Trans effects in the Heck reaction – A model study

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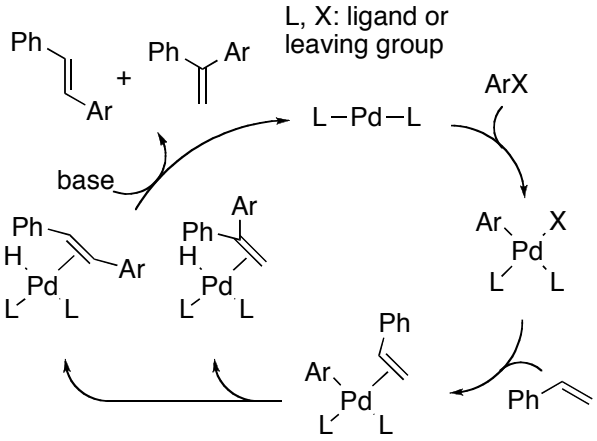
Abstract

The selectivity-determining step in Heck arylation of styrene, the migratory insertion, has been modeled by DFT. In particular, the regioselectivity has been studied as a function of the trans effect of several sets of small model ligands with different σ-donor and π-accepting abilities. It has been shown, both by analyzing the geometries and comparing the activation energies, that the TS for branched product formation is more sensitive than the TS leading to linear product, although most ligand combinations give a preference for the linear product. The branched TS is strongly destabilized by any strong ligand in a position trans to the alkene in the pre-insertion intermediate. For the ligand trans to the migrating group, a strong trans effect accelerates the reaction, more for the branched than for the linear product formation. On electronic grounds, the regio-selectivity and rate can be adjusted by considering not only the trans effect of a ligand, but also by controlling the position they will have in the migratory insertion step. Very importantly, the trans effect change in the selectivity-determining TS will be expected to give rise to Halpern-type selectivity, with the consequence that product distributions cannot be reliably predicted from observable intermediates.

Introduction

Palladium-catalyzed arylation and vinylation of alkenes has been used for more than 30 years in organic synthesis. This methodology is known as the Mizoroki-Heck reaction,[1] or sometimes just the Heck reaction, and since its discovery, it has become one of the most important tools for complex building in organic chemistry.[2,3] It allows formation of new carbon-carbon bonds under relatively mild conditions, and with a high functional group tolerance. Furthermore, it is formally a C–H activation, and as such, more atom economical than most other Pd-catalyzed coupling reactions. However, like many other C–H activations,[4] the selectivity can be a problem in the Heck reaction. Depending on the substrate, selectivity issues can include regiochemistry of the newly formed C–C bond, position and stereochemistry of the product alkene, and possibly also stereochemistry of newly formed asymmetric centers.

The scope and mechanism of the Heck reaction has been thoroughly studied.[5] The basic steps are schematically exemplified in Scheme 1. In particular the investigations by Cabri in the 90's have outlined empirical rules for selecting appropriate reaction conditions with various substrate combinations.[2] The experimental observations have also been augmented by detailed computational studies that help aid the understanding of the reaction at an atomic level.[6,7,8,9]



Scheme 1 A schematic representation of Heck arylation of styrene.

The Heck reaction can broadly be divided into two classes. When the reaction is run with monodentate ligands (e.g., PR_3) in the presence of coordinating anions like halides, the alkene substrate will substitute a neutral ligand, leading to an overall neutral intermediate and subsequent transition state for the selectivity-determining carbopalladation step. In this mode, the so-called neutral Heck, the insertions tend to favor linear products.[2] On the other hand, the Heck reaction can be run in cationic mode by using bidentate neutral ligands (usually bis-phosphines), and excluding coordinating anions by using, for example, triflates as leaving groups. In this case, the pre-insertation square planar complex and the insertion TS will be cationic, with two neutral ligands, the alkene, and an aryl group coordinating to Pd^{II}. When the substrates are very electron rich alkenes, like vinyl ethers, the cationic Heck reaction frequently yields good selectivity for branched products.[2] However, the inherent regioselectivity is not very strong, and the final product distribution is easily

influenced by other factors, like solvent, steric repulsion,[9] substrate electron density,[10] subtle changes in ligand structure,[11] ligand bite angle,[12] or intramolecular geometry constrains.[13]

We have recently undertaken computational and experimental studies of the reaction mechanism of the Heck reaction,[7-10] aimed at increasing our understanding of the factors influencing product selectivity, and thereby facilitating the choice of reaction conditions for any substrate. In particular, it has been shown that DFT calculations can explain the observed product distribution from competing β-hydride elimination[7] and elimination-readdition[9] pathways, and also that the stereoselectivity in asymmetric Heck can be rationalized at the same level of theory.[8] As the next step in our continuing investigations, we here return to the fundamental level of ligand electronic influence on the carbopalladation, the selectivity-determining step in many applications of the Heck reaction. In order to aid future reaction design, we want to separate the effects influencing the selectivity, and here we have chosen to neglect steric factors in order to clarify the purely electronic effects. We have therefore selected to study only small ligand models, where the steric repulsions have been eliminated. When the underlying electronic effects are clarified, suitable experimental systems can then be designed by also considering steric factors.

The electronic properties of a ligand are mainly manifested as trans influences or trans effects in metal complexes.[14,15] In square planar or octahedral complexes, the trans influence (sometimes called the steric trans effect) is understood as the elongation of a particular coordination bond caused by the ligand in a trans position, whereas the trans effect (or the kinetic trans effect) is a weakening of the same coordination, manifested as a lower barrier to substitution. In here, we will use the term "trans effect" also for structural effects in transition states. In structurally similar situations, longer bonds are usually weaker, and therefore the trans influence and effect are closely correlated, but not identical. However, both can be most easily understood in terms of the 3-center-4-electron bond (ω-bond).[16] Two ligands in a trans relationship σ-donate to the same metal-centered ds-hybrid orbital[17] (similar in shape to the familiar d_{Z^2} orbital, Figure 1), and any increase in bonding to one ligand must therefore be accompanied by a bonding decrease with the trans ligand. Thus, strong trans effects result from very basic lone pairs, like in alkyl groups which need a strong overlap with the central metal to stabilize the localized carbanion, or from lone pairs in orbitals of optimum size for maximizing the overlap with the metal, like phosphines. Attenuating factors include the ability of the ligand to accept π-backbonding, like in CO and to a lesser extent in phosphines, where the backdonation allows a stronger σ-donation without causing charge separation. Two strongly π-accepting ligands in a trans relationship will of course also compete for the same filled orbital on the metal, but this factor is probably less important than the σ-donation, and it is not obvious that only ligands in trans positions will compete.

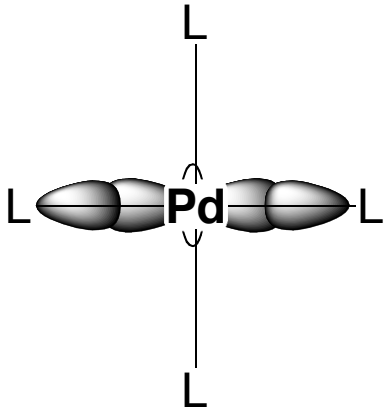


Figure 1 Two ligand lone pairs competing for the same orbital on Pd, an ω-bond.

The trans effect is usually seen as a property of an isolated ligand, but in reality it is a pair function; a strongly trans influencing ligand will reduce the influence of a second ligand trans to itself, and vice versa.[15] In terms of stability, when two strong ligands are trans to each other, the complex will be destabilized, and thus be disfavored in equilibria with geometries where only weak ligands are trans to strong ones. However, it should be realized that in Curtin-Hammett situations,[18] where all complexes are in rapid equilibrium compared to the rate of subsequent reactions, the destabilized complexes could still be important, since they also have a much higher reactivity. In fact, it was recently shown in the asymmetric Heck reaction that most of the observed product arose from the unstable and unobservable isomer intermediate.[8] This is an example of Halpern selectivity,[19] that is, that the major product arises from a preceding minor intermediate.

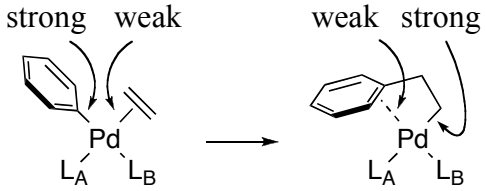


Figure 2 Trans effect changes in the carbopalladation step.

The Halpern selectivity in the asymmetric Heck reaction can be understood in terms of how the trans effect changes during the course of the reaction. Figure 2 illustrates this change in a selectivity-determining step of the Heck reaction, the carbopalladation (or migratory insertion). It is easily seen that a strong ligand in any position must destabilize either the reactant or the product. Since the transition state is somewhere between these two states, it is not self-evident what the total effect on the barrier will be. In the previously studied case,[8] it turned out that, from the aspect of trans effects, the TS was more product-like, despite the strong exothermicity of the step. This is an indication that the TS is asynchronous, with the different bonds formed to unequal degree at the TS. From Figure 2, it is obvious that for any case where the TS is product-like, the reaction will show Halpern selectivity, that is, the destabilized and less populated isomer of the intermediate will give rise to most of the observed product. However, it is by no means certain that the earlier result can be generalized to other types of systems. We have therefore embarked upon a study of how the regioselectivity of both the cationic and neutral versions of the Heck reaction

will be expected to vary with ligands of different trans-inducing power. As a model system, we have chosen to work with an experimentally well-studied reaction, phenylation of styrene. The system is interesting because the trans influences in the two carbopalladated intermediates leading to the regioisomeric products will be quite different (Figure 3). In the intermediate leading to the linear product, the alkyl group is stabilized by conjugation with the styrene phenyl, giving a moderate trans influence, whereas in the intermediate leading to the branched product, the unstabilized alkyl group is a very strong σ-donor. Thus, we can expect sensitivity to the nature of the ligand. In any experimental system, the analysis will be complicated by the fact that we cannot *a priori* know which ligand is preferred in which position in the TS, but in a computational study, all preferences can be easily separated. In line with the earlier study,[8] we will assume Curtin-Hammett conditions. In computational terms, this means that no intermediates have to be calculated since all selectivities are obtained directly from the TS energies.

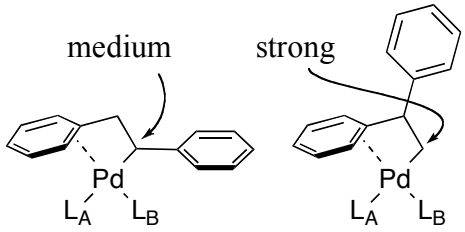


Figure 3 Alkyl trans influence in carbopalladation products from styrene.

Methods

Presentation of Model Systems

The purpose of the present study is to elucidate how the trans effect of the ligand affects the regio-selectivity in the Heck reaction. Therefore, we want the exclude other factors that influence the regio-selectivity as much as possible. It is obvious that steric effects will have an important influence on the regio-selectivity. Therefore, we have chosen as small ligands as possible – still with significant differences in trans effects – to exclude the steric effects as a factor of regio-selectivity. Also, the ligands should have similar sizes so that the interchange of two ligands will not affect the palladium complex from a structural point of view. We also desire a system that has a limited number of possible conformations, in order to minimize the necessary conformational scanning.

As our model system, we have chosen a well-studied reaction, phenylation of styrene, Scheme 1. The investigation includes both the cationic and neutral Heck reaction, and we concentrate on small systems that can be seen as models of bidentate ligands. For the cationic system, we have selected a series of three different ligands with different trans-influencing capacities: phosphine (PH_3), carbon monoxide (CO) and ammine (NH_3). PH_3 is a relatively strong σ donor and a modest π acceptor, that is, a relatively strong trans influencing ligand. CO is a strongly π-accepting ligand but a modest σ donor; generally, it shows strong trans effects. NH_3 is the weakest ligand, with relatively poor σ-donating and negligible π-accepting ability.[15] The square

planar pre-insertion intermediate for all cationic systems are depicted in Figure 4. Experimentally, the most frequently used ligands are phosphines. Structure **1** is used as a model for bidentate phosphines as well as for an excess of monodentate phosphines in the absence of coordinating anions. Structure **2** simulates replacing one of the phosphines with a neutral carbenoid, like the popular N-heterocyclic carbene ligands,[20] whereas **3** represents the frequently employed PN-ligands.[8]

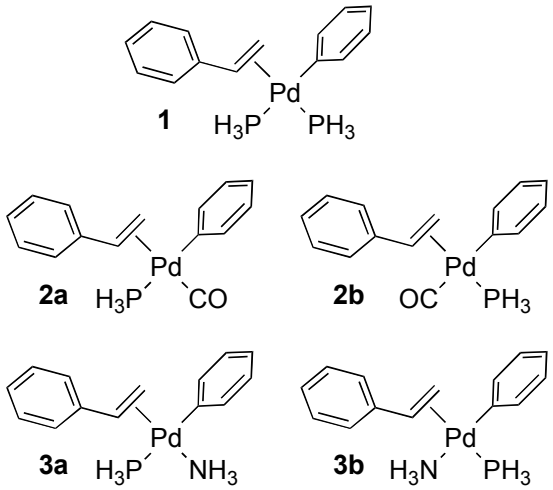


Figure 4 Cationic pre-insertion intermediates.

