575141000 9.532184000 10.488857000
1 6.511589000 6.717350000 10.013178000
84
EXTRA ESI - Conformer B
1 7.731252000 6.870461000 7.499318000
6 6.901151000 4.596740000 6.195704000
1 7.870211000 4.789100000 6.660749000
6 6.693255000 3.422235000 5.444133000
1 7.512056000 2.710858000 5.328222000
6 5.462067000 3.200903000 4.877729000
1 5.263726000 2.301452000 4.289506000
6 4.431911000 4.153321000 5.067889000
6 3.124940000 3.994514000 4.543190000
1 2.900817000 3.102553000 3.953357000
6 2.150981000 4.939107000 4.778862000
1 1.145319000 4.802569000 4.376436000
6 2.445722000 6.084848000 5.546934000
1 1.661110000 6.818178000 5.750574000
6 3.711905000 6.275753000 6.062317000
6 4.731203000 5.313085000 5.838206000
6 7.852491000 8.891315000 5.598453000
1 8.657256000 8.263215000 5.986429000
6 8.136709000 9.930347000 4.689154000
1 9.166288000 10.090301000 4.366076000
6 7.111236000 10.728935000 4.244574000
1 7.296938000 11.553917000 3.552309000
6 5.793673000 10.479633000 4.697544000
6 4.677615000 11.266031000 4.314572000
1 4.835391000 12.104505000 3.632124000
6 3.420259000 10.989147000 4.801165000
1 2.571297000 11.611595000 4.511702000
6 3.217298000 9.897077000 5.672515000
1 2.217239000 9.684480000 6.057784000
6 4.280567000 9.103025000 6.049219000
6 5.595193000 9.391852000 5.593458000
6 2.906687000 7.296469000 9.283415000

```
6         2.764883000      5.918801000      9.301348000
1         2.549749000      5.392572000      8.371092000
6         2.940794000      5.217060000     10.503331000
6         3.222430000      5.955174000     11.652711000
1         3.371989000      5.426996000     12.593556000
6         3.337618000      7.356733000     11.648846000
6         3.170627000      8.027241000     10.437395000
1         3.273265000      9.108576000     10.354338000
6         2.876183000      3.689678000     10.482155000
6         3.066853000      3.086821000     11.873594000
1         3.006952000      1.990005000     11.815255000
1         4.049383000      3.340970000     12.299337000
1         2.288356000      3.423811000     12.574490000
6         1.513872000      3.241676000      9.934607000
1         0.692957000      3.616525000     10.564244000
1         1.342879000      3.602001000      8.909076000
1         1.454009000      2.142505000      9.914565000
6         3.997009000      3.169790000      9.566216000
1         3.979829000      2.069505000      9.526137000
1         3.892107000      3.544433000      8.536022000
1         4.985275000      3.481747000      9.939089000
6         3.705888000      8.086855000     12.940490000
6         2.674264000      7.758560000     14.028680000
1         2.932928000      8.275184000     14.965720000
1         1.666601000      8.082531000     13.727391000
1         2.631247000      6.681283000     14.245516000
6         3.745882000      9.603320000     12.750529000
1         4.508422000      9.905768000     12.015924000
1         2.772764000     10.001211000     12.424685000
1         3.999707000     10.089750000     13.703869000
6         5.099782000      7.615447000     13.383913000
1         5.123499000      6.533168000     13.579476000
1         5.851487000      7.835841000     12.609392000
1         5.400974000      8.129659000     14.309667000
7         5.970233000      5.514052000      6.385765000
7         6.636831000      8.622170000      6.038830000
8         2.884637000      7.976274000      8.063121000
15        4.204945000      7.661377000      7.128318000
28        6.339867000      7.182023000      7.511283000
6         8.746037000      7.007062000      9.773644000
6         7.604698000      6.004439000     10.000494000
6         6.376712000      6.697479000      9.467819000
6         6.636251000      8.065630000      9.295219000
6         8.057550000      8.378619000      9.693578000
1         9.258105000      6.786633000      8.823321000
1         7.438680000      5.835939000     11.080843000
