Reliable and Efficient Reaction Path and Transition State Finding for Surface Reactions with the Growing String Method

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Abstract

The computational challenge of fast and reliable transition state and reaction path optimization requires new methodological strategies to maintain low cost, high accuracy, and systematic searching capabilities. The growing string method using internal coordinates has proven to be highly effective for the study of molecular, gas phase reactions, but difficulties in choosing a suitable coordinate system for periodic systems has prevented its use for surface chemistry. New developments are therefore needed, and presented herein, to handle surface reactions which include atoms with large coordination numbers that cannot be treated using standard internal coordinates. The double-ended and single-ended growing string methods are implemented using a hybrid coordinate system, then benchmarked for a test set of 43 elementary reactions occurring on surfaces. These results show that the growing string method is at least 45% faster than the widely used climbing image-nudged elastic band method, which also fails to converge in several of the test cases. Additionally, the surface growing string method has a unique single-ended search method which can move outward from an initial structure to find the intermediates, transition states, and reaction paths simultaneously. This powerful explorative feature of single ended-growing string method is demonstrated to uncover, for the first time, the mechanism for atomic layer deposition of TiN on Cu(111) surface. This reaction is found to proceed through multiple hydrogen-transfer and ligand-exchange events, while formation of H-bonds stabilizes intermediates of the reaction. Purging gaseous products out of the reaction environment is the driving force for these reactions.

Keywords: growing string method, surface chemistry, atomic layer deposition, titanium nitride, transition states

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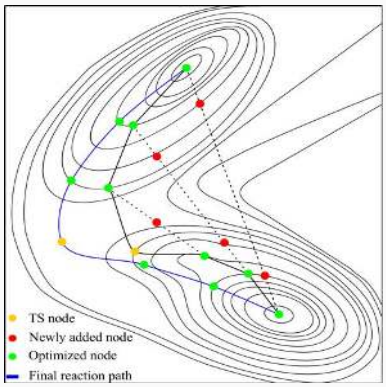

The growing string method is a powerful tool for locating reaction paths and transition states, using little user input. Herein, we present a new implementation of the growing string method for surface reactions and its application to the atomic layer deposition of titanium nitride.

INTRODUCTION

The information contained in transition state (TS) structures and reaction paths (RP) provides the fundamental atomistic details of reaction mechanisms. From a computational viewpoint, TSs are first-order saddle points on a potential energy surface (PES) representing the connection of two intermediates along a path. The high dimensionality of most PESs, however, makes TS-finding an impossible task unless fast, reliable, and accurate methods are available. Given the great interest in simulation of reactions on surfaces, such as atomic layer deposition (ALD),[1] heterogeneous catalysis,[2,3] and electrochemical CO_2 reduction,[4] novel tools for TS and RP finding are in demand.

The algorithms designed to locate TSs and RPs are usually classified as single-ended[5–54] or double-ended.[55–98] Single-ended methods start from a single initial state and refine it systematically to locate a TS. Many single-ended methods require an initial guess-geometry lying close to the desired TS structure, which limits the effectiveness of these approaches. Double-ended methods, on the other hand, connect two structures in a discretized RP and are usually more reliable than single-ended methods due to the endpoints of the path being fixed, so double-ended methods are less likely to diverge to undesired search regions. Most double-ended algorithms do not compute the exact saddle point, so they are usually followed by a local search method (such as the dimer method,[15] mode-tracking,[52] or eigenvector following method[14,34]) to refine the apparent TS structure to the exact TS.[99]

Given the multitude of methods available for TS and RP finding, these techniques are best summarized by the key components that afford their success. We classify these in four groups: 1.) Strategies for quickly approaching the vicinity of the saddle point, 2.) Estimation of the direction of negative curvature, 3.) Optimizer, and 4.) Coordinate system, which should all operate synergistically to rapidly and reliably locate TSs. In an ideal search algorithm, the combination of these four components should operate with little input from the user. These four areas will now be discussed to set the context for our proposed method.