In the neutral Heck reaction, one neutral and one formally anionic ligand coordinates to Pd in the insertion step. We have herein investigated the case of cyanide (CN^-) and alkyl (CH_3^-) as the negatively charged ligand. These anionic ligands where combined with the same series of ligands as in the cationic Heck reaction (CO, PH_3 and NH_3). The cyanide can be seen as an anionic analogue of CO, exhibiting a somewhat stronger σ-donating but slightly weaker π-accepting capacity (**4**-**6**). In contrast, CH_3^- is a very strong σ-donor, with no π-accepting ability (**7**-**9**).[15] In particular, the combination of CH_3^- with PH_3 (**8**) can be seen as a model of cyclometallated phosphine ligands.[21]

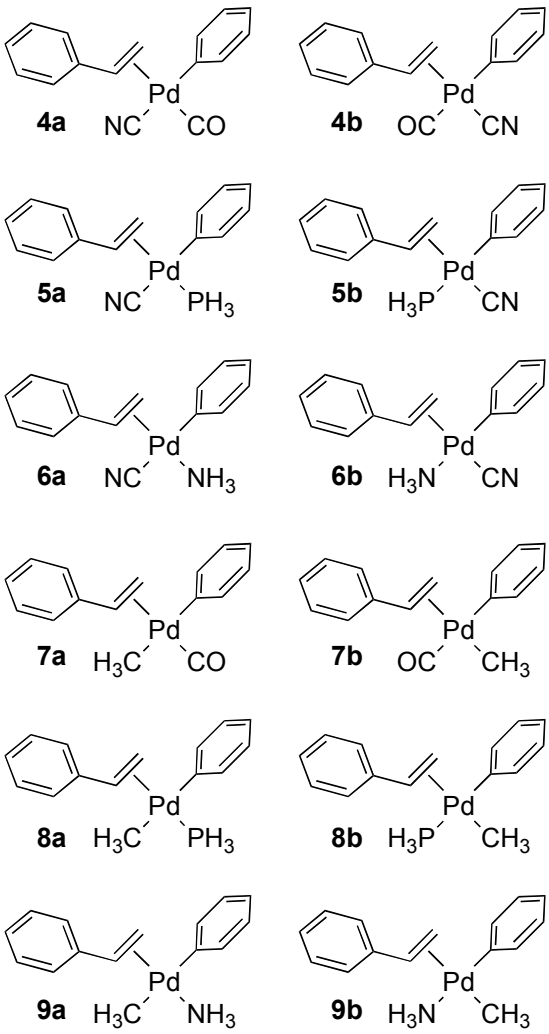


Figure 5 Neutral pre-insertion intermediates.

Computational Method

All calculations herein were performed with Jaguar[22] using the hybrid functional B3LYP[23] in combination with the LACVP* basis set.[24] All optimized geometries were characterized and saddle points were verified by frequency calculation. Harmonic vibrational frequencies have been used to calculate the thermodynamic contributions to the enthalpies and free energies.

Results and Discussion

The migratory insertion step in the cationic and neutral Heck reactions has been investigated for 17 different model systems (Figure 4 and Figure 5). The bond lengths and the full geometries can be found in Supporting Information. Starting with system **1** (Figure 4), the symmetrically substituted intermediate where both ligands are PH_3, the transition states leading to branched and linear products are shown in Figure 6.

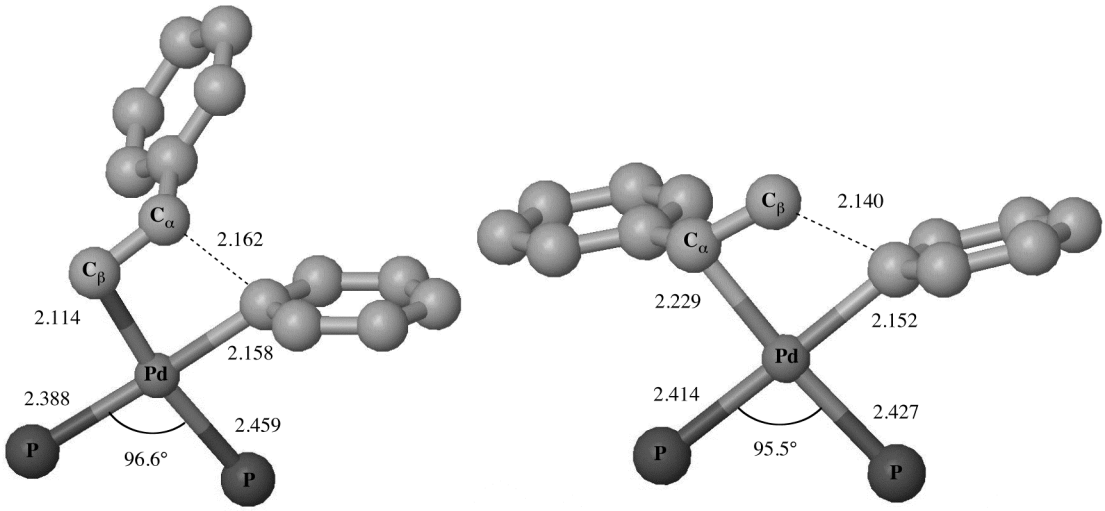


Figure 6 Branched and linear TS from cationic **1**. Hydrogens are hidden for clarity.

It can be seen from the Table 1 that the two transition states are very similar in energy. This agrees well with the observation that phenylation of styrene is relatively unselective when sterically unencumbered phosphines (*e.g.*, dppp) are employed.[2,10] When analyzing the geometries in Figure 6, we notice that the length of the developing Pd–C bond differ substantially. In the branched case, the new bond is forming to the β-carbon, where a free negative charge would be very unstable, and as a result the interaction with Pd is strong. In the linear TS, the forming negative charge on the α-carbon can be stabilized by conjugation, and therefore the interaction with Pd is weaker and the forming bond is longer by 0.115 Å.

We also see that the Pd–P bond trans to the forming Pd–C bond is longer in the branched TS (by 0.032 Å), in good agreement with the qualitative picture in Figure 3. On the other hand, the breaking bond between Pd and the phenyl group is very similar in the two cases, only longer by 0.006 Å in the branched form. Despite this, the Pd–P bonds trans to the phenyl differ by 0.026 Å, indicating that more of the negative charge has been transferred to the alkene in the branched TS. Qualitatively, the differences between branched and linear TS seen in Figure 6 can be found in all transition states analyzed here, for both the cationic and neutral pathways; only a few examples will be shown (*vide infra*), but all structures are available as supporting information.

Table 1 Differential activation energies (kJ mol^{-1}) for cationic systems, relative to the lowest energy TS for each ligand combination (**1**, **2**, or **3**).

Intermediate	Variable ligand	ΔE		ΔG	
		Linear	Branched	Linear	Branched
1	PH_3	0	3	0	1
2a	CO	5	3	7	0
2b		0	0	0	2
3a	NH_3	0	1	0	3
3b		1	13	3	11

Exchanging one phosphine for CO (intermediate **2)**, we can see that the two products still can be formed via low energy pathways, but interestingly enough, for the linear TS, the geometry with CO trans to the phenyl (**2b**) is strongly preferred. In the branched TS, there is little free energy difference between the two coordination geometries. Viewed from a synthetic perspective, if geometry **2b** could be selectively disfavored by sterically demanding substituents, it should be possible to achieve a strong preference (>10:1) for the branched product. However, in a Curtin-Hammett situation without steric demands, the results with a CO-type ligand should closely mirror those obtained with only phosphines.

In the PN-model, **3**, we can see an inherent preference for transition states with the strong phosphine ligand trans to the phenyl group. This result, already seen in a study of the asymmetric Heck reaction,[8] shows that from an electronic viewpoint, the TS can be characterized as "late", despite the strong exergonicity. Obviously, enough electron density has been transferred from the phenyl group so that the forming Pd–C bond dominates the trans effect, and thus prefers the ammine in a trans position. Interestingly enough, the PN-system shows a preference for linear products. Synthetically, this effect could be maximized by favoring geometry **3b,** which shows a large linear preference of 8 kJ mol^{-1}.

The neutral Heck reaction has been modeled with two simple anionic ligands, cyanide and methyl. Transition states for an example model system, **5a**, are shown in Figure 7. Overall, it can be seen that the geometries are very similar to those of the cationic system in Figure 6, but the transition states are "later"; the forming C–C and Pd–C bonds are shorter, and the breaking Pd–C bond is longer for both structures in Figure 7 compared to their counterparts in Figure 6.

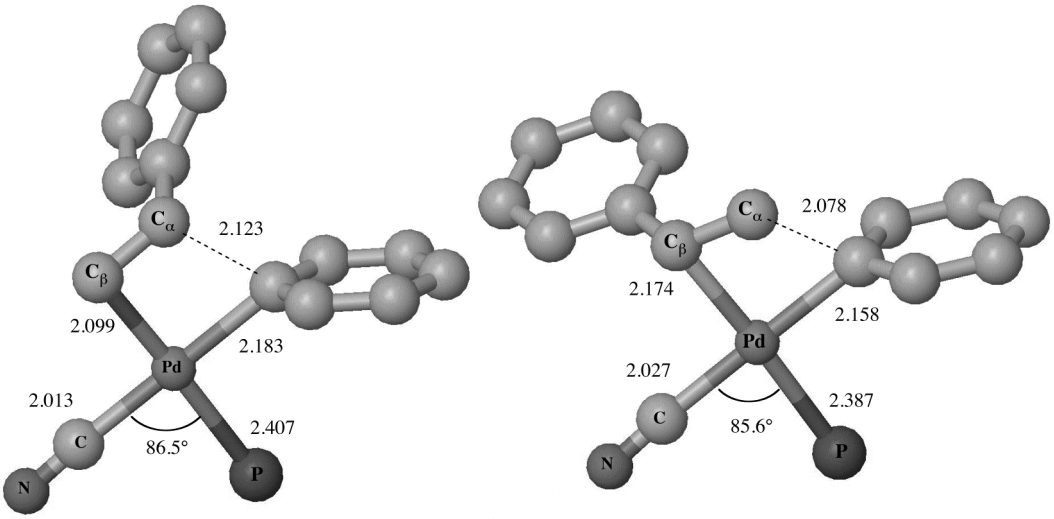


Figure 7 Branched and linear TS from neutral **5a**. Hydrogens are hidden for clarity.

The relative energies for the migratory insertion transition states for all cyanide-containing systems are shown in Table 2. The most obvious trend is that the strong cyanide ligand prefers a position trans to the migrating phenyl group. Again, this is not what would have been expected from the pre-insertion intermediate, where a trans position of the two strong ligands phenyl and cyanide should be disfavored, but it agrees well with the effect seen in the cationic case (*vide supra*), especially for the PN-system **3**.[8] It is also clear from Table 2 that the preference for the weak ligand trans to the forming Pd–C bond is much stronger for the branched TS. In the linear TS, the developing negative charge on the β-carbon is stabilized by the aromatic substituent, somewhat mitigating the effect. Another way to view the same effect is that the branched TS is "later" than the linear TS, and thus has a more marked preference for the strong ligand trans to the phenyl, which has lost much of its trans effect thanks to charge transfer to the alkene.

It can also be seen that the observed linear preference for the neutral Heck reaction[2] is reproduced by the calculations, at least for the two cases where the neutral ligands are substantially weaker than the cyanide, **5** and **6**. We note that system **5** is the one most closely reminiscent of the "classical" neutral Heck system, a monodentate phosphine together with an anionic ligand. We also see that the linear preference will be much stronger in cases where path **b** can be favored. This could happen in specific cases due to steric interactions, but also for any reaction that does *not* obey Curtin-Hammett kinetics. The latter would occur in experiments where the oxidative addition is rate limiting and shows a preference for the most stable intermediate (*e.g.,* **5b**), and where no cis/trans-isomerization path is open to the intermediate.

Table 2 Differential activation energies (kJ mol^{-1}) for neutral systems with one cyanide ligand, relative to the lowest energy TS for each ligand combination (**4**, **5**, or **6**).

Intermediate	Neutral ligand	ΔE		ΔG	
		Linear	Branched	Linear	Branched
4a	CO	0	2	0	0
4b		13	21	13	21
5a	PH_3	0	6	0	4
5b		13	27	14	27
6a	NH_3	0	4	0	4
6b		17	40	20	36

For the systems with a very strong methyl ligand (**7**-**9**), we have chosen to illustrate the disfavored path **b**, where the methyl group is trans to the developing Pd–C bond (Figure 8). We can see a few important differences from the favored path **a** in Figure 7. First of all, the developing Pd–C bond is much longer than in any of the previously depicted transition states. This is not due to an "earlier" TS, but rather to the very strong trans effect of the methyl group. In fact, the length of the developing C–C bond indicates that the TS is "later", as would be expected according to the Bell-Evans-Polanyi relationship when the product is destabilized.[25] This is verified also by the breaking Pd–C bond, which is substantially longer in **8b** compared to either **1** (Figure 6) or **5a** (Figure 7), despite having only a phosphine in the trans position.

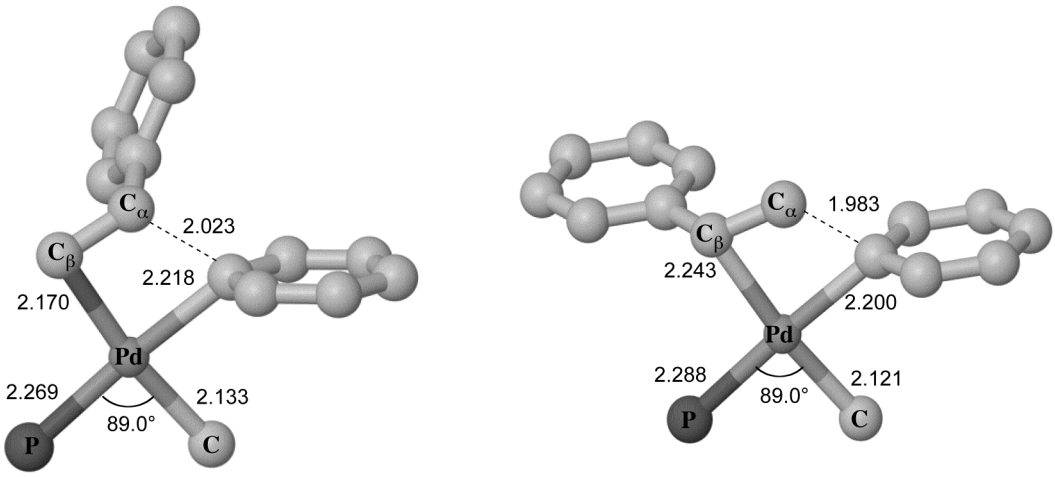


Figure 8 Electronically disfavored branched and linear TS from neutral **8b**. Hydrogens are hidden for clarity.

The relative migratory insertion barriers for all systems with a methyl ligand (**7**, **8**, and **9**) are shown in Table 3. Compared to the values obtained for the cyanide ligand (Table 2), we can see that the trends correlate, but the linear preference is substantially larger, even for the favored path **a**. In fact, the linear preference obtained for **8a** (ca 20:1) is close to the experimental preference seen with a phosphapalladacycle ligand,[21] the closest experimental analog to **8a**.