1         7.791365000      5.012784000      9.560098000
1         5.382603000      6.288143000      9.665905000
1         5.862950000      8.835908000      9.367274000
1         8.026798000      8.860023000     10.688554000
1         8.566339000      9.088826000      9.023818000
1         9.511462000      6.963502000     10.561271000
84
EXTRA ESI - Conformer C
```

1	7.950094000	6.781817000	8.221917000
6	6.842574000	4.582348000	6.605666000
1	7.780248000	4.642917000	7.163575000
6	6.538548000	3.419535000	5.873909000
1	7.247061000	2.590429000	5.869229000
6	5.350373000	3.357509000	5.185584000
1	5.078619000	2.469176000	4.609916000
6	4.464877000	4.460473000	5.227221000
6	3.214506000	4.477028000	4.557310000
1	2.919493000	3.601198000	3.974739000
6	2.386215000	5.572372000	4.640863000
1	1.424702000	5.573207000	4.123765000
6	2.772796000	6.700938000	5.397169000
1	2.108206000	7.566548000	5.460570000
6	3.982951000	6.718987000	6.055916000
6	4.852512000	5.598857000	5.986200000
6	7.056078000	8.780744000	3.878366000
1	7.745655000	7.940855000	3.737604000
6	7.116655000	9.894362000	3.007703000
1	7.849303000	9.909877000	2.198990000
6	6.246743000	10.941511000	3.203147000
1	6.266515000	11.819379000	2.552192000
6	5.312441000	10.877227000	4.265785000
6	4.369172000	11.894165000	4.563748000
1	4.345322000	12.792960000	3.942644000
6	3.496967000	11.753808000	5.619608000
1	2.777032000	12.544048000	5.841787000
6	3.519887000	10.593060000	6.427901000
1	2.829770000	10.489816000	7.267597000
6	4.421092000	9.586547000	6.153779000
6	5.337331000	9.708531000	5.075102000
6	3.446926000	7.602748000	9.426555000
6	3.807748000	6.264411000	9.451370000
1	4.038037000	5.746109000	8.522102000
6	3.855139000	5.572365000	10.671167000
6	3.510695000	6.266469000	11.828720000
1	3.543154000	5.748028000	12.786128000
6	3.123144000	7.618541000	11.813750000
6	3.094593000	8.283799000	10.589204000
1	2.818094000	9.334280000	10.509390000
6	4.339175000	4.121109000	10.682575000
6	4.111818000	3.450914000	12.037761000
1	4.442071000	2.402401000	11.996167000
1	4.683139000	3.940619000	12.840220000
1	3.047855000	3.456760000	12.318783000
6	3.602553000	3.307497000	9.609451000
1	2.515245000	3.322802000	9.777933000
1	3.791595000	3.686709000	8.593407000
1	3.936739000	2.258933000	9.633776000
6	5.846330000	4.120284000	10.379053000
1	6.235235000	3.090153000	10.347313000
1	6.056621000	4.596585000	9.408804000
1	6.402815000	4.671800000	11.152253000
6	2.778420000	8.317058000	13.129869000

```
6         1.620975000      7.572133000     13.810544000
1         1.359855000      8.063370000     14.760536000
1         0.725096000      7.566680000     13.171305000
1         1.879536000      6.527450000     14.037263000
6         2.359906000      9.771372000     12.914479000
1         3.166702000     10.368172000     12.461711000
1         1.467863000      9.849874000     12.274405000
1         2.113194000     10.233946000     13.881415000
6         4.015586000      8.295930000     14.040228000
1         4.343079000      7.270206000     14.265014000
1         4.858918000      8.824290000     13.569019000
1         3.794262000      8.792838000     14.997360000
7         6.043752000      5.635592000      6.668448000
7         6.202551000      8.686525000      4.871966000
8         3.441392000      8.326831000      8.247630000
15        4.599410000      8.071479000      7.104884000
28        6.465709000      7.281766000      7.648028000
6         6.864280000      8.038357000     10.760471000
6         6.571432000      9.236298000      9.859682000
6         7.129609000      8.814224000      8.515053000
6         8.205487000      7.805956000      8.758830000
6         8.228163000      7.547082000     10.271395000
1         6.096758000      7.262298000     10.602771000
1         7.120160000     10.127624000     10.216938000
1         5.506936000      9.510487000      9.831142000
1         7.320446000      9.604808000      7.776510000
1         9.180664000      8.008835000      8.292836000