Starting from an initial state, there are three often-used algorithmic strategies to approach the saddle point region. Minimum-mode following methods find the lowest curvature direction of the Hessian and follow this eigenvector towards the saddle point.[48,100] Alterna-

tively, coordinate driving techniques push the initial structure towards an approximate TS structure along a specified reaction direction.[23,31,101] When the initial and final states are known, the highest energy point along an approximate reaction path from a double-ended method can be used as a good estimate of the exact TS.[60,99]

After obtaining an approximate TS geometry, the direction corresponding to the transition vector must be estimated. While in principle the exact Hessian can be calculated and diagonalized to find the negative curvature direction, the computational cost can be expensive or prohibitive. To reduce this cost, approximate Hessians can be constructed and diagonalized via subspace iteration methods,[48,102–104] or alternatively, the reaction tangent at the guess TS from a RP can provide an estimate of this direction.[99]

In addition to the two prerequisites of a good initial TS structure and reaction direction, an efficient optimizer[34] is necessary to direct the TS searches and refine reaction paths. In practice, quasi-Newton[34] methods are widely used because they update approximate Hessians at each optimization step, entirely skipping Hessian computations while still benefiting from PES curvature information. For TS searches, eigenvector following optimizers[99] maximize the energy along the lowest Hessian mode while minimizing in all other directions. These methods tend to converge when the Hessian contains a reasonably accurate eigenvector representing the reaction direction.

The fourth component of interest is the coordinate system which forms the basis in which RPs and TSs are optimized. Cartesian coordinates are often chosen due to their simple implementation, despite internal coordinates (IC) being superior in many respects: chemical bonds are included as intrinsic coordinates, the curvilinear motion of angle bending or torsions are better represented by internals, and ICs have reduced intercoordinate coupling which allows faster optimization. Further advantages include that the interpolation of a RP in ICs avoids the collision of atoms or intersections of bonds,[9,11,12,23,34,54,57,86,99] and ICs can accelerate convergence of optimization by a factor of four.[18,57,58,105]

Two common surface-compatible reaction finding methods are the nudged elastic band[62] (NEB) and the dimer[15] method. NEB and its variations[59,60,63,64] interpolate between two structures in Cartesian coordinates to optimize a chain-of-states representation of the reaction path. NEB therefore is frequently used to form the guess for a transition state

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optimization by the dimer method in a two-step procedure. Multi-step computational procedures are inherently less user-friendly, suggesting new methods for simultaneous RP and TS finding with increased efficiency, reliability, and usability as promising additions to the computational toolkit.

Herein a novel means for systematic TS search and RP finding is implemented in a powerful tool for the study of surface reactions. The method is inspired by GSM[54,65,86,99] and designed as a combined RP optimization and TS search algorithm. When the reactant and product structures are known, the new double-ended GSM (DE-GSM) can be used to calculate a RP and TS at low cost and high fidelity. In cases where the final structure is unknown, single-ended GSM (SE-GSM) can explore a new reaction space based on simple reaction coordinates as input. Detailed comparisons of three investigated methods (DE-, SE-GSM, and CI-NEB) are provided to benchmark their computational cost and reliability. The high usability of SE-GSM for exploring new reactions is demonstrated by showing an atomistic mechanism for the initiation and growth of titanium nitride on Cu(111) surface.

METHOD

Growing String Method with Exact TS Search

i. Overview

GSM develops a RP by iteratively adding new nodes and optimizing them until a complete RP with a TS and a stable intermediate on each side of the string are present. The string consists of a discretized set of structures along the RP connecting the reactant and product geometries, and is constructed starting only from the endpoints. By incremental addition of new nodes, GSM rapidly leads to a reasonably well converged RP since it avoids placing nodes at high-energy regions of the PES.[65]

Based on our experience using GSM for molecular systems,[54,86,99] we have developed a new method to overcome challenges of RP and TS finding for periodic systems and surface reactions. This method operates through three overall phases: growth, optimization, and exact TS search (Figure S1), which now will be discussed in detail.

ii. Growth Phase

During the growth phase, new nodes are added along the reaction tangent direction and minimized in directions perpendicular to the reaction tangent. The reaction tangent is defined either by interpolation or driving coordinates (see below), and used as constraint to prevent nodes from falling back to local minima. New nodes are added after the gradient at the frontier node drops below a predefined threshold, and the growth phase terminates when either two string fragments are connected (double-ended) or an intermediate on the other side of the string is found (single-ended).