Table 3 Differential activation energies (kJ mol^{-1}) for neutral systems with one methyl ligand, relative to the lowest energy TS for each ligand combination (**7**, **8**, or **9**).

Intermediate	Neutral ligand	ΔE		ΔG	
		Linear	Branched	Linear	Branched
7a	CO	0	7	0	2
7b		8	26	7	26
8a	PH_3	0	10	0	8
8b		11	35	12	36
9a	NH_3	0	9	0	8
9b		19	59	20	56

Like in the cyanide case, the linear preference would become huge if the experimental system could be constrained to follow path **b**. How to do this is not easily envisioned, since the preference for path **a** is strong, but bidentate ligands like the aforementioned palladacycle, decorated with selective steric bulk could offer a possible way to accomplish this.

Summary and Conclusions

DFT has been utilized to investigate the influence of the trans effect of ligands for the migratory insertion selectivity in the cationic and neutral Heck reaction. Small model systems have been utilized to exclude interference of any other factors that may affect the insertion selectivity. The geometries and activation energies of the transition state for the branched and linear forms have been investigated and compared. The following general trends have been observed in the systems investigated here.

i) Due to the product-like electronic nature of the migratory insertion TS, the favored TS will frequently arise from the least favored intermediate, leading to Halpern-type selectivity.[19,8] Thus, the selectivity can *not* be reliably predicted from observable intermediates.

ii) The TS is very sensitive to the trans effect of the ligand in a position trans to the migrating aryl moiety. A strong ligand in this position will accelerate the reaction, more so for the branched TS, but rarely to a point where the branched product is favored.

iii) The forming Pd–C bond is generally shorter in the branched than in the linear TS, implying a stronger interaction. This is a result of the lower basicity of the α-carbon due to stabilization of the forming negative charge by the neighboring aryl group.

iv) A related observation is that the bond length of palladium and the ligand trans to the forming Pd–C bond is more elongated in the branched form compared to the linear form. This is true no matter if the ligand has a strong or weak trans effect. This can be traced to the more σ donating nature of the β-carbon atom in the branched form. In the linear form the negative charge can be distributed into the π system turning the α-carbon into a weaker σ donor. We conclude that the branched product formation would benefit from a less competitive ligand opposite to the alkene in the pre-insertion intermediate. The effect is clearly seen in the bond lengths, and we also observe a minor difference in activation energy in the cationic system going from a weak, to a moderate σ donating group.

v) The Pd-L bond trans to the migrating phenyl group is always shorter in branched than in linear transition states, implying that the trans effect of the phenyl group has decreased more in the branched TS, and that this therefore is "later" than the linear TS. Similarly, the breaking Pd–C bond to the phenyl group is always slightly longer in the branched TS, for the same reason, but this effect is much smaller.

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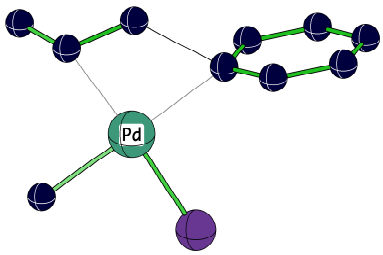

Selectivity and trans effects

The selectivity determining step of the Heck reaction has been studied by DFT for a range of model ligands. The trans effect of the ligands is found to have a profound and sometimes non-intuitive influence on the reaction selectivity. In particular, the change in trans effect during the reaction leads to a strong Halpern effect.

Keywords

Heck couplings
Density functional calculations
Homogenous catalysis
Palladium
Reaction mechanisms

Supporting information

Calculated potential and free energies and lowest frequency for all transition states

Ligand combination, file names	**E** (au)	**G** (au)	**Freq** (cm^{-1})
CN_NH3			
TRANs_CN_NH3_Trans_to_the_Phenyl_TS_igen_ochfreq.out	-817.4264116	-817.201314	-337
GEM_CN_NH3_Trans_to_the_Phenyl_TS_2_TS_SP.ou	-817.4176061	-817.193804	-347
TRANs_CN_NH3_TS_SP.out	-817.4329997	-817.209002	-288
GEM_CN_NH3_TS_SP.out	-817.431591	-817.207596	-286
CN_PH3			
TRANS_CN_trans_to_phenyl_TS_SP.out	-1104.011761	-1103.799793	-316
GEM_CN_trans_to_phenyl_TS_SP.out	-1104.009614	-1103.798181	-307
TRANS_CN_TS_SP.out	-1104.00674	-1103.794331	-328
GEM_CN_TS_SP.out	-1104.001591	-1103.789655	-331
CN_CO			
TRANS_CO_transOlefin_CN_transPhenyl_TS_SP.out	-874.1828011	-873.990009	-311
GEM_CN_CO_transOlefin_TS_SP.out	-874.1819924	-873.989858	-292
TRANS_CO_transPhenyl_CN_transOlefin_TS_SP.out	-874.1777537	-873.985237	-329
GEM_CO_transPhenyl_CN_tranOlefin_TS_2_SP.out	-874.1746606	-873.982184	-322
CH3_NH3			
TRANS_CH3_trans_to_olefin_TS_SP_cont.out	-764.4675254	-764.215018	-358
GEM_CH3_trans_to_olefin_TS_SP.out	-764.4522523	-764.201262	-383
TRANS_NH3_trans_to_olefin_CH3_transOlefin_TS_SP.out	-764.4747281	-764.222463	-267
GEM_NH3_trans_to_olefin_CH3_transPhenyl_TS_SP.out	-764.4713439	-764.219416	-273
CH3_PH3			
TRANS_CH3_trans_to_olefin_PH3_trans_Ph_TS_SP.out	-1051.052602	-1050.812363	-351
GEM_CH3_trans_to_olefin_PH3_trans_Ph_TS_SP.out	-1051.043446	-1050.80355	-368
TRANS_CH3_trans_to_phenyl_TS_SP.out	-1051.056856	-1050.817121	-296
GEM_CH3_trans_to_phenyl_TS_SP.out	-1051.052993	-1050.813971	-1051
CH3_CO			
TRANS_CO_transOlefin_CH3_transPhenyl_TS_SP.out	-821.23591	-821.014266	-291
GEM_CO_trans_OLefin_CH3_transPhenyl_TS_SP.out	-821.2332375	-821.013504	-286
TRANS_CO_transPhenyl_CH3_transOlefin_TS4_SP.out	-821.23272	-821.011485	-353
GEM_CO_transPhenyl_CH3_tranOlefin_TS2_SP.out	-821.2258494	-821.004205	-363
PH3_CO			
TRANS_CO_transPhenyl_PH3_transOlefin_TS_SP.out	-1124.294413	-1124.083667	-282
GEM_CO_transPhenyl_PH3_tranOlefin_TS_2_SP.out	-1124.294332	-1124.082993	-279
TRANS_CO_transOlefin_PH3_transPhenyl_TS2_SP.out	-1124.292406	-1124.08111	-257
GEM_CO_trans_OLefin_TS_SP.out	-1124.293364	-1124.083783	-270
PH3_NH3			
TRANS_NH3_trans_to_phenyl_TS_SP.out	-1067.550429	-1067.306126	-296
GEM_NH3_trans_to_phenyl_TS_SP.out	-1067.546065	-1067.303236	-311
TRANS_NH3_TS_SP.out	-1067.550867	-1067.307329	-236
GEM_NH3_TS_SP_cont2.out	-1067.550467	-1067.306223	-256[a]
PH3_PH3			
PD_2PH3_Ph_Styrene_TS_SP.out	-1354.126867	-1353.896059	-283
PD_2PH3_Ph_Styrene_gem_TS_fix_IGEN2.out	-1354.125713	-1353.895809	-288

[a]One additional negative eigenvalue (-30 cm^{-1}) corresponding to PH_3 rotation

Geometries for all transition states:

TRANS_CH3_trans_to_olefin_PH3_trans_Ph_TS_SP.out

Pd1	0.3622897028	-0.3159447538	0.0115857788
C2	0.0813758070	1.8729810343	-0.3881082784
C3	1.4814475247	1.8636806285	-0.0741434355
H5	2.1629715895	2.2026483987	-0.8488386488
H6	1.7402201615	2.2495526970	0.9067976431
H7	-0.5872156568	2.1720842196	0.4179456225
X8	0.7630015000#	1.8708020000#	-0.1961420000#
H19	-2.4238656589	-1.6176343383	0.9506491535
H20	-2.8777374549	-0.0459174837	-0.4321188034
C17	5.1503353646	-0.7383329354	0.4832929573
C18	4.3986921067	-0.3614911901	1.5992661926
C19	3.0913633388	0.0980588359	1.4406927169
C20	2.5004309630	0.1795264270	0.1665599765
C21	3.2777924520	-0.1918308131	-0.9472702159
C22	4.5845480935	-0.6516760113	-0.7920167230
H23	6.1723625190	-1.0877371609	0.6048467841
H24	4.8340999969	-0.4206485935	2.5941371476
H25	2.5240946374	0.4046411383	2.3173109111
H26	2.8561969884	-0.1213259218	-1.9477583320
H27	5.1640615928	-0.9396372321	-1.6662838501
C27	-1.5654463941	2.4889562944	-4.3185125387
C28	-0.2500665512	2.0397568034	-4.1769927877
C29	0.2990707288	1.8354683608	-2.9134426293
C30	-0.4522862381	2.0749180600	-1.7432693779
C31	-1.7782446877	2.5294400795	-1.9076122298
C32	-2.3250124796	2.7338698744	-3.1724032916
H33	-1.9904612505	2.6473404860	-5.3060749231
H34	0.3548401387	1.8458132498	-5.0598079061
H35	1.3235952030	1.4813965908	-2.8345571943
H36	-2.3764094375	2.7407880250	-1.0229729882
H37	-3.3478074575	3.0924791613	-3.2631831875
H38	0.0593480907	-3.0560633857	0.3983955161
H39	1.6091136816	-2.6292827030	-0.3720795185
C36	0.8864490408	-2.3347276377	0.3960191481
H40	1.3750952534	-2.3530214579	1.3760265876
P36	-1.8288313775	-0.9567198690	-0.1484184200
H41	-2.1403275494	-1.9184869560	-1.1355151484

GEM_CH3_trans_to_olefin_PH3_trans_Ph_TS_SP.out

Pd1	0.4958643176	-0.2489337985	0.0029913116
C2	0.4595034360	1.8957176831	0.3325769943
C3	1.8923414320	1.8474004293	0.1662749378
H6	2.4692415979	2.1710332604	1.0273561237
H7	0.0871975054	2.1204288589	1.3316806124
X8	0.4806690000#	1.8054860000#	0.3130400000#
H18	-2.3619732471	-1.4258447527	0.6902302010
H19	-2.7026213310	0.4026371405	-0.3431298041
C17	4.9065164352	-1.4067620884	1.4031756840
C18	3.9446091674	-0.9594752112	2.3135787398
C19	2.8334279233	-0.2498652043	1.8581610785
C20	2.6470032269	-0.0018679017	0.4847767812
C21	3.6295495226	-0.4429306924	-0.4143047853
C22	4.7477131167	-1.1431050608	0.0402320573
H23	5.7812494316	-1.9474160746	1.7559132421
H24	4.0676399825	-1.1528909934	3.3768069005
H25	2.1056544908	0.1217143445	2.5775525469
H26	3.5218235795	-0.2385035259	-1.4758346065
H27	5.4964567369	-1.4848704159	-0.6708681015
H28	-0.1240671567	2.3415481496	-0.4697410661
C37	3.6586296092	3.2597437651	-3.5015164061
C38	4.2513135214	3.5414582513	-2.2701807928

C39	3.6795543867	3.0607482708	-1.0920361994
C40	2.5012251376	2.3007244306	-1.1207534221
C41	1.9190033927	2.0173496854	-2.3658924577
C42	2.4915045160	2.4932341619	-3.5443481553
H43	4.1054907825	3.6279870878	-4.4214679470
H44	5.1623351474	4.1329917247	-2.2252796619
H45	4.1510432595	3.2787581065	-0.1361194958
H46	1.0213771272	1.4049140455	-2.4084671137
H47	2.0281631404	2.2605009112	-4.4999090454
H35	-0.0331400912	-2.9596599023	-0.4767355980
H36	1.4455493139	-2.3891884393	-1.2842642360
C36	0.8528785738	-2.3200004362	-0.3637063764
H37	1.4513638220	-2.7000427897	0.4710720241
P36	-1.7239298803	-0.6227059607	-0.2828292744
H38	-2.1433192430	-1.3456392789	-1.4231713439

TRANS_CO_transPhenyl_PH3_transOlefin_TS_SP.out

Pd1	0.3248405665	-0.2952667123	0.0745855727
C2	0.0617197665	1.9001666050	-0.3510527971
C3	1.4132886532	1.9078701974	0.0718642401
H4	2.1856980315	2.2211292277	-0.6185906592
H5	1.6114107411	2.1395092532	1.1122597941
H6	-0.6777054519	2.1226647679	0.4172698728
C7	5.1042264081	-0.8081613589	0.2034552652
C8	4.4317469686	-0.5156932902	1.3923482878
C9	3.0986733558	-0.0947454040	1.3630110393
C10	2.4369600719	0.0166995295	0.1326608467
C11	3.1126966240	-0.2636513558	-1.0638821888
C12	4.4442349944	-0.6826883968	-1.0224751886
H13	6.1427187828	-1.1242391481	0.2306861666
H14	4.9437499998	-0.6049369389	2.3463349613
H15	2.5895539399	0.1468576987	2.2924761664
H16	2.6108379969	-0.1625719711	-2.0226701175
H17	4.9660704306	-0.9028668154	-1.9496834303
C18	-1.3732829666	2.4913333388	-4.3427105671
C19	-0.0190015632	2.2127144040	-4.1363047560
C20	0.4676901817	2.0121689110	-2.8479571717
C21	-0.3970629318	2.0832562619	-1.7380895373
C22	-1.7585369620	2.3663809922	-1.9621003623
C23	-2.2413916544	2.5720117166	-3.2508373639
H24	-1.7482866381	2.6506710274	-5.3494895525
H25	0.6596763693	2.1595657084	-4.9826083053
H26	1.5264525415	1.8124054244	-2.7093121647
H27	-2.4383559037	2.4382102125	-1.1154107864
H28	-3.2922726898	2.7987303703	-3.4045092013
O32	-2.7975858916	-0.7524814695	0.0460817644
C33	-1.6773922469	-0.5619463798	0.0569647142
P32	0.8389862230	-2.6707972897	0.4680126456
H33	-0.0857549563	-3.7060211162	0.2089173108
H34	1.9599715186	-3.1655915894	-0.2258347029
H35	1.2026855823	-3.0119914332	1.7864800430