1         9.031825000      8.164314000     10.704334000
1         8.443660000      6.501701000     10.536655000
1         6.860045000      8.283908000     11.831981000
84
EXTRA ESI - Conformer D
1         6.032605000      5.677094000      7.767060000
6         5.387941000      5.003714000      3.240116000
1         6.438878000      5.210422000      3.008482000
6         4.660523000      4.082298000      2.450238000
1         5.149302000      3.584574000      1.610920000
6         3.345442000      3.828985000      2.762580000
1         2.753415000      3.120980000      2.176893000
6         2.752242000      4.498889000      3.860789000
6         1.406776000      4.319496000      4.273978000
1         0.771812000      3.622067000      3.722114000
6         0.906565000      5.012275000      5.353641000
1        -0.129884000      4.865461000      5.664310000
6         1.721902000      5.919678000      6.070012000
1         1.319030000      6.462596000      6.928894000
6         3.032097000      6.115329000      5.687523000
6         3.574892000      5.408454000      4.581589000
6         7.874084000      8.568196000      5.047796000
1         8.692575000      7.942888000      5.403171000
6         8.137907000      9.633272000      4.167125000
1         9.164366000      9.815721000      3.846863000
6         7.097754000     10.422993000      3.743040000
1         7.266649000     11.267749000      3.070667000
```

6	5.785124000	10.131821000	4.182153000
6	4.656707000	10.892986000	3.785028000
1	4.809492000	11.747966000	3.122294000
6	3.393813000	10.561671000	4.218673000
1	2.532058000	11.154634000	3.906360000
6	3.206069000	9.443008000	5.057237000
1	2.198189000	9.167230000	5.377404000
6	4.284033000	8.688899000	5.471622000
6	5.598856000	9.024027000	5.056603000
6	3.600132000	7.171522000	9.060920000
6	3.491670000	5.798570000	9.224807000
1	3.175688000	5.180437000	8.382231000
6	3.766746000	5.217923000	10.472796000
6	4.142388000	6.064039000	11.515628000
1	4.357796000	5.633248000	12.492743000
6	4.263241000	7.456446000	11.358943000
6	3.986261000	8.005969000	10.106891000
1	4.061944000	9.074971000	9.912390000
6	3.649742000	3.700821000	10.628177000
6	3.980364000	3.241450000	12.047907000
1	3.884295000	2.147858000	12.117119000
1	5.011273000	3.500437000	12.334017000
1	3.295390000	3.680365000	12.788763000
6	2.213412000	3.270695000	10.296506000
1	1.492485000	3.756891000	10.970914000
1	1.934513000	3.527450000	9.263263000
1	2.105231000	2.180871000	10.409028000
6	4.627775000	3.022215000	9.656808000
1	4.549107000	1.926967000	9.735958000
1	4.422319000	3.294725000	8.609878000
1	5.667316000	3.303283000	9.886968000
6	4.701415000	8.312047000	12.548270000
6	3.666143000	8.170065000	13.673895000
1	3.961406000	8.779347000	14.542126000
1	2.673351000	8.508271000	13.340537000
1	3.570490000	7.128562000	14.014307000
6	4.819486000	9.790494000	12.178226000
1	5.562685000	9.955387000	11.382651000
1	3.857316000	10.209409000	11.846641000
1	5.143726000	10.367809000	13.056568000
6	6.071891000	7.824554000	13.041085000
1	6.044495000	6.773635000	13.364223000
1	6.830291000	7.914623000	12.248155000
1	6.404102000	8.427529000	13.900152000
7	4.871156000	5.643268000	4.263856000
7	6.663724000	8.268368000	5.492491000
8	3.334827000	7.754723000	7.830636000
15	4.192089000	7.221305000	6.523228000
28	6.328298000	6.819896000	6.707889000
6	7.911897000	7.335555000	9.358567000
6	7.367206000	5.913588000	9.487194000
6	7.205684000	5.463106000	8.033961000
6	8.093108000	6.298966000	7.210516000
6	8.814110000	7.273044000	8.123913000

1 8.432858000 7.680331000 10.263043000
1 6.441559000 5.849603000 10.075662000
1 8.114398000 5.255800000 9.961452000
1 7.196825000 4.380953000 7.842340000
1 8.646470000 5.832079000 6.384711000
1 8.996793000 8.262407000 7.674304000
1 9.806692000 6.866003000 8.392872000
1 7.073975000 8.032544000 9.177871000
84
EXTRA ESI - I_tN' - Coordination of the cyclopentene
C 5.98370 4.01052 4.74932