The tangent definition during the growth phase depends on whether the algorithm is double-ended or single-ended. For DE-GSM, reaction tangent for node i pointing to node j is defined as

$$U_C = \alpha_c \sum_k \langle \Delta q | U_k^{(i)} \rangle U_k^{(i)} \tag{1}$$

where U_C is the (constrained) tangent direction, Δq is defined to be $\Delta q = q^{p,(j)} - q^{p,(i)}$, q^p are the primitive (hybrid) coordinates, α_c is a normalization factor, and the vectors U_k are the non-redundant (hybrid) coordinates vectors (see Coordinate System for Surfaces). Following the constrained optimization in delocalized IC introduced by Baker et al,[12] Δq is projected onto the non-redundant DOF and then normalized to form a vector space with one extra DOF. The new vector set undergoes Schmidt orthonormalization to form a new coordinate set spanning the constraint vector U_C and the remaining non-redundant DOF. This procedure allows a reaction path to be represented in any combination of internal and Cartesian coordinates without any problems caused by an over-specified (redundant) set of coordinates.

SE-GSM requires a modification in the tangent definition for the growth phase

$$U_C = \alpha_c \sum_{k=1}^{3N-6} \langle \delta q | U_k^{(i)} \rangle U_k^{(i)} \tag{2}$$

where δq is a primitive coordinate vector describing desired changes in connectivity (bond lengths, angles, and torsions). During the growth phase, new nodes are added, one at a time, along the vector U_C and only this frontier node is optimized using U_C as a constraint.

Combining GSM with IC therefore allows an opportunity of using driving coordinates to

find TSs starting from a single initial state. The resulting method, SE-GSM, can explore the chemical reaction space without having prior knowledge about the final state. In practice, δq includes reaction coordinates (combination of bonds, angles, and torsions) representing any desired reaction. This includes coordinates not present in the primitive internals of the starting structure, as any reaction coordinates can be trivially added to the coordinate system when needed.

iii. Optimization

When the string is fully grown, all the nodes on the string undergo optimization cycles under the constraint U_C of Equation (1), which depends on the node's location along the string. During optimization, an approximate Hessian matrix is used to accelerate convergence. This Hessian is formed when a node is created from a diagonal primitive coordinate Hessian,[99] and updated using the BFGS[106–109] scheme as optimization proceeds. Diagonalization of the Hessian at each node in the non-redundant coordinates provides a set of eigenvectors and eigenvalues which are used in the eigenvector optimizer:

$$\Delta v_i = \frac{-g_i}{H_{ii} + \lambda} \tag{3}$$

v_i are the eigenvectors of the Hessian in coordinates U_k, H_{ii} are the corresponding eigenvalues, g_i is the gradient in the eigenvector basis, and λ is a scaling factor.

After the reaction path is converged to a specified threshold, a CI search begins.[60] At the TS node, perpendicular directions are optimized as described by Equation (3) while the U_C direction of the highest energy node is maximized according to:

$$\Delta U_C = \frac{g_c}{\beta} \tag{4}$$

U_C is the constraint climbing direction, g_c is the gradient along the U_c, and β is a scaling constant.

The CI search (Equation 4) moves the highest energy node towards the vicinity of the saddle point, which is vital to providing an accurate TS guess prior to the exact TS search. At this point, the reaction tangent (U_C) also provides a good approximation to the TS eigenmode.

vi. Exact TS search

After the CI search has begun and the RP converges to a predefined gradient threshold, the eigenvector following TS search commences. The eigenvector of the Hessian with highest overlap with the reaction tangent $\left(\max_i \langle U_C | v_i \rangle\right)$ at the TS node is followed to find the exact TS

$$\Delta v_{RP} = \frac{g_{RP}}{H_{RP} + \lambda} \tag{5}$$

where subscript RP refers to the vector with maximum overlap. This strategy ensures the correct mode is followed,[99] but requires that the RP be available during the TS search. Therefore GSM with exact TS search has a particular advantage over typical saddle point finding methods which do not simultaneously optimize the RP.

Prior to beginning the TS optimization, the Hessian has no negative eigenvalues because the BFGS scheme enforces a positive definite Hessian. To initiate the exact TS search, the curvature along RP is approximated using the reaction path tangent defined by the nodes neighboring the TS. Projecting this curvature into the Hessian results in a single negative eigenvalue and its corresponding eigenvector, while avoiding the (expensive) computation of the exact Hessian. Details on building this Hessian can be found in the Appendix.