GEM_CO_transPhenyl_PH3_tranOlefin_TS_2_SP.out

Pd1	0.4523664782	-0.2954940116	0.0590516964
C2	0.4825202234	1.7957883986	0.4003138031
C3	1.8952483067	1.9111070304	0.1678713880
H4	2.5050423130	2.1491022978	1.0323362106
H5	0.1434375464	1.9291695498	1.4272208389
C6	4.8722934260	-1.4346153649	1.2883234146
C7	3.9432364894	-1.0256214056	2.2492897617
C8	2.7828119336	-0.3549165570	1.8558744338
C9	2.5443468310	-0.1204842611	0.4909174333
C10	3.4897803268	-0.5045140886	-0.4706244919

C11	4.6474945333	-1.1730543909	-0.0679611288
H12	5.7815118274	-1.9420881129	1.5972657042
H13	4.1276595318	-1.2118724595	3.3034938682
H14	2.0773398506	-0.0140398754	2.6099010163
H15	3.3332410470	-0.2729192322	-1.5207245115
H16	5.3788079405	-1.4797044484	-0.8106941796
H17	-0.1823671588	2.2254383892	-0.3456915171
C18	3.6181365562	3.3138985436	-3.4832656363
C19	4.3035828602	3.4456640440	-2.2738522151
C20	3.7358208821	2.9609477137	-1.0984976261
C21	2.4675969809	2.3524809093	-1.1130059246
C22	1.7884208700	2.2204843641	-2.3393536775
C23	2.3614568080	2.6991553912	-3.5136819235
H24	4.0614500221	3.6868529833	-4.4021635515
H25	5.2782654128	3.9237411210	-2.2470147892
H26	4.2723883310	3.0606802301	-0.1578209702
H27	0.8136185063	1.7409972527	-2.3788743390
H28	1.8306968934	2.5961239736	-4.4555930842
O29	-2.6590789838	-0.3642589482	-0.2743151499
C30	-1.5286400655	-0.3373197255	-0.1584580310
P31	0.8136266376	-2.7094556300	-0.4336134787
H32	-0.2389448187	-3.6501567963	-0.4425242854
H33	1.3929254996	-3.0165883191	-1.6823760993
H34	1.7201802658	-3.3813091354	0.4098495894

GEM_CO_trans_OLefin_TS_SP.out

Pd1	0.3597563075	-0.3418829924	0.0982207779
C2	0.3729142850	1.7618451712	0.1236777141
C3	1.7972980027	1.9250630339	0.0652437644
H6	2.2868025360	2.1555466467	1.0051649861
H7	-0.0917319129	2.0076612436	1.0799258981
P17	-2.0493888408	-0.3998701169	-0.1537136968
H18	-2.8039759228	-1.0748937278	0.8275042657
H19	-2.7587841916	0.8175963651	-0.1950885965
H20	-2.5772626121	-1.0138854750	-1.3083838877
C17	4.9454218078	-1.3423794625	0.8722296828
C18	4.1534665532	-0.9054922438	1.9382700867
C19	2.9230388137	-0.2932283196	1.6889550449
C20	2.4892558056	-0.1273685309	0.3641906153
C21	3.2889593895	-0.5502664484	-0.7060592274
C22	4.5134317907	-1.1679651144	-0.4468018399
H23	5.9070851951	-1.8077142360	1.0687364913
H24	4.4962765006	-1.0310673533	2.9614721917
H25	2.3174273871	0.0571287929	2.5212222983
H26	2.9757456818	-0.3807184684	-1.7325770736
H27	5.1342508538	-1.5026828923	-1.2731918354
H28	-0.1989330721	2.0975964470	-0.7395426772
C37	3.9710029397	3.3965378832	-3.3043116351
C38	4.5064500141	3.4808789966	-2.0170141574
C39	3.7927945364	2.9750244462	-0.9345838108
C40	2.5255197908	2.3915101973	-1.1205458450
C41	1.9978845827	2.3108320655	-2.4231956729
C42	2.7173537887	2.8089369722	-3.5047403358
H43	4.5284024389	3.7867541930	-4.1511275384
H44	5.4781381729	3.9390880071	-1.8583966771
H45	4.2136561151	3.0354643193	0.0663179346
H46	1.0272946754	1.8533856786	-2.5958680339
H47	2.3028282276	2.7426247925	-4.5063735678
O33	0.8203936462	-3.4976994468	0.1273599300
C34	0.6259483763	-2.3790275014	0.1110317911

TRANS_CO_transOlefin_PH3_transPhenyl_TS2_SP.out

Pd1	0.3460549255	-0.2773247089	0.0096286508
C2	0.1081919632	1.9129876295	-0.3346117155
C3	1.4777957030	1.9008761769	0.0042611319

H4	2.2188227497	2.1356123345	-0.7493089119
H5	1.7557899468	2.1516443157	1.0209023309
H6	-0.5787653395	2.1649493513	0.4729806744
P7	-2.0863445815	-0.5633979525	-0.1685738389
H8	-2.6926822903	-1.6720148028	0.4582164152
H9	-2.9510430634	0.4558383135	0.2774386914
H10	-2.5809647672	-0.7342178243	-1.4766332766
C11	5.1130058894	-0.9216163646	0.4382743656
C12	4.3691693167	-0.5929466567	1.5740495874
C13	3.0493188462	-0.1476367139	1.4491382714
C14	2.4829949388	-0.0425963813	0.1751513133
C15	3.2193679983	-0.3654160783	-0.9699971187
C16	4.5378608358	-0.8081412076	-0.8304157364
H17	6.1396808264	-1.2597722522	0.5404512504
H18	4.8127870926	-0.6764337740	2.5621789768
H19	2.4819382261	0.1148742059	2.3379808900
H20	2.7826941968	-0.2805171789	-1.9613572072
H21	5.1132091515	-1.0607485011	-1.7166881904
C22	-1.5074046414	2.5480987333	-4.2571461971
C23	-0.2018742374	2.0664424606	-4.1210714654
C24	0.3404096330	1.8545383919	-2.8568983546
C25	-0.4187171252	2.1160424768	-1.7000750876
C26	-1.7304636385	2.6056175949	-1.8515408525
C27	-2.2678431095	2.8231653441	-3.1188094978
H28	-1.9257174461	2.7144885998	-5.2454237750
H29	0.3957187143	1.8599009900	-5.0041818170
H30	1.3587655351	1.4847701003	-2.7728267141
H31	-2.3206054069	2.8435940903	-0.9687930123
H32	-3.2765414700	3.2136175661	-3.2174152140
O34	0.9584934739	-3.3446164528	0.4627262259
C35	0.7110489337	-2.2505615423	0.2855757071

GEM_CN_NH3_Trans_to_the_Phenyl_TS_2_TS_SP.out

Pd1	0.4902237750	-0.2351349082	0.0240421622
C2	0.4555960672	1.8487134272	0.3740840427
C3	1.8822620376	1.8627773138	0.1817269406
H6	2.4718281269	2.1694757961	1.0396260990
H7	0.0956622710	2.0562944792	1.3821382740
X8	0.4656231486#	1.7848511480#	0.2631404320#
H18	-2.1767538080	-0.3834808959	0.5962885834
H19	-2.0657639259	0.0988142485	-0.9784032688
C17	4.8419887338	-1.4601675530	1.2940833140
C18	3.9293387779	-0.9960873291	2.2452549874
C19	2.8071159975	-0.2768605799	1.8369663048
C20	2.5711315194	-0.0372940637	0.4704790675
C21	3.5046549563	-0.4898520384	-0.4749148156
C22	4.6289940071	-1.2036582618	-0.0633577528
H23	5.7220367977	-2.0139926805	1.6107262316
H24	4.0958916991	-1.1885069030	3.3022193355
H25	2.1103541097	0.1005211038	2.5824052572
H26	3.3449230278	-0.2970927653	-1.5308210945
H27	5.3364387036	-1.5687320699	-0.8035120355
H28	-0.1582841851	2.2816846049	-0.4146943863
C37	3.6197128766	3.2578075026	-3.4977404978
C38	4.2193497365	3.5462662782	-2.2711803390
C39	3.6534047953	3.0723274165	-1.0879277413
C40	2.4741833662	2.3133884935	-1.1091265824
C41	1.8840985998	2.0233622412	-2.3492905576
C42	2.4511286188	2.4924856188	-3.5322514340
H43	4.0642633691	3.6177054633	-4.4219077309
H44	5.1318789452	4.1355476506	-2.2342306789
H45	4.1304489509	3.2930187122	-0.1355005355
H46	0.9922774514	1.4022278993	-2.3866340371
H47	1.9861285049	2.2509371215	-4.4845014684
N36	-1.6498048712	-0.5000175323	-0.2675504765

H38	-1.7329490881	-1.4723989363	-0.5663188470
N34	0.4873358997	-3.3628215047	-0.7291429982
C35	0.6198238174	-2.2401931481	-0.4235740368

TRANs_CN_NH3_Trans_to_the_Phenyl_TS_igen_ochfreq.out

Pd1	0.4032342828	-0.2435611944	-0.0353108555
C2	0.1389523808	1.8893791351	-0.3624496943
C3	1.5445088401	1.9089474410	-0.1105679143
H4	2.2079108317	2.1864189820	-0.9229829709
H5	1.8539296671	2.3093791211	0.8485018245
H6	-0.4990619059	2.1805624890	0.4726430345
H7	-2.2157304244	-0.7096030027	0.5472777833
H8	-1.7115698023	-1.6870810918	-0.6724569321
C9	5.0846193502	-0.8342684542	0.6085925055
C10	4.2990792465	-0.4439458795	1.6963538994
C11	3.0141216629	0.0556098875	1.4890561765
C12	2.4877995466	0.1555937657	0.1890849444
C13	3.2936773470	-0.2272955301	-0.8984014079
C14	4.5789444333	-0.7234767192	-0.6895402611
H15	6.0880624909	-1.2188549443	0.7709734966
H16	4.6879012041	-0.5304280437	2.7078664967
H17	2.4117898275	0.3598487354	2.3419193078
H18	2.9079241242	-0.1517782138	-1.9124683481
H19	5.1852123812	-1.0280984357	-1.5391719642
C20	-1.7867895978	2.2831593479	-4.1910106648
C21	-0.4275219654	1.9635332113	-4.1283305245
C22	0.2183221437	1.8445017822	-2.9005248073
C23	-0.4794906648	2.0424871075	-1.6916698499
C24	-1.8492156346	2.3701503950	-1.7741006477
C25	-2.4935805066	2.4895698485	-3.0053856772
H26	-2.2864423445	2.3716008201	-5.1516731269
H27	0.1341510725	1.8015928330	-5.0450351220
H28	1.2731482914	1.5836501663	-2.8815090424
H29	-2.4047362152	2.5539297900	-0.8553971754
H30	-3.5488973521	2.7498800252	-3.0368780107
N31	0.6426122383	-3.3993649245	0.3838967914
C32	0.6645051474	-2.2369342033	0.2529989040
X33	0.7759635033	1.8648363278	-0.2126517589
N34	-1.6948955818	-0.7277488388	-0.3281829826
H35	-2.1543964526	-0.1137110950	-1.0020582703

TRANs_CN_NH3_TS_SP.out

Pd1	0.3561612962	-0.2606022745	0.0396420297
C2	0.0136856107	1.8076981627	-0.3467439583
C3	1.3824774749	1.8391394434	0.0674416901
H5	2.1312872079	2.1946176427	-0.6309658231
H6	1.5796574689	2.1195978027	1.0969552356
H7	-0.7251551777	2.0545859732	0.4123509238
X8	0.6800432499#	1.8403976244#	-0.1166524474#
C17	5.0740060341	-0.9750141426	0.3693094510
C18	4.3643011408	-0.6334066994	1.5232393371
C19	3.0715127368	-0.1108824395	1.4246256472
C20	2.4642776982	0.0577035318	0.1700189972
C21	3.1957629851	-0.2644014484	-0.9851170055
C22	4.4866192070	-0.7881115181	-0.8848158566
H23	6.0817310406	-1.3743764165	0.4461169870
H24	4.8187720832	-0.7670462355	2.5021623659
H25	2.5327281091	0.1630596557	2.3294425472
H26	2.7521904003	-0.1152762134	-1.9671554753
H27	5.0357330067	-1.0459424381	-1.7873796837
C27	-1.3928866780	2.5654849819	-4.3423211249
C28	-0.0278081739	2.3765676959	-4.1193040660
C29	0.4477170833	2.1254619705	-2.8329667814

C30	-0.4334386524	2.0561145581	-1.7402340307
C31	-1.8055019734	2.2452539008	-1.9813293924
C32	-2.2797156313	2.4980560455	-3.2652424751
H33	-1.7623035266	2.7596174974	-5.3459354299
H34	0.6717142036	2.4266292566	-4.9501159524
H35	1.5158032970	1.9846145484	-2.6869870464
H36	-2.5038878224	2.1620404046	-1.1530599993
H37	-3.3458648172	2.6349407845	-3.4261462798
H38	0.7950887532	-2.8963571614	-0.4897109507
H40	-0.1543052651	-2.7807559055	0.8501220348
N34	-2.7425650093	-1.0191516666	0.0366557433
C35	-1.6223794271	-0.6843796180	0.0045763746
N35	0.6811784335	-2.4111244443	0.3989202501
H39	1.4973212946	-2.6036015660	0.9778134054