H 7.07140 3.99708 4.86465
C 5.32832 2.96200 4.07113
H 5.91438 2.14732 3.64348
C 3.95749 2.98520 3.98458
H 3.41105 2.18326 3.48184
C 3.23921 4.06042 4.56238
C 1.82440 4.14601 4.53603
H 1.25897 3.35128 4.04362
C 1.17264 5.20547 5.12461
H 0.08214 5.25562 5.10982
C 1.90853 6.23738 5.74535
H 1.38145 7.07364 6.21124
C 3.28744 6.19490 5.77754
C 3.98524 5.09144 5.20176
C 7.41540 7.51001 3.78284
H 8.09921 6.67774 3.96014
C 7.57986 8.32992 2.64800
H 8.38853 8.11699 1.94768
C 6.73490 9.39830 2.46980
H 6.85504 10.07708 1.62175
C 5.67943 9.60762 3.38992
C 4.73974 10.66342 3.27266
H 4.85070 11.37733 2.45324
C 3.70243 10.78508 4.16984
H 2.98814 11.60514 4.07273
C 3.53540 9.83293 5.19922
H 2.68485 9.90825 5.88178
C 4.43882 8.80109 5.34427
C 5.55648 8.69649 4.47534
C 4.26653 8.48907 8.85925
C 4.59610 7.62155 9.89669
H 4.19801 6.60776 9.87368
C 5.43499 8.06516 10.91872
C 5.90421 9.38927 10.86082
H 6.55919 9.73929 11.65761
C 5.56631 10.26924 9.83275
C 4.72955 9.79180 8.81139
H 4.44026 10.42788 7.97375
N 5.34947 5.03273 5.28518
N 6.47321 7.69700 4.68616
O 3.48577 7.99976 7.80715
P 4.35796 7.43857 6.53695
Ni 6.27992 6.55225 6.37125

```
H          5.79103        5.88073        7.52449
C          8.17908        6.08150        7.05717
C          7.67577        7.21262        7.69812
H          8.04996        5.06851        7.45082
H          7.11925        7.19635        8.63846
C          9.44728        7.97966        6.23640
H         10.46145        8.35887        6.42482
H          9.16070        8.37570        5.25258
C          8.45321        8.44570        7.31777
H          8.97411        8.80955        8.22053
H          7.80755        9.27536        6.99009
C          9.40977        6.43758        6.25457
H          9.45301        5.98542        5.24889
H         10.28738        6.02843        6.78521
C          5.87128        7.15816       12.07005
C          6.06313       11.71504        9.77762
C          5.43542        7.78513       13.40226
H          5.73992        7.14290       14.24305
H          5.88852        8.77498       13.55956
H          4.34216        7.90492       13.44229
C          7.40088        7.01802       12.03906
H          7.73639        6.56615       11.09206
H          7.90533        7.98952       12.14652
H          7.74245        6.37207       12.86266
C          5.25528        5.76304       11.96471
H          4.15571        5.79712       11.99798
H          5.55912        5.24904       11.03936
H          5.59141        5.14430       12.80976
C          6.84016       11.93610        8.47145
H          6.22045       11.73874        7.58340
H          7.18967       12.97818        8.40724
H          7.72163       11.27905        8.42325
C          4.85197       12.65819        9.82206
H          4.17284       12.49355        8.97203
H          4.27393       12.51284       10.74705
H          5.18353       13.70755        9.78713
C          6.98584       12.05161       10.94922
H          6.47395       11.94696       11.91761
H          7.88320       11.41410       10.96147
H          7.32362       13.09528       10.86720
84
EXTRA ESI - TS_I_II_tN' - TS for the C-H bond formation
C          5.85966        3.96025        4.49754
H          6.95104        3.91042        4.56175
C          5.14768        2.96686        3.79243
H          5.69179        2.16148        3.29691
C          3.77575        3.03084        3.76585
H          3.18621        2.27209        3.24504
C          3.11363        4.09291        4.42906
C          1.70220        4.22042        4.46578
H          1.09315        3.46963        3.95665
C          1.10726        5.26564        5.13460
H          0.01910        5.34773        5.16756
C          1.89863        6.24199        5.77678
```

H	1.41742	7.06759	6.30676
C	3.27558	6.15698	5.74929
C	3.91702	5.06628	5.08958
C	7.45075	7.44518	3.76159
H	8.10772	6.58554	3.89857
C	7.63037	8.30239	2.65738