Coordinate System for Surfaces

As many studies have shown,[9,11–13,18,27,32,34,57,86,110] the motion of molecular systems is best described by IC, which are composed of primitive coordinates such as bonds, angles, and torsions. A specifically useful type of ICs are delocalized ICs[12] which are constructed from a set of primitive internals[9] and fully span the nonredundant coordinate space. These coordinates can be used whenever a set of primitives is available, and provide the significant benefit for optimization of systems including atoms with low coordination numbers.

Use of any type of IC becomes significantly more cumbersome, however, when treating periodic systems which include a large number of atoms with high coordination numbers. For instance with metallic systems, optimizing using ICs is impractical due to the huge number of primitive coordinates that can be present. A mixed coordination system involving Cartesians on high coordination number atoms, and ICs elsewhere, is straightforward.[110–112]

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Such a mixed coordinate system is justified because in a surface reaction only certain atoms require ICs, while others are largely immobile. For instance in a typical reaction, adsorbate atoms move significantly while surface atoms remain relatively immobile and act as binding sites for adsorbate species. Furthermore, only the surface's topmost layer is actively involved in a reaction and bottom layers are stationary supports. As a result, there is no obvious need to include all atoms in the IC set, as Cartesians will easily be able to describe relatively immobile atoms.

Fortunately, a hybrid coordinate system is fully compatible with the delocalized internal coordinates procedure. For each reaction, we define the active surface atoms involved, and assign ICs to these atoms along with all molecular species in the system. All atoms embedded in the surface are assigned Cartesian coordinates, as shown in Figure 1. Once the (redundant) set of Cartesians and ICs are available, the delocalized hybrid coordinates are formed with the usual procedure (see Appendix).

Computational Details

All energy and gradient calculations are performed in a plane wave basis set under periodic boundary conditions as implemented in the Vienna Ab Initio Simulation Package (VASP).[113–116] The PBE functional and projector-augmented wave methods are used to describe the exchange-correlation energy and electron-ion interactions, respectively. An energy cutoff of 300 eV and a smearing parameter of 0.2 eV were employed for the plane waves. The Brillouin zone is sampled using a $1 \times 1 \times 1$ Monkhorst-Pack mesh for all reactions except reactions 5, 7, and 9 where a $2 \times 2 \times 1$ k-point grid is used for the integration and the energy cutoff is set to 400 eV. GSM is implemented in C++ and invokes the Atomistic Simulation Environment (ASE)[117] to provide the quantum mechanical gradients through VASP.

For both single-ended and double-ended GSM the equal spacing of the nodes on each side of the TS node is maintained by a reparameterization step that is performed after each optimization cycle. Reparameterization does not shift the highest energy node after string is fully grown and CI starts.

All CI-NEB calculations used the BFGS optimizer as implemented in ASE and a spring

constant of 0.1 $eV/$Å. CI-NEB were considered converged when the RMS gradient on the TS node was below 0.0136 $eV/$Å $\simeq$ 0.0005 Hartree/Å and the total gradient over all the active images was below 2.7 $eV/$Å $\simeq$ 0.1 Hartree/Å to match the GSM's convergence criteria. The calculations that required more than 200 gradient computations per active node (>1,800 gradient calculations for double-ended methods) were terminated and considered unsuccessful.

The chemical structures for this study are created using ASE and the CI-NEB method is employed as implemented in ASE. Reactant and product structures were optimized using the BFGSLineSearch optimizer and were converged when the maximum force on each atom was below 0.05 $eV/$Å.

In the examples that follow, 11 nodes including the two fixed endpoints (9 active nodes) were used to represent the reaction path for double-ended calculations (DE-GSM & CI-NEB) except reaction 1, which has 7 nodes. The input reactant and product structures for the double-ended methods are identical for both methods. The number of nodes for SE-GSM is determined by the method automatically, and typically ranges from 7 to 11 nodes in the reported tests. The three methods under study are compared based on the number of gradient computations required for the convergence of the reaction paths and calculated activation barriers. More details can be found in section 1 of SI.

Surface Reaction Validation Test Set

To confirm the efficiency and reliability of the proposed method, an extensive test set of elementary reactions was created. A variety of reaction types, including molecular and dissociative adsorptions, desorptions, and bimolecular and unimolecular reactions, are covered in this set. Most of these reactions have been investigated previously using the NEB method by other researchers.[118–133] In summary, 43 elementary reactions which consists of 9 different metals, one metal oxide, and 7 different surface terminations were studied. Summaries of the reactions are given in Table 1.