GEM_CN_NH3_TS_SP.out

Pd1	0.4780797063	-0.2198042206	0.0272655453
C2	0.3897391763	1.8326040463	0.3084634782
C3	1.8186316368	1.8238102217	0.1453520139
H6	2.4000639908	2.0701192950	1.0276785651
H7	-0.0000352668	2.0102912219	1.3096799434
X8	0.4134861759#	1.8392818665#	0.3031877218#
C17	4.8522298037	-1.6345175413	1.1864499628
C18	3.9786575703	-1.1641081809	2.1706377649
C19	2.8610127353	-0.4077212837	1.8093446907
C20	2.5903627756	-0.1382578654	0.4578152371
C21	3.4888011506	-0.5846013936	-0.5209350003
C22	4.6070562454	-1.3418474665	-0.1581030099
H23	5.7275495462	-2.2144527570	1.4672059930
H24	4.1709518451	-1.3790214428	3.2191968001
H25	2.1935237011	-0.0332185425	2.5830437105
H26	3.3193336116	-0.3398365916	-1.5665881623
H27	5.2922451775	-1.6950395596	-0.9253808679
H28	-0.2206624502	2.2565297773	-0.4838454345
C37	3.6896656228	3.1958901525	-3.4718574233
C38	4.3186801323	3.3603492474	-2.2370183536
C39	3.7073869968	2.8920930418	-1.0748034967
C40	2.4539146550	2.2639910630	-1.1246749834
C41	1.8316718752	2.0993960251	-2.3734172774
C42	2.4456780791	2.5624642866	-3.5354461238
H43	4.1667391576	3.5545817366	-4.3801459070
H44	5.2870392575	3.8501322401	-2.1776156620
H45	4.2050085408	3.0149820537	-0.1152843923
H46	0.8705004475	1.5958497596	-2.4355162894
H47	1.9521659095	2.4263151698	-4.4941657191
H35	0.3558956754	-2.8788453788	0.6006007036
H36	-0.0671482112	-2.6805215616	-0.9738343940
N34	-2.6338026565	-0.5707878003	-0.5074739133
C35	-1.5010584088	-0.3787539747	-0.2891434907
N35	0.6135195130	-2.4092993872	-0.2660689204
H37	1.5398020378	-2.7305250588	-0.5436217578

TRANS_CN_trans_to_phenyl_TS_SP.out

Pd1	0.3175766789	-0.2863445175	0.0841058272
C2	0.0048328352	1.8221487460	-0.3457718083
C3	1.3552536645	1.8586465028	0.1124669136
H5	2.1200485305	2.2514841390	-0.5467445309
H6	1.5130786917	2.1023739670	1.1581073768
H7	-0.7654309805	2.0416550500	0.3892126426
X8	0.7630015000#	1.8708020000#	-0.1961420000#
C17	5.1006258071	-0.8296594949	0.1729410801
C18	4.4557924625	-0.5020872303	1.3683262414
C19	3.1379368598	-0.0395121757	1.3520422137
C20	2.4426623861	0.0876240252	0.1398779905
C21	3.1064730925	-0.2223494223	-1.0591331261

C22	4.4221933294	-0.6891736083	-1.0407527553
H23	6.1274765436	-1.1848723894	0.1859694190
H24	4.9793120628	-0.6050776965	2.3157375918
H25	2.6483928286	0.2188449271	2.2885970066
H26	2.5901695311	-0.1118118536	-2.0098832457
H27	4.9185153658	-0.9392214017	-1.9754360100
C27	-1.2539188191	2.5359516057	-4.3942052264
C28	0.1045131967	2.3747025331	-4.1152259657
C29	0.5326987704	2.1351840415	-2.8104107600
C30	-0.3925258705	2.0502349404	-1.7539275894
C31	-1.7579566384	2.2102691692	-2.0518353331
C32	-2.1832020918	2.4522828993	-3.3546410374
H33	-1.5856012569	2.7220077443	-5.4123925275
H34	0.8357729597	2.4384927461	-4.9171739089
H35	1.5963294219	2.0193655324	-2.6204084367
H36	-2.4880670887	2.1139944051	-1.2528870870
H37	-3.2441691142	2.5685072653	-3.5598903934
H38	-0.0436931492	-3.4941745562	-0.4211190489
H39	1.7736840766	-3.2799280162	0.6990366822
P36	0.5320524020	-2.6220336694	0.5266239922
H40	-0.1288890566	-3.1062199894	1.6751567629
N34	-2.8193024380	-0.8899294827	0.0916470727
C35	-1.6792437638	-0.6315473009	0.0658254165

GEM_CN_trans_to_phenyl_TS_SP.out

Pd1	0.4678983340	-0.2403261071	0.0206878744
C2	0.4134861759	1.8392818665	0.3031877218
C3	1.8395916684	1.8331063121	0.1394741918
H6	2.4199296242	2.0901611275	1.0189489447
H7	0.0205070617	2.0075873638	1.3042194276
X8	0.4806690000#	1.8054860000#	0.3130400000#
C17	4.8805759852	-1.5541573245	1.2646711484
C18	3.9658250476	-1.1074778161	2.2226562778
C19	2.8390771994	-0.3821060781	1.8278737210
C20	2.6008198502	-0.1216361689	0.4683507501
C21	3.5371825593	-0.5455578990	-0.4831947948
C22	4.6652463150	-1.2693304347	-0.0867731208
H23	5.7628964292	-2.1095402387	1.5712192114
H24	4.1330813709	-1.3153365031	3.2767970524
H25	2.1397793279	-0.0252079998	2.5816839501
H26	3.3874008211	-0.3143104238	-1.5345437781
H27	5.3786254579	-1.6077663342	-0.8345276898
H28	-0.2026619728	2.2491723885	-0.4911866548
C37	3.6861425745	3.2077900558	-3.4885198616
C38	4.3217890897	3.3746384499	-2.2573411539
C39	3.7193604378	2.9036495967	-1.0916545007
C40	2.4681229200	2.2704116477	-1.1346375776
C41	1.8394384152	2.1031337186	-2.3797267107
C42	2.4446403449	2.5689398756	-3.5452197938
H43	4.1559245758	3.5694509834	-4.3994194250
H44	5.2880795977	3.8690962606	-2.2035789535
H45	4.2216892490	3.0293473740	-0.1350055901
H46	0.8790454613	1.5974842757	-2.4375459092
H47	1.9459035909	2.4315047305	-4.5009988464
H35	-0.4060521257	-3.3771334086	0.4684367249
H36	-0.0327783114	-3.0581143051	-1.6029188254
P36	0.4543898521	-2.6180951079	-0.3530350466
H37	1.6001155045	-3.4468193737	-0.2766851092
N34	-2.6707938121	-0.4185113692	-0.4620732566
C35	-1.5227510824	-0.3064429194	-0.2720078975

TRANS_CN_TS_SP.out

Pd1	0.3627072990	-0.2788674460	0.0118083143
C2	0.0812722231	1.8601161962	-0.3736406838
C3	1.4706547836	1.8695564595	-0.0516628341

H5	2.1745802498	2.1725868388	-0.8186349339
H6	1.7363512353	2.2109256080	0.9426206782
H7	-0.5958299295	2.1542434512	0.4275411053
P17	-1.8954028091	-0.9064059025	-0.1721052115
H18	-2.4567940705	-1.6229624515	0.9033719738
H19	-2.9462836449	0.0120103813	-0.4128628817
H20	-2.1673130024	-1.8197277030	-1.2097979434
C17	5.1198218726	-0.8307985688	0.4669184809
C18	4.3770823840	-0.4623564442	1.5909770529
C19	3.0699204034	0.0031548210	1.4467377609
C20	2.4873018609	0.0938585762	0.1741697646
C21	3.2429167916	-0.2681711933	-0.9517554625
C22	4.5492258648	-0.7330095954	-0.8047048632
H23	6.1391103225	-1.1899388864	0.5804817760
H24	4.8145001265	-0.5398320157	2.5831138215
H25	2.5007522014	0.2871233265	2.3284665414
H26	2.8086702789	-0.2034856685	-1.9464625415
H27	5.1204797146	-1.0216751730	-1.6835097871
C27	-1.5492553531	2.4737483971	-4.3089702396
C28	-0.2339964443	2.0253081587	-4.1657115895
C29	0.3110776070	1.8245819510	-2.8997901838
C30	-0.4477375973	2.0662596356	-1.7382526346
C31	-1.7703137558	2.5216374456	-1.9009543382
C32	-2.3137491477	2.7236852976	-3.1681391098
H33	-1.9718531419	2.6277797204	-5.2980458413
H34	0.3717906253	1.8282533282	-5.0465970825
H35	1.3338423279	1.4673265496	-2.8152707867
H36	-2.3716905871	2.7300183930	-1.0180809282
H37	-3.3361525904	3.0805681626	-3.2639769273
N34	0.7191272207	-3.4069467402	0.5695158250
C35	0.6677450510	-2.2562187670	0.3683055987

GEM_CN_TS_SP.out

Pd1	0.4734802268	-0.2419281458	0.0179930189
C2	0.4445677406	1.8592476236	0.3447471088
C3	1.8679218893	1.8477846102	0.1564495872
H6	2.4629529682	2.1155797281	1.0223326702
H7	0.0825814879	2.0599187293	1.3525900997
P17	-1.8151044906	-0.5756481980	-0.2812070725
H18	-2.4148656101	-1.4909234860	0.6066756524
H19	-2.7905559528	0.4500585118	-0.2203856964
H20	-2.2062162706	-1.1682271077	-1.4985674312
C17	4.8897274214	-1.4703938478	1.2878049016
C18	3.9699631198	-1.0205320405	2.2383478120
C19	2.8318330518	-0.3246080699	1.8299113077
C20	2.5951210347	-0.0959856074	0.4650258256
C21	3.5276074651	-0.5347762775	-0.4825370574
C22	4.6677279642	-1.2249358691	-0.0697858628
H23	5.7812655367	-2.0051335452	1.6049028631
H24	4.1418581355	-1.2046158199	3.2959823374
H25	2.1280564065	0.0386734206	2.5759307732
H26	3.3618255480	-0.3495206691	-1.5391597640
H27	5.3803615897	-1.5786495050	-0.8105766489
H28	-0.1632308307	2.3011068445	-0.4418424631
C37	3.6656219054	3.2072421373	-3.5034054154
C38	4.2795995036	3.4485600127	-2.2737580909
C39	3.6934936826	2.9834149004	-1.0973137752
C40	2.4788090754	2.2824293896	-1.1281219229
C41	1.8734232161	2.0399585410	-2.3715739303
C42	2.4621679243	2.4987105210	-3.5480610341
H43	4.1254193487	3.5604704851	-4.4226085836
H44	5.2185897524	3.9939361826	-2.2294521637
H45	4.1813420059	3.1652994123	-0.1422909072
H46	0.9504117130	1.4672264456	-2.4188867307
H47	1.9852855061	2.2950972034	-4.5032191991

N34	0.6188153837	-3.3865174978	-0.6387947491
C35	0.6344051894	-2.2462652071	-0.3787944224

GEM_CO_trans_OLefin_CH3_transPhenyl_TS_SP.out

Pd1	0.3839321754	-0.2462062005	0.0311670215
C2	0.3499884680	1.8570950897	0.2634372279
C3	1.7775700982	1.8266875808	0.1625423394
H4	2.3286187960	2.0261516575	1.0750592736
H5	-0.0752750926	2.0542199802	1.2458202192
C6	-1.7199113743	-0.1639943095	-0.2458914874
H7	-2.2065394530	-1.0346110115	0.2032897738
H8	-2.1299778279	0.7452637430	0.1991215090
H9	-1.9136129330	-0.1613848098	-1.3244501930
C10	4.9446526857	-1.5740721146	1.1090339288
C11	4.0752602148	-1.1379927460	2.1124171423
C12	2.9107497552	-0.4418433049	1.7751476187
C13	2.5961706275	-0.1860809950	0.4326818554
C14	3.4807594251	-0.6097753488	-0.5651699041
C15	4.6443551850	-1.3084589727	-0.2292505549
H16	5.8547046736	-2.1083208861	1.3693003911
H17	4.3054758542	-1.3337185201	3.1574363986
H18	2.2460429490	-0.0995111148	2.5671218581
H19	3.2698050708	-0.3934291613	-1.6096029474
H20	5.3185470737	-1.6423872824	-1.0147896987
H21	-0.2196735496	2.2746541437	-0.5617834298
C22	3.8405924639	3.2066913127	-3.3442214214
C23	4.4143627335	3.3422616191	-2.0792886568
C24	3.7426709614	2.8690107876	-0.9535367414
C25	2.4807366541	2.2657859917	-1.0687032072
C26	1.9148206360	2.1312987233	-2.3472803160
C27	2.5902174861	2.5966630127	-3.4736432611
H28	4.3657128114	3.5685792473	-4.2242704813
H29	5.3879025090	3.8125740272	-1.9684754820
H30	4.1990750747	2.9664255425	0.0289183638
H31	0.9492445150	1.6458776341	-2.4610709226
H32	2.1406768697	2.4801964821	-4.4564320730
O33	0.2303513781	-3.3065712947	-0.3807253124
C34	0.3418636129	-2.1780710512	-0.2233287641

TRANS_CO_transOlefin_CH3_transPhenyl_TS_SP.out

Pd1	0.3018118635	-0.2803729652	0.0568441562
C2	0.0231003023	1.8641997158	-0.3359317074
C3	1.3867229961	1.8457557852	0.0674812959
H4	2.1461583389	2.1707144772	-0.6339753690
H5	1.6063293946	2.0887476979	1.1017718807
H6	-0.7066450174	2.1163027565	0.4300421085
C7	-1.8170535127	-0.4829128759	-0.1022374806
H8	-2.1599995357	-1.5148759483	0.0032836189
H9	-2.2722756176	0.1272468250	0.6845858682
H10	-2.0985324431	-0.0997054625	-1.0860738003
C11	5.1695985858	-0.8693805246	0.2909199484
C12	4.4880433779	-0.5252931241	1.4601326132
C13	3.1653139717	-0.0784468314	1.3967912655
C14	2.5026960640	0.0216521678	0.1669225049
C15	3.1983180964	-0.3176392350	-1.0030682716
C16	4.5202506567	-0.7651948526	-0.9415686554
H17	6.2002015619	-1.2112947664	0.3387735994
H18	4.9856140206	-0.6037802083	2.4241304827
H19	2.6501980727	0.1914992770	2.3169473163
H20	2.7083288004	-0.2420045562	-1.9717034271
H21	5.0433245967	-1.0309447285	-1.8575073445
C22	-1.3096019154	2.6896491431	-4.3448827552
C23	0.0072174690	2.2796428340	-4.1220361447
C24	0.4530735850	2.0054639527	-2.8316483135
C25	-0.4073143561	2.1337812822	-1.7246152124