H	8.42882	8.09440	1.94391
C	6.81182	9.39736	2.52254
H	6.94521	10.10433	1.69992
C	5.76150	9.59369	3.45165
C	4.83559	10.66463	3.36972
H	4.95687	11.40482	2.57544
C	3.79532	10.76585	4.26633
H	3.08846	11.59476	4.19304
C	3.61529	9.78204	5.26298
H	2.76019	9.84161	5.94141
C	4.51111	8.73986	5.37999
C	5.62618	8.65011	4.50747
C	4.35121	8.42140	8.84518
C	4.72415	7.59972	9.90479
H	4.36889	6.56987	9.91311
C	5.54102	8.11024	10.91329
C	5.95529	9.45008	10.81442
H	6.59663	9.85140	11.59821
C	5.58367	10.28106	9.75791
C	4.75942	9.74084	8.75832
H	4.44039	10.34233	7.90692
N	5.27959	4.96729	5.11449
N	6.52453	7.62757	4.68271
O	3.56929	7.87409	7.82427
P	4.40665	7.33340	6.52307
Ni	6.29935	6.43709	6.32608
H	5.73506	5.74855	7.43009
C	8.27278	5.93524	6.79631
C	7.66268	6.56300	7.87873
H	8.32560	4.84571	6.69697
H	7.21893	6.03067	8.72156
C	9.00412	8.22740	6.80452
H	9.88412	8.86294	6.97613
H	8.36729	8.75336	6.07708
C	8.20772	7.95119	8.08534
H	8.86917	7.91927	8.97074
H	7.43208	8.69879	8.30763
C	9.37507	6.83454	6.27503
H	9.55022	6.81074	5.18976
H	10.32176	6.48859	6.72992
C	6.00041	7.26281	12.10070
C	6.05016	11.73223	9.63266
C	5.49676	7.90656	13.40087
H	5.81509	7.31049	14.27008
H	5.89013	8.92510	13.53322
H	4.39791	7.96599	13.41077
C	7.53516	7.20478	12.11336
H	7.92074	6.74151	11.19164

```
H          7.98471        8.20468       12.20127
H          7.88763        6.60517       12.96673
C          5.46295        5.83359       12.02592
H          4.36279        5.80781       12.03819
H          5.81102        5.30999       11.12151
H          5.81569        5.25780       12.89417
C          6.85354       11.88643        8.33169
H          6.25500       11.62676        7.44501
H          7.19153       12.92755        8.21248
H          7.74465       11.23962        8.33906
C          4.82317       12.65446        9.59271
H          4.16847       12.43144        8.73687
H          4.22379       12.55247       10.50993
H          5.13825       13.70581        9.50546
C          6.93792       12.15385       10.80335
H          6.40740       12.08359       11.76487
H          7.85154       11.54331       10.86656
H          7.24967       13.20090       10.67465
84
EXTRA ESI - II_tN' - Ni-Alkyl post TS. Agostic interaction
C          5.10563        4.87479        2.92754
H          6.03038        5.20891        2.44396
C          4.32452        3.85826        2.32842
H          4.64617        3.41427        1.38475
C          3.17117        3.44600        2.95429
H          2.54557        2.66067        2.52224
C          2.79238        4.05094        4.17784
C          1.62959        3.70993        4.91605
H          0.96742        2.93037        4.53140
C          1.33904        4.34886        6.10053
H          0.44305        4.07602        6.66180
C          2.18838        5.36169        6.60562
H          1.95371        5.86264        7.54714
C          3.31937        5.71692        5.90222
C          3.64899        5.06606        4.68435
C          7.81831        8.74336        4.52599
H          8.74780        8.25859        4.82209
C          7.84909        9.82059        3.62189
H          8.80892       10.15241        3.22434
C          6.67118       10.43273        3.27090
H          6.65767       11.27975        2.58051
C          5.45571        9.95473        3.81393
C          4.19787       10.53292        3.50485
H          4.16769       11.38365        2.82013
C          3.03887       10.03518        4.05398
H          2.07613       10.48854        3.81015
C          3.09094        8.93198        4.93248
H          2.16786        8.53454        5.36276
C          4.29766        8.34872        5.25508
C          5.50774        8.85098        4.71133
C          4.59370        8.16574        8.72080
C          4.83624        7.61228        9.97597
H          4.39453        6.64375       10.20746
C          5.62221        8.30788       10.89579
```

```
C          6.15919        9.54745       10.50626