RESULTS AND DISCUSSION

Overall Performance of Reaction Path Optimization Methods

To evaluate the performance and stability of the three reaction finding methods, their computational cost and success rate will be compared first. Robust methods should converge relatively fast on a wide variety of reactions and successfully calculate a RP and TS in a small number of gradient calculations. The success rate and average number of gradient calls for convergence of DE-GSM, SE-GSM, and CI-NEB are shown in Figure 2. DE-GSM was successful in all cases (43 out of 43) while SE-GSM succeeded for 41. CI-NEB converged in 33 out of 43 test cases within 1,800 total gradient calculations, and the reasons for the failures will be discussed in the subsequent section. The average number of gradient calls were 614, 338, and 366 for CI-NEB, DE-GSM, and SE-GSM, respectively, demonstrating that GSM is on average at least 1.8 times faster than CI-NEB.

Taking a closer look at the convergence behavior of the methods provides some insight into the faster convergence of GSM. An example is shown in Figure 3 where an addition reaction on Pd(111) (Reaction 8-b) takes place between a hydrogen atom and an ethyl fragment to form ethane. The initially interpolated RP from CI-NEB has a higher RMS gradient compared to DE-GSM's and therefore requires a larger number of optimization iterations to converge. GSM, on the other hand, does not generate all of the nodes at once, which avoids distorted chemical structures with high gradients. This property of maintaining low gradients and small numbers of optimization steps is well-known for GSM,[65] and is fully taken advantage of in DE- and SE-GSM for surfaces.

Additionally, the initial linear path by CI-NEB does not capture the correct asynchronicity in hydrogen and carbon movements. On average, the carbon atom moves 0.03 Å higher on the surface in CI-NEB's initial path compared to DE-GSM. At the same time, the hydrogen is 0.04 Å closer to the surface in CI-NEB. The root mean square deviations (RMSD) in RPs indicate that DE-GSM's initial reaction path is similar to its final path (RMSD = 0.097), while CI-NEB's deviates more significantly (RMSD = 0.209). In CI-NEB, this difference is seen in the unnecessary half-circular motion of hydrogen adatom on surface before its addition to the ethyl group (Figures S16, S15 and Table S1). Overall, the high quality of

GSM's initial RP results in improved performance compared to CI-NEB.

Comparison of Reaction Paths from DE-GSM and CI-NEB

To further demonstrate the reliability and robustness of DE-GSM, it will now be compared in more detail to the CI-NEB method. As shown in Figure S3, the activation energies predicted by these two methods are similar, with a linear regression of slope 0.995 and R^2 of 0.989. This correlation shows that DE-GSM with its exact TS search produces similar barriers compared to those from CI-NEB. Some deviation is expected, however, because GSM performs an exact saddle point search, while CI-NEB provides an approximate TS. The maximum difference in calculated activation energies by two double-ended methods occurs for water dissociation on W(111) (Reaction 15-a), which differs by 4.6 kcal/mol between DE-GSM and CI-NEB. In section 2 of SI we show that this difference occurs because the two methods find distinct reaction pathways, which should not have the same barrier.

There are two cases where CI-NEB did not compute a realistic RP, specifically two copper surface rearrangements,[134] reactions 6-b and 6-c. Such reaction steps are known to be important for copper-promoted graphene growth[135] and silicon device production,[136] and otherwise represent standard reactions that should be resolvable by double-ended methods. In Reaction 6-c, two Cu atoms exchange positions on Cu(110) surface, but the linear Cartesian interpolation of the CI-NEB's initial RP causes the moving atoms to sit directly on top of one another (section 2 of SI). From this geometry, convergence of the DFT density and energy fails, and optimization cannot proceed. DE-GSM, by incrementally adding and optimizing nodes, never reaches such problematic structures and optimizes smoothly to the desired RP. Reaction 6-b similarly has a problem with the initial interpolation in CI-NEB, which is discussed in section 2 of SI.

Comparison of DE-GSM and SE-GSM

In the case of SE- and DE-GSM, the reaction tangent definitions are different and can lead to unique RPs being found for the same qualitative reaction. This can occur in reactive systems with more than a few degrees of freedom, where there are often multiple pathways

from a given initial state to a single product structure.[34] Usually, TS finding methods locate only one such path at a time, and thus offer no guarantee that all connecting TSs will be found. Cases where two different RPs were found by SE- and DE-GSM are discussed in this section.