C26	-1.7289302748	2.5503744535	-1.9663208428
C27	-2.1746306639	2.8241491384	-3.2583322283
H28	-1.6557546694	2.9007544572	-5.3530933864
H29	0.6921095021	2.1706718359	-4.9594832087
H30	1.4796460908	1.6791035360	-2.6874696437
H31	-2.4114493661	2.6614674208	-1.1273447293
H32	-3.2016515501	3.1445809613	-3.4146566559
X33	0.7703436313#	1.8649657583#	-0.1981727120#
O34	0.3522458071	-3.2993104156	0.6376030128
C35	0.3936063753	-2.1763421456	0.4195619202

GEM_CN_CO_transOlefin_TS_SP.out

Pd1	0.4496506092	-0.2560349479	0.0272773054
C2	0.3973822832	1.8226131082	0.3384275853
C3	1.8184602540	1.8527345064	0.1607917140
H6	2.4090846608	2.0829078675	1.0402364512
H7	0.0132437085	1.9649242400	1.3468642509
C17	4.9062952374	-1.5316194508	1.2119198896
C18	4.0024803149	-1.1068843500	2.1896245520
C19	2.8529156296	-0.4042110439	1.8199643573
C20	2.5908577430	-0.1412416811	0.4670576309
C21	3.5101309632	-0.5465116619	-0.5070232485
C22	4.6592535424	-1.2494193173	-0.1345546208
H23	5.8043244678	-2.0716669009	1.4992153102
H24	4.1935397057	-1.3163777897	3.2391287083
H25	2.1597513936	-0.0668675164	2.5880905577
H26	3.3322868527	-0.3193187689	-1.5547530442
H27	5.3617365553	-1.5763722115	-0.8971729453
H28	-0.2351447482	2.2391305944	-0.4389282460
C37	3.6430058287	3.2523907159	-3.4623431374
C38	4.2926724139	3.3954773379	-2.2352467004
C39	3.6963417539	2.9147653259	-1.0709836994
C40	2.4362037113	2.2976952132	-1.1115247236
C41	1.7928380209	2.1552833341	-2.3527733464
C42	2.3935922297	2.6289288899	-3.5170575225
H43	4.1086817543	3.6208123597	-4.3725286115
H44	5.2649342276	3.8780420082	-2.1843813552
H45	4.2087901186	3.0200624025	-0.1173428436
H46	0.8255423885	1.6632492700	-2.4107267298
H47	1.8855324528	2.5099259308	-4.4701700080
O33	0.4225268190	-3.3557066952	-0.4922734757
C34	0.4996096238	-2.2354150390	-0.3011174427
N31	-2.7053548158	-0.1974264670	-0.4430262340
C32	-1.5524015841	-0.2147368125	-0.2591461997

TRANS_CO_transOlefin_CN_transPhenyl_TS_SP.out

Pd1	0.2875129832	-0.2616764222	0.1349882207
C2	0.0231116269	1.8588220403	-0.3354738610
C3	1.3560986647	1.8926202527	0.1544488253
H4	2.1496013932	2.2636834526	-0.4809074602
H5	1.4977142600	2.1040336389	1.2094590879
H6	-0.7661129098	2.0837302299	0.3766497980
C8	5.0773613190	-0.8468684003	0.0427063235
C9	4.4783925031	-0.5400854252	1.2668732355
C10	3.1596519434	-0.0814400833	1.3089826646
C11	2.4268698261	0.0643849147	0.1238026531
C12	3.0365626490	-0.2311441591	-1.1050047420
C13	4.3539311776	-0.6928199981	-1.1424934912
H14	6.1041193490	-1.2010321405	0.0119039000
H15	5.0364037729	-0.6604669263	2.1919726720
H16	2.7024918147	0.1542939762	2.2671280494
H17	2.4824078689	-0.1120874922	-2.0328086018
H18	4.8141692833	-0.9309747198	-2.0982578825
C19	-1.1225282971	2.4799207204	-4.4317748302

C20	0.2316515799	2.4063399300	-4.1009149484
C21	0.6232179628	2.1976453257	-2.7792979991
C22	-0.3361832847	2.0572441663	-1.7600474558
C23	-1.6972856128	2.1302740253	-2.1089299891
C24	-2.0849139918	2.3410859074	-3.4287787929
H25	-1.4254350522	2.6416312242	-5.4629449143
H26	0.9878916986	2.5160702998	-4.8739953955
H27	1.6839987739	2.1546460219	-2.5484933147
H28	-2.4496757921	1.9817005263	-1.3397616001
H29	-3.1420937975	2.3878860962	-3.6759895072
O31	0.4572455958	-3.3180771277	0.7705716064
C32	0.4697248938	-2.2019748853	0.5432283682
N32	-2.9066050393	-0.5368829977	0.2037094978
C33	-1.7427099220	-0.4473200664	0.1618038530

TRANS_CO_transPhenyl_CN_transOlefin_TS_SP.out

Pd1	0.3540685321	-0.2623740800	0.0238658835
C2	0.0890643981	1.8966670984	-0.3541923556
C3	1.4689317701	1.9157901365	-0.0056072125
H4	2.1885459327	2.2364480846	-0.7495966917
H5	1.7141086497	2.2241568186	1.0043100160
H6	-0.6073937580	2.1672614700	0.4380472067
C7	5.1110053780	-0.7968765004	0.4105811784
C8	4.3772931942	-0.4589709071	1.5501296536
C9	3.0660126297	-0.0001980631	1.4285023157
C10	2.4722946759	0.1128220306	0.1626558289
C11	3.2179999964	-0.2185199081	-0.9794445914
C12	4.5287944452	-0.6759201901	-0.8538718117
H13	6.1331645460	-1.1525723035	0.5069150896
H14	4.8240455331	-0.5571432441	2.5359727477
H15	2.5014892993	0.2563295895	2.3213512782
H16	2.7718432353	-0.1395068183	-1.9675592261
H17	5.0936575250	-0.9431267913	-1.7432058718
C18	-1.5017701176	2.4578223673	-4.3100705740
C19	-0.1564637165	2.1211020377	-4.1487902998
C20	0.3784871308	1.9395271325	-2.8748792238
C21	-0.4236632293	2.0873848929	-1.7285709215
C22	-1.7767627407	2.4300696280	-1.9084117858
C23	-2.3095271419	2.6144203657	-3.1811926507
H24	-1.9169081659	2.5954114106	-5.3046768489
H25	0.4813132202	1.9966238879	-5.0200280270
H26	1.4273280192	1.6730485796	-2.7767114430
H27	-2.4153945100	2.5503149929	-1.0352707433
H28	-3.3577628099	2.8792927150	-3.2925779346
N30	0.9211650270	-3.3780651255	0.5194033716
C31	0.7473216909	-2.2372524489	0.3403066539
O32	-2.6515243722	-1.0458906162	-0.0764807568
C33	-1.5665876076	-0.6992786737	-0.0458345118

GEM_CO_transPhenyl_CN_tranOlefin_TS_2_SP.out

Pd1	0.4732669248	-0.2557750178	0.0240322643
C2	0.4553538655	1.8436917747	0.4309114067
C3	1.8717100850	1.8587903342	0.2046810848
H4	2.4891780390	2.1102379310	1.0591916272
H5	0.1152325048	1.9984763476	1.4536230567
C6	4.8801830584	-1.4601911055	1.3351714038
C7	3.9344424623	-1.0431117830	2.2747906580
C8	2.7952372470	-0.3556741175	1.8552609409
C9	2.5842394787	-0.1092340787	0.4889006129
C10	3.5430259530	-0.5140567608	-0.4476322617
C11	4.6848933299	-1.1923836266	-0.0227130796
H12	5.7723703428	-1.9880552449	1.6613302155
H13	4.0865344112	-1.2452583927	3.3318684803
H14	2.0714134077	-0.0158450570	2.5930061675
H15	3.3941743369	-0.3147994966	-1.5041322591

H16	5.4185044034	-1.5222611250	-0.7535259938
H17	-0.1805214983	2.2973751987	-0.3252035255
C18	3.5725903757	3.2627313754	-3.4790530043
C19	4.2208810319	3.4836683493	-2.2631133314
C20	3.6654084249	3.0019127599	-1.0789086189
C21	2.4468532257	2.3063772748	-1.0889566167
C22	1.8061232312	2.0849078099	-2.3190257170
C23	2.3655225700	2.5590861412	-3.5032803564
H24	4.0086000740	3.6289742965	-4.4046012446
H25	5.1619807300	4.0261852864	-2.2359801490
H26	4.1786952718	3.1675155880	-0.1343648771
H27	0.8783430023	1.5191716568	-2.3527058365
H28	1.8625111175	2.3724078327	-4.4481903585
O29	-2.5581499236	-0.6460066844	-0.4150815263
C30	-1.4468108787	-0.4513931352	-0.2483549068
N31	0.8625880532	-3.3534279723	-0.7651644859
C32	0.7389141270	-2.2323432665	-0.4615739624

GEM_NH3_trans_to_phenyl_TS_SP.out

Pd1	0.4586022821	-0.2898967409	0.0354090146
C2	0.4656231486	1.7848511480	0.2631404320
C3	1.8900083245	1.9159727115	0.1213582705
H6	2.4340716680	2.1917192542	1.0183186607
H7	0.0594449291	1.9749117547	1.2577442781
X8	0.4806690000#	1.8054860000#	0.3130400000#
H18	-2.1698093136	-0.9794912051	0.4532406136
H19	-2.1556405988	0.5755530835	-0.0611716794
C17	4.8880551063	-1.3930283307	1.1702813935
C18	3.9966568567	-0.9590588271	2.1564775158
C19	2.8283573713	-0.2870731436	1.7931433563
C20	2.5365234259	-0.0672105403	0.4336385113
C21	3.4499779476	-0.4800702900	-0.5501768151
C22	4.6149580842	-1.1534442560	-0.1808252427
H23	5.8046865598	-1.9017408644	1.4549054067
H24	4.2189294501	-1.1290326547	3.2062473000
H25	2.1519124211	0.0705336515	2.5657261716
H26	3.2599673914	-0.2628161655	-1.5976817093
H27	5.3158615560	-1.4785378228	-0.9448874117
H28	-0.1499143959	2.1658312736	-0.5513027507
C37	3.8049972594	3.3646183828	-3.4255520751
C38	4.4055351696	3.5210812877	-2.1750606115
C39	3.7777317432	3.0249689252	-1.0346952283
C40	2.5333588424	2.3779653116	-1.1252490884
C41	1.9409541281	2.2222023523	-2.3911310581
C42	2.5724447941	2.7125373471	-3.5307700532
H43	4.2953126290	3.7462571153	-4.3166051368
H44	5.3622142205	4.0277414568	-2.0881531315
H45	4.2507388300	3.1450250928	-0.0627506060
H46	0.9880892536	1.7079357349	-2.4890857172
H47	2.1057009813	2.5869634491	-4.5035619628
H35	-0.2346647498	-3.6892924084	-0.1457107797
H36	1.2990277967	-3.1632049119	-1.5259681490
P36	0.7908392662	-2.7233717154	-0.2836370617
H37	1.7518293112	-3.3267587955	0.5538897381
N36	-1.7325598410	-0.3403585135	-0.2111088495
H38	-2.0081382917	-0.6452892662	-1.1450807029

TRANS_NH3_trans_to_phenyl_TS_SP.out

Pd1	0.3826048316	-0.2705450609	-0.0109474587
C2	0.1338241281	1.8795804367	-0.3764006829
C3	1.5198255474	1.9192410422	-0.0845149096
H5	2.2203126061	2.1761534124	-0.8702571335
H6	1.8134030866	2.2470778290	0.9054862780
H7	-0.5314865582	2.1194645861	0.4545609127
X8	0.7630015000#	1.8708020000#	-0.1961420000#

H19	-2.3297687221	-0.5274245577	0.5475772520
H20	-2.1387630175	0.1755790335	-0.9329880179
C17	5.1126927555	-0.8272315185	0.4656708623
C18	4.3659831227	-0.4690985519	1.5914977610
C19	3.0516484031	-0.0173747421	1.4499400417
C20	2.4716713688	0.0594508559	0.1730004471
C21	3.2306233806	-0.2859697869	-0.9576169342
C22	4.5437984394	-0.7343552538	-0.8077327495
H23	6.1383361935	-1.1658341506	0.5789957492
H24	4.8085259071	-0.5303059392	2.5818820975
H25	2.4863243269	0.2775160020	2.3305530411
H26	2.8020519577	-0.2072123437	-1.9537157230
H27	5.1239962267	-1.0019772445	-1.6865838551
C27	-1.6933087101	2.4375283250	-4.2213508465
C28	-0.3492089875	2.0572616223	-4.1466596787
C29	0.2645554301	1.8733587602	-2.9110399065
C30	-0.4565565746	2.0655530993	-1.7165755232
C31	-1.8089718696	2.4533573427	-1.8070555849
C32	-2.4200700528	2.6403726776	-3.0476212763
H33	-2.1658391981	2.5823747276	-5.1883730811
H34	0.2227768467	1.9068743539	-5.0578866983
H35	1.3102436230	1.5794081411	-2.8777225039
H36	-2.3706018124	2.6520063188	-0.8954100069
H37	-3.4587865436	2.9546632252	-3.0952876794
H38	-0.0884984366	-3.6568967454	0.2139290108
H39	1.9799324914	-3.1633434173	-0.0766256772
P36	0.8184922514	-2.6081134235	0.4973014772
H40	1.0731933906	-2.9184546294	1.8499588258
N36	-1.7897976052	-0.5642222190	-0.3179617628
H41	-2.0090989331	-1.4529163503	-0.7678537863