H          6.78048       10.08836       11.21884
C          5.93042       10.10656        9.24941
C          5.11914        9.39515        8.35342
H          4.87861        9.80441        7.37193
N          4.78445        5.45851        4.05906
N          6.70494        8.27053        5.06418
O          3.80775        7.44914        7.83169
P          4.50945        6.96659        6.41481
Ni         6.68884        6.82411        6.32393
H          6.65407        5.63356        7.36451
C          8.54843        6.45782        6.55053
C          7.86885        5.51512        7.45214
H          9.01337        6.07293        5.63341
H          7.92483        4.44446        7.21038
C          8.58321        7.40217        8.74630
H          9.18703        7.77383        9.58598
H          7.66558        8.01433        8.71049
C          8.20469        5.92865        8.88568
H          9.07178        5.33209        9.21403
H          7.38745        5.75195        9.60005
C          9.30283        7.46577        7.39800
H          9.32614        8.48269        6.97358
H         10.35725        7.14930        7.50383
C          5.90608        7.77002       12.29973
C          6.52954       11.44158        8.80465
C          5.30251        8.73910       13.32776
H          5.48498        8.37314       14.35007
H          5.74218        9.74437       13.24894
H          4.21519        8.83518       13.18755
C          7.42276        7.66895       12.51693
H          7.88020        6.96839       11.80170
H          7.92377        8.64169       12.40528
H          7.63628        7.30178       13.53252
C          5.29558        6.38554       12.51777
H          4.19947        6.39901       12.42075
H          5.69714        5.64395       11.80928
H          5.53085        6.03157       13.53224
C          7.40278       11.20474        7.56249
H          6.82006       10.78951        6.72620
H          7.84914       12.15178        7.22143
H          8.22114       10.50287        7.78581
C          5.39417       12.41404        8.45484
H          4.76457       12.03372        7.63617
H          4.74391       12.58855        9.32513
H          5.80624       13.38414        8.13628
C          7.39634       12.07377        9.89311
H          6.81583       12.29076       10.80224
H          8.24327       11.42756       10.17008
H          7.81138       13.02642        9.53210
84
EXTRA ESI - I_tP - Coordination of the cyclopentene
H          3.12373       -0.55691       -1.58255
C          1.74349       -2.82274       -1.92417
```

H	2.80527	−2.78435	−1.67439
C	1.18909	−3.98723	−2.49049
H	1.83218	−4.84923	−2.67266
C	−0.14755	−4.00618	−2.80767
H	−0.60910	−4.88847	−3.25807
C	−0.93950	−2.86615	−2.53283
C	−2.33214	−2.80773	−2.79062
H	−2.81882	−3.67349	−3.24584
C	−3.06242	−1.68809	−2.46165
H	−4.13586	−1.65614	−2.65792
C	−2.43200	−0.58421	−1.84959
H	−3.02526	0.28457	−1.55293
C	−1.07509	−0.60169	−1.60158
C	−0.30008	−1.73729	−1.94687
C	2.51470	1.25388	−3.71892
H	3.26438	0.45865	−3.70387
C	2.54791	2.24472	−4.72161
H	3.31763	2.19911	−5.49341
C	1.62170	3.26062	−4.69124
H	1.63318	4.05663	−5.44005
C	0.63963	3.27239	−3.67209
C	−0.35216	4.27931	−3.54298
H	−0.36476	5.10087	−4.26302
C	−1.27765	4.22748	−2.52591
H	−2.02825	5.01454	−2.42965
C	−1.27476	3.15437	−1.60523
H	−2.01701	3.10950	−0.80518
C	−0.32785	2.15963	−1.71233
C	0.66479	2.21176	−2.72577
C	−1.35218	0.28483	1.65537
C	−0.97561	−1.05216	1.63749
H	−0.58773	−1.50252	0.72426
C	−1.08407	−1.82832	2.79516
C	−1.58190	−1.21982	3.95082
H	−1.67167	−1.81068	4.85891
C	−1.96689	0.12822	3.98092
C	−1.84682	0.88012	2.80731
H	−2.12081	1.93560	2.77179
N	1.04084	−1.73118	−1.67057
N	1.61616	1.23230	−2.75304
O	−1.23677	1.08634	0.53086
P	−0.18554	0.69236	−0.67669
Ni	1.91539	−0.02836	−1.02994
C	1.80493	1.84109	1.77963
C	2.64816	2.40429	0.62188
C	3.21302	1.18772	−0.06683
C	3.00138	0.03987	0.69982
C	2.27178	0.38701	1.97307
H	0.73554	1.87846	1.53596