The activation energies computed by SE-GSM and DE-GSM (Figure S8) are usually similar, but less closely related than DE-GSM compared to CI-NEB. The comparison of SE- to DE-GSM yields a slope of 0.899 and R^2 value of 0.875. Because the optimization process is identical for the two methods after the string endpoints are connected, this slight dissimilarity is due to differences in the initial reaction tangent and RP. Specifically, since DE-GSM uses curvilinear interpolation in ICs between the two frontier nodes to estimate a RP, it does not generally have the same tangent as SE-GSM, where the tangent consists of a few specific ICs used as driving coordinates.

This difference in tangent definition and its influence on the outcome of a calculation is most pronounced in Reactions 10-a, 14-c, 15-a, and 16-b. Reaction 10-a is a representative example that describes addition of a hydrogen atom to oxygen of CO on Ni(111) surface to release H_2O and deposit C on the surface. SE-GSM's initial RP is formed under a more free reaction tangent compared to DE-GSM, because its reaction tangent consists of only one driving coordinate (addition of hydrogen and oxygen).

This freedom of movement in SE-GSM ultimately results in variations in energies and chemical structures of the TSs. In this example, SE-GSM results in a lower activation barrier and a more stable product (Figure 4). This occurs because the CO molecule is stationary in DE-GSM, while it moves from its starting binding site to a neighboring fcc site in the SE-GSM case (Figure S9). Chemical structures of this example are quantitatively compared in Table 2. A similar situation happens in other cases (reactions 14-c, 15-a, 16-b) where the products form on different binding sites or in different relative positions on the surface.

In addition to different single elementary step transformations, we observed that reactions 4 and 5-b proceed in different number of elementary steps through the two GSM growth strategies. For example in reaction 4, CO and O combine on a Ru(0001) surface to release carbon dioxide. For this case the DE-GSM's RP consists of two elementary steps, in which a CO−O complex is formed on the surface followed by its desorption. On the other hand,

the SE-GSM's RP proceeds through a single elementary step that combines CO_2 formation and desorption (Figure 5) through the asymmetric dissociation of Ru−O bonds (Figure S10 and TS structures of Figure 5b).

When a system has many degrees of freedom, multiple pathways connecting the same two qualitative chemical structures can be present. SE- and DE-GSM provide two varying growth methods due to their tangent definitions, which enables exploring alternative paths for a given reaction. This will be especially the case if multiple SE-GSM trials are attempted, which is a subject of future research and will be reported subsequently.

Atomic Layer Deposition of TiN on Cu(111)

Titanium Nitride (TiN) has many desirable properties that make it a good candidate as a wear-resistant coating or copper diffusion barrier in microelectronics.[137] To build TiN layers of controlled thickness, ALD is an especially useful technique. In ALD, alternating cycles of two self-limiting and complementary reactions utilize gaseous precursors to form ultrathin, conformal, and uniform films with monolayer control over the thickness.[138] Experimental studies[139,140] have shown that tetrakis(dimethylamido)titanium (TDMAT) and ammonia (NH_3) are good precursors for ALD of TiN. By first reacting NH_3 onto the surface in the form of NH_x units and their derivatives (N, N_2), the subsequent ALD cycle using TDMAT precursors attaches Ti-containing species to these surface sites. Upon repeating these cycles, TiN layers can be formed in a controlled fashion.

Little mechanistic information is available for this ALD reaction, hindering our ability to extend the scope and availability of new precursors and conditions for reaction. While some mechanistic information for related processes are available,[141,142] these fail to capture any specific details of the TiN ALD mechanism. Given this lack of information, SE-GSM is ideally suited for investigating this process because it starts from a single initial state and locates the TS, RP, and the product in one computation. This capability enables systematic exploration of the reactive space, without requiring a guess transition structure close to the saddle point or even a complete set of reactive intermediates. Studying ALD of TiN will therefore serve to demonstrate the capabilities and advantages of SE-GSM for reactions that are not already well-known.