PD_2PH3_Ph_Styrene_TS_SP.out

Pd1	0.3453000000	-0.3036320000	0.0281060000
C2	0.0770570000	1.8726900000	-0.3732580000
C3	1.4489460000	1.8689140000	-0.0190260000
H5	2.1853100000	2.1412310000	-0.7645980000
H6	1.7038320000	2.1493840000	0.9961850000
H7	-0.6167710000	2.1262080000	0.4277060000
X8	0.7379980000#	2.4121280000#	0.0181420000#
P13	0.8407220000	-2.6255110000	0.5308280000
H14	1.1580680000	-2.8942750000	1.8783600000
H15	-0.0635810000	-3.6886770000	0.3061130000
H16	1.9873830000	-3.1624290000	-0.0867700000
P17	-2.0338460000	-0.6250610000	-0.2251130000
H18	-2.6758680000	-1.7169590000	0.3980830000
H19	-2.9292820000	0.3975130000	0.1499010000
H20	-2.4760850000	-0.8330110000	-1.5474850000
C17	5.1305680000	-0.8532050000	0.3706400000
C18	4.4111890000	-0.5169030000	1.5200310000
C19	3.0849740000	-0.0839390000	1.4216940000
C20	2.4721670000	-0.0021570000	0.1637450000
C21	3.1963040000	-0.3285390000	-0.9920680000
C22	4.5210880000	-0.7582870000	-0.8838330000
H23	6.1637480000	-1.1774160000	0.4502720000
H24	4.8818010000	-0.5799870000	2.4972880000
H25	2.5417040000	0.1928870000	2.3218000000
H26	2.7376560000	-0.2516270000	-1.9746770000
H27	5.0774640000	-1.0100610000	-1.7826250000
C27	-1.4960400000	2.5959590000	-4.2994330000
C28	-0.1921700000	2.1104090000	-4.1595970000
C29	0.3353090000	1.8660980000	-2.8950820000
C30	-0.4355660000	2.0986970000	-1.7398430000
C31	-1.7453840000	2.5920170000	-1.8958890000
C32	-2.2689360000	2.8412790000	-3.1633080000
H33	-1.9024960000	2.7887370000	-5.2879720000

H34	0.4158990000	1.9269730000	-5.0408460000
H35	1.3526340000	1.4941970000	-2.8085590000
H36	-2.3453760000	2.8093900000	-1.0145150000
H37	-3.2765820000	3.2344500000	-3.2629270000

PD_2PH3_Ph_Styrene_gem_TS_fix_IGEN2.out

Pd1	0.4569059570	-0.2875153343	0.0176864674
C2	0.4806686718	1.8054855592	0.3130402053
C3	1.9003820355	1.8959978627	0.1304863013
H6	2.4838383959	2.1227014732	1.0156344673
H7	0.1092193779	1.9669963728	1.3251120181
X8	0.7379980000#	2.4121280000#	0.0181420000#
P13	0.8147417710	-2.6850818957	-0.3948668423
H14	1.7243233593	-3.3310002298	0.4666379706
H15	-0.2171403870	-3.6515223442	-0.3852712826
H16	1.4031400164	-3.0289367466	-1.6306487704
P17	-1.9171773580	-0.3160870496	-0.2379496407
H18	-2.6697075445	-1.0443367277	0.7074896699
H19	-2.6334856864	0.8988841499	-0.2003338236
H20	-2.4727191217	-0.8580996531	-1.4169040958
C17	4.9019297917	-1.4449427421	1.2455997239
C18	3.9771528715	-1.0341746990	2.2103308559
C19	2.8119581547	-0.3680703494	1.8228231746
C20	2.5635667741	-0.1350231818	0.4600977617
C21	3.5032365433	-0.5229138710	-0.5039211032
C22	4.6659558987	-1.1885801197	-0.1086519245
H23	5.8144730473	-1.9492670023	1.5501122160
H24	4.1692164021	-1.2166908280	3.2640174298
H25	2.1096844888	-0.0288078228	2.5806241324
H26	3.3401544180	-0.2954227746	-1.5540296631
H27	5.3914343008	-1.4959831692	-0.8570474547
H28	-0.1475602525	2.2355151423	-0.4640097311
C37	3.7599473099	3.3042513371	-3.4571542472
C38	4.4060989864	3.4209025468	-2.2249655559
C39	3.7958315319	2.9349171128	-1.0710792484
C40	2.5234687712	2.3390726823	-1.1292737394
C41	1.8853607549	2.2225809856	-2.3778058588
C42	2.4996292600	2.7021475473	-3.5309522919
H43	4.2364512444	3.6780861844	-4.3589740970
H44	5.3844322379	3.8883577014	-2.1634596132
H45	4.3036213282	3.0232876007	-0.1134585093
H46	0.9095020679	1.7490687061	-2.4512017611
H47	1.9979310868	2.6081886644	-4.4897711468

TRANS_NH3_TS_SP.out

Pd1	0.3745829046	-0.2746312736	0.0081892368
C2	0.0817942344	1.8728619916	-0.3607714825
C3	1.4588930283	1.8570695251	-0.0355739415
H5	2.1891273808	2.0856992442	-0.8021452881
H6	1.7472391958	2.1391819867	0.9700876509
H7	-0.5934083911	2.1438960950	0.4505465487
P17	-2.0099350558	-0.6484119743	-0.2080752524
H18	-2.5911288658	-1.8052812841	0.3588221660
H19	-2.9208153240	0.3061788785	0.2897449571
H20	-2.5200600476	-0.7710261708	-1.5169061906
C17	5.0706374425	-1.0357749673	0.4864191704
C18	4.3258716345	-0.6708374268	1.6107206535
C19	3.0271623153	-0.1706457170	1.4653812968
C20	2.4699174508	-0.0552749779	0.1847274038
C21	3.2212139829	-0.4027558458	-0.9457345390
C22	4.5182245235	-0.9004385585	-0.7895680051
H23	6.0823869554	-1.4125418199	0.6033209704
H24	4.7567930711	-0.7618383251	2.6040603986
H25	2.4649043652	0.1311665762	2.3456224299
H26	2.8076801843	-0.2888960675	-1.9448526246

H27	5.0973874257	-1.1729665115	-1.6677495596
C27	-1.5610135075	2.6037879003	-4.2586250182
C28	-0.2632631069	2.0958862270	-4.1438037925
C29	0.2868167980	1.8501158924	-2.8890991367
C30	-0.4550138960	2.1040826743	-1.7202294932
C31	-1.7587313118	2.6174703905	-1.8502315173
C32	-2.3053842312	2.8683892990	-3.1080422004
H33	-1.9850806318	2.7976188059	-5.2395300205
H34	0.3222497606	1.8957563314	-5.0366501333
H35	1.2986688100	1.4590787773	-2.8215194238
H36	-2.3367393828	2.8464737495	-0.9570926183
H37	-3.3085164967	3.2771029008	-3.1885305468
N34	0.8055366252	-2.4383445325	0.3484585062
H38	0.0830217505	-2.9870150993	0.8148770739
H39	1.0262667495	-2.9061839215	-0.5313917020
H40	1.6465380157	-2.4808867998	0.9257164933

GEM_NH3_TS_SP_cont2.out

Pd1	0.4109966189	-0.3133872761	0.0579597405
C2	0.3752740549	1.7750678429	0.1881637821
C3	1.8010904665	1.8942719444	0.0976824972
H6	2.3210605589	2.1030318388	1.0262396266
H7	-0.0612115838	1.9926418693	1.1639750942
P17	-1.9632986046	-0.4392329615	-0.1899174503
H18	-2.7367970120	-0.7101120412	0.9597593169
H19	-2.6684829302	0.6906770403	-0.6561015773
H20	-2.5261210348	-1.4074955613	-1.0507446776
C17	4.9052532738	-1.4854408439	0.9452835658
C18	4.0905533990	-1.0460247119	1.9921889210
C19	2.8976151561	-0.3717375926	1.7151810402
C20	2.5125047794	-0.1545981508	0.3826104424
C21	3.3457245341	-0.5682817395	-0.6668443778
C22	4.5331655431	-1.2477489906	-0.3823431865
H23	5.8389487268	-1.9961989991	1.1627305274
H24	4.3884601227	-1.2143233192	3.0235186801
H25	2.2800981847	-0.0137126594	2.5357268064
H26	3.0855717222	-0.3434818356	-1.6981087207
H27	5.1767612197	-1.5731693122	-1.1953950542
H28	-0.2079746144	2.1547982101	-0.6486468028
C37	3.9110432136	3.3585773500	-3.3222489414
C38	4.4755676206	3.4372898389	-2.0473912838
C39	3.7831827815	2.9345066726	-0.9489492868
C40	2.5092420745	2.3596226339	-1.1058033986
C41	1.9525932364	2.2832707172	-2.3956436195
C42	2.6497200194	2.7789353282	-3.4935723183
H43	4.4518904744	3.7456954647	-4.1812097455
H44	5.4540989914	3.8880490490	-1.9099950702
H45	4.2276900170	2.9911847865	0.0419776332
H46	0.9763017667	1.8293530995	-2.5449944199
H47	2.2113976873	2.7158151479	-4.4854238516
N34	0.7532147825	-2.5306175088	-0.0349678010
H35	0.1052088049	-3.0883982613	-0.5906387322
H36	1.6869861935	-2.6699888783	-0.4229983944
H37	0.7640985732	-2.9261832936	0.9061786443

TRANS_CH3_trans_to_olefin_TS_SP_cont.out

Pd1	0.4520797473	-0.2680589159	-0.1145914853
C2	0.2044780181	1.9435521250	-0.4259333805
C3	1.6340091783	1.9042544424	-0.2810122017
H5	2.2235081369	2.1121463113	-1.1704687889
H6	2.0209263207	2.4218941347	0.5916457538
H7	-0.3589191930	2.2771858411	0.4454353280
X8	0.7630015000#	1.8708020000#	-0.1961420000#
H19	-2.1176859347	-0.9025961268	0.4501836383
H20	-2.0946779082	-0.0212377170	-0.9579486744

C17	5.0739897383	-0.8103993448	0.8200228342
C18	4.2190499255	-0.3534873541	1.8282641865
C19	2.9729206278	0.1777808141	1.5007628509
C20	2.5351387820	0.2437690370	0.1607291113
C21	3.4222549907	-0.2035979238	-0.8397822889
C22	4.6714642965	-0.7295041182	-0.5166313769
H23	6.0505759085	-1.2147738676	1.0730927200
H24	4.5290619838	-0.4058382938	2.8694714149
H25	2.3264934629	0.5507009712	2.2927807948
H26	3.1243985492	-0.1422332160	-1.8845508637
H27	5.3328136116	-1.0783186353	-1.3064929779
C27	-2.0127664477	2.1780118414	-4.1085239175
C28	-0.6539731790	1.8473343547	-4.1313074026
C29	0.0855919659	1.7774105024	-2.9543269701
C30	-0.5082614665	2.0411633867	-1.6979138539
C31	-1.8845382750	2.3735777255	-1.6974680785
C32	-2.6208588936	2.4426627507	-2.8799796611
H33	-2.5843036696	2.2302241377	-5.0311032460
H34	-0.1642406794	1.6394142161	-5.0800276675
H35	1.1378655214	1.5111612922	-3.0079271963
H36	-2.3658732136	2.6109309978	-0.7494617903
H37	-3.6738791155	2.7130349907	-2.8398056896
H38	0.0044989837	-2.8432014127	0.5481486599
H39	1.1254590390	-2.7431345234	-0.8395638962
C36	0.8722625727	-2.3061373456	0.1361373032
H40	1.7224034581	-2.4428758805	0.8116524486
N36	-1.6239624941	-0.7599837547	-0.4295825667
H41	-1.6805700401	-1.6275303325	-0.9598557674

GEM_CH3_trans_to_olefin_TS_SP.out

Pd1	0.5361081068	-0.2254717810	0.0106213720
C2	0.5127807321	1.9081457262	0.3806282140
C3	1.9487552424	1.8570953271	0.1855647204
H6	2.5390890966	2.2215075680	1.0230228419
H7	0.1648116894	2.1489283419	1.3859444819
X8	0.4806690000#	1.8054860000#	0.3130400000#
H18	-1.9325967587	-1.0526811477	0.4885649374
H19	-2.1174965413	0.3523184153	-0.3624047426
C17	4.8503933289	-1.4389945045	1.4075054352
C18	3.8984328083	-0.9665005549	2.3156281297
C19	2.8179316387	-0.2143775708	1.8584156392
C20	2.6424609086	0.0532046052	0.4841818355
C21	3.6215267791	-0.4165471277	-0.4103797925
C22	4.7105451931	-1.1577643174	0.0453718715
H23	5.7035328984	-2.0127740537	1.7611917530
H24	4.0067987057	-1.1739717083	3.3778160613
H25	2.1014992161	0.1819712753	2.5757407369
H26	3.5263514827	-0.2036872464	-1.4709218431
H27	5.4515092113	-1.5209562277	-0.6631940120
H28	-0.0773048779	2.3640740499	-0.4137363136
C37	3.5921498637	3.2649813983	-3.5449173172
C38	4.1731719385	3.6272378461	-2.3292647244
C39	3.6420037115	3.1516956470	-1.1298408428
C40	2.5167522439	2.3153992683	-1.1217236039
C41	1.9463596240	1.9517809565	-2.3510307955
C42	2.4770954230	2.4231946717	-3.5504857158
H43	4.0087665321	3.6278616443	-4.4810951494
H44	5.0443959848	4.2774271993	-2.3128275229
H45	4.1046386584	3.4339162743	-0.1863487654
H46	1.0950590121	1.2743401023	-2.3593317268
H47	2.0248045670	2.1253332899	-4.4933571623
H35	-0.1201533246	-2.8305320685	-0.5490422625
H36	1.4390686278	-2.4140094778	-1.2974195959
C36	0.8258436778	-2.2832367951	-0.3954818746
H37	1.3557721098	-2.7549493786	0.4418150644
N36	-1.5726222000	-0.5045370317	-0.2908065720