H	3.49895	3.00109	0.99620
H	2.08237	3.07218	−0.04792
H	4.03371	1.28968	−0.78233
H	3.63308	−0.85083	0.64518
H	3.00538	0.31043	2.79620

```
H          1.45310       -0.30179        2.22624
H          1.91657        2.43329        2.69856
C         -0.64017       -3.29157        2.73791
C         -2.48567        0.80551        5.25131
C         -0.87644       -4.01472        4.06331
H         -1.94099       -4.01732        4.34191
H         -0.55258       -5.06274        3.98011
H         -0.30595       -3.55767        4.88574
C         -1.42720       -4.01767        1.63621
H         -2.50912       -3.97954        1.83393
H         -1.25187       -3.57462        0.64342
H         -1.12561       -5.07554        1.58618
C          0.86046       -3.34265        2.41088
H          1.08639       -2.85980        1.44701
H          1.45063       -2.83412        3.18854
H          1.20463       -4.38714        2.35226
C         -2.58484       -0.16925        6.42513
H         -3.27556       -0.99938        6.21259
H         -1.60508       -0.59332        6.69237
H         -2.96638        0.35858        7.31153
C         -1.51995        1.93587        5.63797
H         -0.50970        1.54190        5.82773
H         -1.44276        2.69755        4.84773
H         -1.86786        2.43842        6.55375
C         -3.88130        1.38653        4.98337
H         -3.86754        2.13716        4.17935
H         -4.58976        0.59514        4.69490
H         -4.26912        1.87810        5.88897
84
EXTRA ESI - TS_I_II_tP - TS for the C-H bond formation
H          8.12766        6.73556        6.38110
C          6.59715        4.57505        6.22473
H          7.68096        4.55844        6.34922
C          5.91752        3.42890        5.77039
H          6.48728        2.52548        5.54940
C          4.55422        3.47945        5.60806
H          3.99550        2.61219        5.24761
C          3.86356        4.67142        5.92956
C          2.45465        4.79776        5.83598
H          1.87468        3.94573        5.47372
C          1.82585        5.96411        6.20779
H          0.73960        6.04807        6.13891
C          2.58048        7.05105        6.69719
H          2.07173        7.96225        7.02233
C          3.95403        6.96589        6.78591
C          4.62479        5.77919        6.39705
C          7.11590        8.46900        4.00977
H          7.77212        7.59884        3.91418
C          7.05981        9.43533        2.98160
H          7.66424        9.29997        2.08335
C          6.25532       10.53928        3.14336
H          6.20278       11.31450        2.37465
C          5.48454       10.66996        4.32401
C          4.62458       11.76550        4.59715
```

H	4.54592	12.57090	3.86307
C	3.90298	11.81587	5.76810
H	3.25167	12.66836	5.97114
C	3.98645	10.76685	6.71379
H	3.40456	10.80612	7.63718
C	4.81006	9.69009	6.47116
C	5.59086	9.63037	5.28676
C	3.92027	7.87618	9.89921
C	4.38166	6.56527	9.91935
H	5.00917	6.19161	9.10847
C	4.05308	5.72238	10.98486
C	3.26498	6.24079	12.01639
H	3.00228	5.59634	12.85131
C	2.79970	7.56320	12.01119
C	3.13842	8.38171	10.92869
H	2.80650	9.41932	10.86795
N	5.99046	5.71541	6.51615
N	6.41556	8.55996	5.12118
O	4.21412	8.73905	8.85858
P	5.02954	8.23902	7.51694
Ni	6.99723	7.35313	6.99986
C	7.50582	8.47659	10.03244
C	7.62428	9.57573	8.96706
C	8.14640	8.85083	7.74721
C	8.71741	7.63537	8.12981
C	8.50934	7.39603	9.60562
H	6.49039	8.05872	10.04214
H	8.38768	10.32171	9.25541
H	6.69194	10.14008	8.81091
H	8.46279	9.39643	6.85266
H	9.57641	7.18790	7.62819
H	9.49034	7.53953	10.09473
H	8.18792	6.37448	9.85820
H	7.69494	8.85073	11.04804
C	4.54696	4.27477	10.95270
C	1.93924	8.13551	13.14000
C	4.17215	3.51085	12.22224
H	3.08189	3.45108	12.35735
H	4.55328	2.48055	12.16371
H	4.60595	3.97549	13.12048
C	3.91130	3.56731	9.74562
H	2.81336	3.56837	9.82179
H	4.18039	4.06034	8.79892
H	4.25081	2.52098	9.69031