In particular, the initiation steps to form three atomic layers of TiN on Cu(111) will be studied. The reactive process proposed here proceeds through three general steps: Step 1.) Addition of ammonia to nucleate surface sites and release H_2 gas. Step 2.) Deposition of titanium via a ligand-exchange with TDMAT extruding dimethylamine gas. Step 3.) Addition of ammonia to the titanium-terminated surface. Repeating steps 2 and 3 provides access to additional layers of TiN. In order to reduce the computation complexity, $-N(CH_3)_2$ ligands are truncated to $-NH_2$ except when the ligand is involved directly in a reaction. A summary of activation energies, proposed reactions, and chemical structures are shown in Table 3 and Figures 6 to 9 and S11 to S14. The asterisk (*) on chemical moieties means they are adsorbed on surface.

i. Nitrogen nucleation during first NH_3 cycle

During the first deposition cycle, molecular NH_3 is chemisorbed on the surface in a barrierless transformation that is exothermic by 10.6 kcal/mol (T1, Figure 6). Three different orientations of adsorbed NH_3 are possible on surface which yield slightly different activation energies for the subsequent reactions. Reaction T1 is followed by progressive dehydrogenation of NH_3 to form NH_x* species (x=2, 1, 0) and subsequent release of H_2 gas from hydrogen adatoms present on the surface (Reactions T2-T4 of Figure 6) as suggested by experimental studies.[139] During the first dehydrogenation step (T2, Figure 6 and Figure S12a), NH_3* moves from atop position to form NH_2* in a higher-coordinated bridge site and H* in fcc through a barrier of 31.4 kcal/mol and is endothermic by 16.8 kcal/mol. A second hydrogen dissociation and migration from NH_2* proceeds through a very similar process with a barrier of 30.5 kcal/mol and is also endothermic by 27.6 kcal/mol (T3, Figure 6 and Figure S12b).

Although the barriers for fragmentation of surface bound ammonia are too high to proceed at room temperature, the experimental conditions can exceed 150 ℃, making these barriers surmountable. The barrier for reductive-coupling of two surface-bound hydrogen adatoms is 22.6 kcal/mol, which allows release of hydrogen gas and provides an entropic driving force for these reactions (T4, Figure 6 and Figure S12c).

ii. Ti layer formation

The second ALD cycle introduces TDMAT to the reaction. A previous report[140] on this process proposes that NH* moieties on surface likely serve as nucleation sites for TDMAT deposition, rather than open Cu surface sites. This step is therefore driven by the electron-rich dimethylamido ligands on TDMAT which serve as strong H-bond acceptors for NH* groups. This characteristic also means that its dimethylamido ligands make TDMAT preferable to other titanium precursors such as $Ti(NH_2)_4$. As a result, deposition of titanium on the surface (T5, Figure 7) is initiated by the gradual formation of a strong H-bond between one of the dimethylamido ligands and an NH*. As the reaction approaches the transition state, the hydrogen from NH* is formally transferred to dimethylamine, resulting in elongation of the titanium-amino bond by 0.20 Å. Additionally, the distance between the titanium center and the N*, 2.95 Å , is too long to be a covalent bond, highlighting the importance of a strong H-bond interaction to stabilize these types of species (Figure S11). The resulting $Ti(N(CH_3)_2)_3(NH(CH_3)_2)$ intermediate is stabilized by interaction between one of the dimethylamido ligands on TDMAT and a surface amine, in this case N*. The final step of tethering titanium onto the surface, via ligation of N*, proceeds through a concerted ligand-exchange with a barrier of 7.9 kcal/mol, displacing one of the dimethylamido ligands via a dissociative transformation (Figure S13a). This mechanism is in agreement with the experimental observation of the build-up of dimethylamine gas during this process.[139,140]

Once the titanium is surface-bound through N*, it is plausible that further hydrogen-transfer/ligand-exchange reactions could lead to the formation of complex Ti−N bonding-networks. Such networks are suggested by the crystal structure of TiN, where titanium is coordinated to six nitrogens. Specifically, a dimethylamido ligand on titanium can undergo a hydrogen-transfer reaction with its neighboring unreacted NH_2* fragments (Reaction T6, Figure 7) through concerted hydrogen-transfer/ligand-exchange. This transformation, which is similar to the initial TDMAT attachment step, adds another tethering site for titanium to bind to the surface. This second N-ligand-exchange with titanium has a barrier of 19.3 kcal/mol and is endothermic by 4.4 kcal/mol with a thermodynamic driving-force via release of the gaseous dimethylamine. Similar to Reaction T5, formation of N−H H-bonds in the

reactant and TS structures facilitates proton transfer from NH_2* to $N(CH_3)_2$ ligand in a dissociative concerted mechanism. After completion of proton transfer, a new bond between Ti and N* starts to form while breaking the Ti dimethylamine bond, resulting in a five coordinated titanium center before desorption of dimethylamine gas.