H38	-1.7051787960	-1.0540809071	-1.1376279549

TRANS_CH3_trans_to_phenyl_TS_SP.out

Pd1	0.3226241641	-0.2936756535	0.0306092287
C2	0.0241458219	1.8313393635	-0.3590023683
C3	1.4022303418	1.8073232561	0.0172227229
H5	2.1393599496	2.1316425500	-0.7092569950
H6	1.6390262767	2.0952926052	1.0363628947
H7	-0.6850060370	2.1010433084	0.4205070021
X8	0.7630015000#	1.8708020000#	-0.1961420000#
H19	-2.2634531899	0.0838102871	0.6150676724
H20	-2.0707054017	-0.2393185720	-1.1320603399
C17	5.1713316067	-0.8894430705	0.3694283503
C18	4.4624786356	-0.5287060499	1.5177816042
C19	3.1461780647	-0.0693711458	1.4166742358
C20	2.5092459834	0.0256054006	0.1699217550
C21	3.2395472180	-0.3247750497	-0.9778132306
C22	4.5545371981	-0.7858947345	-0.8801774227
H23	6.1977569701	-1.2389279153	0.4460512888
H24	4.9363477502	-0.5999373611	2.4945173574
H25	2.6126691766	0.2198308483	2.3207286438
H26	2.7777754142	-0.2436069316	-1.9602205468
H27	5.0995613210	-1.0595148347	-1.7812402344
C27	-1.3904022030	2.6902264595	-4.3341543367
C28	-0.0761181432	2.2553888266	-4.1438968003
C29	0.3954296026	1.9677150785	-2.8657983834
C30	-0.4342740853	2.1073754846	-1.7362233570
C31	-1.7539957897	2.5474262062	-1.9460704798
C32	-2.2260077010	2.8343665296	-3.2260133385
H33	-1.7567210896	2.9123530542	-5.3330066503
H34	0.5865147850	2.1375808403	-4.9982098464
H35	1.4190486357	1.6217917533	-2.7473475063
H36	-2.4131444599	2.6681001934	-1.0895360255
H37	-3.2507072413	3.1739781396	-3.3562848095
H38	-0.0448056924	-3.4759488378	-0.4911223348
H39	1.7649818519	-3.2220786289	0.6147857423
P36	0.5159205115	-2.5759508881	0.4449796977
H40	-0.1268092408	-3.0926174115	1.5944794096
C36	-1.7773344896	-0.5592533959	-0.1274867685
H41	-2.1233782382	-1.5875834204	0.0316164003

GEM_CH3_trans_to_phenyl_TS_SP.out

Pd1	0.3883495411	-0.2475265913	0.0107545853
C2	0.3453234166	1.8487889703	0.1947015052
C3	1.7785820758	1.7953780670	0.1200118863
H6	2.3093596872	2.0236300431	1.0384237715
H7	-0.0962347125	2.0757571797	1.1635519857
X8	0.4806690000#	1.8054860000#	0.3130400000#
H18	-2.1545543397	-0.8641754991	0.5614891796
H19	-2.1276480183	0.7537425123	-0.1799213322
C17	4.9375537431	-1.5782310150	1.1243821238
C18	4.0640671048	-1.1214485137	2.1157954770
C19	2.9091960353	-0.4188590438	1.7614646959
C20	2.5990429047	-0.1752459899	0.4138240728
C21	3.4939772122	-0.6162371061	-0.5701397390
C22	4.6489412214	-1.3233543000	-0.2188428897
H23	5.8416551446	-2.1164028379	1.3975003702
H24	4.2858264048	-1.3049731463	3.1650709418
H25	2.2435314729	-0.0582605926	2.5445495102
H26	3.2956154406	-0.4050743731	-1.6184640680
H27	5.3275076423	-1.6686261086	-0.9961334552
H28	-0.2014264615	2.2563234145	-0.6509632321
C37	3.8821203542	3.1881983925	-3.3636689021
C38	4.4307644427	3.3427659416	-2.0898205699
C39	3.7473127039	2.8659184962	-0.9719578543

C40	2.4990266264	2.2386755231	-1.1033960925
C41	1.9593814933	2.0844307490	-2.3907837009
C42	2.6454188028	2.5546717476	-3.5089768700
H43	4.4155468632	3.5538282487	-4.2373711249
H44	5.3936451101	3.8317462743	-1.9652939279
H45	4.1842769278	2.9808462199	0.0175473416
H46	1.0045522336	1.5805344899	-2.5152485827
H47	2.2141784656	2.4239811861	-4.4983028618
H35	-0.7292545485	-3.3536102150	-0.2004837419
H36	0.9939912118	-3.1469809198	-1.4237254303
P36	0.4630882428	-2.5905917288	-0.2338108543
H37	1.2160913326	-3.3779175347	0.6709509581
C36	-1.7044024720	-0.2533941202	-0.2310446024
H38	-1.9619169651	-0.6931170598	-1.2031761847

GEM_NH3_trans_to_olefin_CH3_transPhenyl_TS_SP.out

Pd1	0.4031278361	-0.2311019265	0.0362095420
C2	0.3066154725	1.8307894805	0.1886320868
C3	1.7464714534	1.7678898836	0.1164521321
H6	2.2748258756	2.0032192071	1.0354469309
H7	-0.1292942586	2.0858788962	1.1539479534
X8	0.4806690000#	1.8054860000#	0.3130400000#
H18	-2.0815316266	-1.0309090154	0.5610468256
H19	-2.1924742865	0.5677805119	-0.2076231033
C17	4.8669025265	-1.7217077372	1.0293502208
C18	4.0601695057	-1.2116696347	2.0508926790
C19	2.9323006608	-0.4463697981	1.7384659968
C20	2.5786590838	-0.1954653165	0.4026788992
C21	3.4137176986	-0.6843867112	-0.6130847013
C22	4.5413838841	-1.4531930697	-0.3034633763
H23	5.7494460521	-2.3088977798	1.2700771185
H24	4.3129146784	-1.4034797898	3.0918128926
H25	2.3194034236	-0.0458434875	2.5448776669
H26	3.1895713354	-0.4587445557	-1.6535474644
H27	5.1728166380	-1.8326623553	-1.1044691464
H28	-0.2311127242	2.2488515453	-0.6590116078
C37	3.8633317186	3.1539068689	-3.3640536277
C38	4.4128369621	3.3002249383	-2.0898926463
C39	3.7245164900	2.8276684097	-0.9734382126
C40	2.4710445642	2.2116188304	-1.1056658588
C41	1.9305948647	2.0653364011	-2.3933998864
C42	2.6206957444	2.5323920243	-3.5104200182
H43	4.4003389572	3.5164552122	-4.2368880821
H44	5.3804218172	3.7795423643	-1.9639655661
H45	4.1627154691	2.9361810895	0.0162911589
H46	0.9714925415	1.5698180161	-2.5178450200
H47	2.1877371145	2.4083312730	-4.4999704160
H35	-0.1803539674	-2.8138988502	-0.6977860050
H36	1.4570579976	-2.7162678395	-0.4416056022
N36	0.5429428457	-2.4300326649	-0.0928924388
H37	0.4236857757	-2.8323082898	0.8353010122
C36	-1.6659405167	-0.3916321847	-0.2311222334
H38	-1.8610064337	-0.8663917245	-1.2039872421

TRANS_NH3_trans_to_olefin_CH3_transOlefin_TS_SP.out

Pd1	0.3431586028	-0.2743060641	0.0229784620
C2	0.0059182379	1.7896847508	-0.3635309052
C3	1.3971189056	1.7615496194	-0.0045752865
H5	2.1240637870	2.0709518764	-0.7488125241
H6	1.6504196494	2.0771794024	1.0029132873
H7	-0.6848141239	2.0987912134	0.4187022691
X8	0.7630015000#	1.8708020000#	-0.1961420000#
H19	-2.0494398685	-1.0937764297	0.8703130852
H20	-2.3208750723	0.1383030148	-0.3894694229
C17	5.1161216142	-1.0636251877	0.4428368627

C18	4.3956724077	-0.6721372586	1.5734993211
C19	3.1065011450	-0.1470203578	1.4391022329
C20	2.5045443193	-0.0192270198	0.1771613221
C21	3.2507759578	-0.3959824897	-0.9525172016
C22	4.5388407130	-0.9219309882	-0.8219506278
H23	6.1214185759	-1.4642758837	0.5448118869
H24	4.8400585598	-0.7674762452	2.5621301476
H25	2.5648998974	0.1687215418	2.3297373981
H26	2.8216946470	-0.2832396020	-1.9467639663
H27	5.0949367450	-1.2163396702	-1.7097447402
C27	-1.4241355535	2.7158416580	-4.3227095846
C28	-0.1267047252	2.2268768498	-4.1494141261
C29	0.3471722064	1.9150808110	-2.8777775646
C30	-0.4616042806	2.0843564219	-1.7379363318
C31	-1.7633216066	2.5805523468	-1.9305169493
C32	-2.2396981852	2.8900813412	-3.2038809290
H33	-1.7926294248	2.9569678372	-5.3164461830
H34	0.5207891839	2.0856562290	-5.0118376875
H35	1.3565166483	1.5255977635	-2.7720015045
H36	-2.4050742191	2.7297969707	-1.0649695283
H37	-3.2509094174	3.2727550713	-3.3206035225
H38	-0.1631505795	-2.8467277889	0.8034636637
H39	0.9083276723	-2.8883932543	-0.4507040363
N36	0.6703506239	-2.4087186032	0.4159518485
H40	1.4471000116	-2.5336631382	1.0640314083
C36	-1.7040649556	-0.7178786529	-0.1037494850
H41	-1.8388947596	-1.5053607560	-0.8588434779

TRANS_CO_transPhenyl_CH3_transOlefin_TS4_SP.out

Pd1	0.3408219840	-0.3102463198	0.0445528377
C2	0.0623294586	1.8852385772	-0.3627326277
C3	1.4501741086	1.9003501616	-0.0017129510
H4	2.1518701474	2.2890425409	-0.7332453789
H5	1.6671218393	2.2380236467	1.0067555886
H6	-0.6392903969	2.1489793794	0.4266938192
C7	5.1390765962	-0.7105204322	0.3675891086
C8	4.4258034464	-0.3540728982	1.5155395085
C9	3.1132361931	0.1059382996	1.4104993547
C10	2.4792177438	0.2090361379	0.1584335186
C11	3.2187603897	-0.1388715572	-0.9890515382
C12	4.5299319224	-0.6011331341	-0.8860834107
H13	6.1638242436	-1.0629353722	0.4480865539
H14	4.8939559808	-0.4325948659	2.4937949657
H15	2.5752290579	0.3922716970	2.3119624370
H16	2.7623348957	-0.0550754180	-1.9727625884
H17	5.0783556177	-0.8744846993	-1.7843962175
C18	-1.4770260332	2.5421651048	-4.3282366088
C19	-0.1385768511	2.1855113840	-4.1549079548
C20	0.3779076421	1.9677731271	-2.8786741205
C21	-0.4331508377	2.0987976118	-1.7337438393
C22	-1.7820452487	2.4593792546	-1.9295512099
C23	-2.2956442269	2.6792690245	-3.2039250840
H24	-1.8773838417	2.7101801539	-5.3244184377
H25	0.5106373724	2.0751850973	-5.0202339548
H26	1.4241986271	1.6926222475	-2.7749672117
H27	-2.4302836071	2.5700399224	-1.0621509123
H28	-3.3395045414	2.9602762606	-3.3210950006
X29	0.7703436299#	1.8649657632#	-0.1981727132#
O30	-2.5497296570	-1.2921266343	-0.0318883768
C31	-1.4826888846	-0.8750375358	-0.0113168327
C3j	0.9187425865	-2.3217853537	0.4445994380
H33	0.0907434895	-3.0353359804	0.4523258473
H34	1.6397493476	-2.5969902389	-0.3301604156
H35	1.4099279519	-2.3115394851	1.4219037864

GEM_CO_transPhenyl_CH3_tranOlefin_TS2_SP.out

Pd1	0.5052799768	-0.2435447204	0.0052534441
C2	0.4967460826	1.8929251994	0.4382593391
C3	1.9218095988	1.8481487283	0.2227618019
H4	2.5310180924	2.1517855751	1.0683635470
H5	0.1535805909	2.0646685889	1.4571606567
C6	4.8934895689	-1.4416370030	1.4451141544
C7	3.9118688770	-1.0169092320	2.3443723751
C8	2.8108154234	-0.2972333927	1.8803533758
C9	2.6538169208	-0.0215528721	0.5090494369
C10	3.6571903741	-0.4379960934	-0.3787747078
C11	4.7659759208	-1.1460765946	0.0848697440
H12	5.7602997899	-1.9901561164	1.8046912324
H13	4.0110887678	-1.2344162034	3.4051463666
H14	2.0688983657	0.0597578659	2.5928043365
H15	3.5709338061	-0.2106853691	-1.4376422807
H16	5.5314046002	-1.4706912976	-0.6159715833
H17	-0.1154276629	2.3647836937	-0.3255944471
C18	3.5853770530	3.2804885610	-3.4807858480
C19	4.2272506021	3.5294819709	-2.2670643376
C20	3.6858709923	3.0418554068	-1.0778872226
C21	2.4902099507	2.3087533253	-1.0786635382
C22	1.8570755420	2.0579073571	-2.3062951881
C23	2.3999577159	2.5411871754	-3.4958035008
H24	4.0083601205	3.6541151365	-4.4096855995
H25	5.1520609427	4.1002851755	-2.2447552175
H26	4.1944394339	3.2333557445	-0.1353895278
H27	0.9428763509	1.4699456625	-2.3298325681
H28	1.8985296029	2.3362953057	-4.4381668334
O29	-2.4507538359	-0.7557234586	-0.4913461049
C30	-1.3425806885	-0.5288504439	-0.3003821487
C31	0.8961363174	-2.2918227078	-0.4659482813
H32	0.0075061785	-2.8925144893	-0.6790038466
H33	1.5559114404	-2.2957170141	-1.3399362302
H34	1.4262474547	-2.7123917461	0.3936282330