C	6.07558	4.25688	10.80418
H	6.40090	4.72870	9.86400
H	6.56031	4.78952	11.63658
H	6.44664	3.22028	10.79964
C	1.66233	7.10299	14.23307
H	1.11652	6.22990	13.84456
H	2.58982	6.74898	14.70806
H	1.04147	7.55549	15.02033
C	2.67053	9.32906	13.77186
H	3.64266	9.02126	14.18622

```
H          2.85379       10.13203       13.04247
H          2.06936        9.75365       14.59068
C          0.59546        8.60114       12.56036
H          0.72513        9.38189       11.79607
H          0.05357        7.76196       12.09783
H         -0.03904        9.01875       13.35742
84
EXTRA ESI - II_tP - Ni-Alkyl post TS. Agostic interaction
H          2.90666       -0.70049        0.16211
C          1.69302       -2.90079       -1.37491
H          2.63972       -2.86117       -0.83056
C          1.33485       -4.07081       -2.06978
H          2.01028       -4.92702       -2.05854
C          0.13742       -4.10487       -2.74381
H         -0.17544       -4.99728       -3.29158
C         -0.70432       -2.96759       -2.72292
C         -1.96157       -2.92097       -3.37850
H         -2.29572       -3.79915       -3.93583
C         -2.74852       -1.79451       -3.31152
H         -3.71578       -1.77078       -3.81724
C         -2.31299       -0.66417       -2.58498
H         -2.94655        0.22503       -2.53123
C         -1.09435       -0.67440       -1.94220
C         -0.26500       -1.82571       -1.99816
C          1.94248        1.27630       -4.23689
H          2.59817        0.41263       -4.39452
C          2.01071        2.38162       -5.11761
H          2.71523        2.36684       -5.95096
C          1.18430        3.45932       -4.90051
H          1.21171        4.33188       -5.55829
C          0.28537        3.43376       -3.80614
C         -0.61149        4.48440       -3.48280
H         -0.62577        5.38004       -4.10874
C         -1.45100        4.38029       -2.39665
H         -2.13534        5.19615       -2.15543
C         -1.44001        3.22410       -1.58162
H         -2.10401        3.14945       -0.71822
C         -0.58389        2.18557       -1.87973
C          0.29837        2.26984       -2.98979
C         -1.52629        0.24938        1.42897
C         -1.20083       -1.10236        1.44619
H         -1.01788       -1.62665        0.51091
C         -1.12831       -1.79114        2.66091
C         -1.41563       -1.08639        3.83462
H         -1.36225       -1.60806        4.78689
C         -1.76738        0.27010        3.82800
C         -1.82049        0.93521        2.59823
H         -2.07231        1.99475        2.53222
N          0.93622       -1.81593       -1.33245
N          1.12087        1.21760       -3.21415
O         -1.54680        0.96660        0.24607
P         -0.42158        0.67335       -0.92200
Ni         1.42852       -0.16491       -0.39562
C          1.90613        0.64355        2.69306
```

C	1.63497	1.83024	1.77096
C	2.15698	1.36261	0.42691
C	3.20372	0.32515	0.67434
C	3.24387	0.09654	2.19149
H	1.11097	−0.11041	2.56854
H	2.21562	2.71208	2.09993
H	0.57864	2.13523	1.75345
H	2.36090	2.13131	−0.33100
H	4.17694	0.48647	0.18843
H	4.07537	0.69484	2.59763
H	3.42849	−0.94981	2.47543
H	1.93099	0.91423	3.75808
C	−0.66143	−3.24851	2.66883
C	−2.06778	1.04956	5.10980
C	−1.01521	−3.95469	3.97903
H	−2.09808	−3.92526	4.17288
H	−0.70904	−5.01028	3.92973
H	−0.49937	−3.50916	4.84203
C	−1.29776	−4.03053	1.51174
H	−2.39644	−3.99205	1.56071
H	−0.98866	−3.64907	0.52635
H	−0.99115	−5.08647	1.55850
C	0.86700	−3.25027	2.49854
H	1.15819	−2.74948	1.56149
H	1.35663	−2.71975	3.32931
H	1.25474	−4.28115	2.47452
C	−1.95213	0.17461	6.35808
H	−2.66303	−0.66522	6.33846
H	−0.93707	−0.23270	6.48180
H	−2.17631	0.77501	7.25206
C	−1.06596	2.20727	5.23535
H	−0.03309	1.82982	5.28966
H	−1.12692	2.90089	4.38337
H	−1.26472	2.78637	6.15034
C	−3.49658	1.60728	5.03575
H	−3.63083	2.28357	4.17850
H	−4.23203	0.79396	4.94157
H	−3.73129	2.17601	5.94876