Although ligand-exchange pathways described so far have all been concerted, the formation of N*-bridged complex connecting two adjacent titanium species proceeds through a two-step process. The observation of a step-wise hydrogen transfer followed by ligand-exchange is likely a result of increasing steric demand of the incoming NH*. Nevertheless, the first step in this transformation is a hydrogen-transfer from NH* to the dimethylamido of titanium (Reaction T7-a, TS = 24.0 kcal/mol) resulting in a dimethylamine ligand on titanium (Reaction T7a, Figure S13b). The second step which is formation of Ti−N−Ti chain proceeds through a facile (Reaction T7-b, TS = 9.7 kcal/mol) associative ligand-exchange releasing the dimethylamine gas (Reaction T7b, Figure S13c).

iii. Second NH_3 cycle

The alternating cycles of the ALD process require a third step of NH_3 exposure. Through a transamination reaction, SE-GSM shows that the topmost fragments of the deposited layers and the incoming NH_3 react through a step-wise process with an activation energy of 29.9 kcal/mol (Reaction T8, Figure 9). Initially, hydrogen-transfer from NH_3* to one of the dimethylamido ligands of Ti results in a dimethylamine ligand and formation of NH_2*. This step is followed by addition of NH_2* to one of the Ti centers and cleavage of the Ti−$NH(CH_3)_2$ bond to replace a dimethylamido ligand with an amido group (Figure S14a). Similar to Reaction T5, networks of H-bonds stabilize NH_3 over surface during this reaction. Reaction T9 of Figure 9 is the final step in forming the third atomic layer, where a binding site for the incoming TDMAT of the fourth cycle is available. Hydrogen-transfer from the amido group to a dimethylamido ligand of a nearby Ti results in a bridged NH group and desorption of dimetylamine gas, with a barrier of 29.1 kcal/mol (Figure S14b).

These calculations suggest nucleation of the first Cu-N sites is rate-limiting. After this event, formation of H-bonds between ligands, moieties in the gas phase, and intramolecular H-bonds stabilize the various reactive intermediates and allow the deposition to proceed.

Overall, the computed activation barriers are feasible given the high temperature reaction conditions, but desorption of gaseous products is a necessary step for most of these reactions to be favorable thermodynamically.

CONCLUSIONS

Surface reactions cover an important branch of chemistry that contains a wide variety of interesting processes. In this area, GSM is found to be a powerful method for the study of reactions due to its accuracy, reliability, fast convergence, and relative ease of use. The four components for success, strategies for quickly approaching the vicinity of the saddle point, estimation of the direction of negative curvature, optimizer, and coordinate system, were carefully considered, and together integrated into GSM for surfaces to make a method that is highly proficient at reaction path finding.

GSM's efficacy was confirmed by comparison with CI-NEB on an extensive set of reactions characteristic of modern surface chemistry studies. In these cases, GSM reduces the computational cost (in terms of gradient computations) by about 45% on average over CI-NEB.

In addition to high efficiency, GSM has the advantage of operating in single-ended way to enable explorative study of chemical reactions. The strength of the SE-GSM for the study of novel reactions was demonstrated in this article via the first study of ALD of TiN on Cu(111), which provided a wealth of details about the operating mechanism for deposition. In the future, the use of a combinatorial set of driving coordinates in surface SE-GSM to guide a reaction to many different outcomes will be possible through systematic graphical methods.[50,51]

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APPENDIX

Hybrid coordinate system

The B matrix in primitive coordinates is formed using standard techniques[18]

$$B_{ij} = \frac{\partial q_i}{\partial x_j} \tag{6}$$

$$\Delta q = B\Delta X \tag{7}$$

where q are the primitive (hybrid) coordinates and X are Cartesians. The G matrix is formed and diagonalized as described below to produce a set of 3N non-redundant (linearly independent) vector space, U.

$$G = BB^{\top} \tag{8}$$

$$G(U \quad R) = (U \quad R)\begin{pmatrix} \Lambda & 0 \\ 0 & 0 \end{pmatrix} \tag{9}$$

The B matrix in non-redundant (NR) (hybrid) coordinates is formed based on

$$B^{NR} = U^{\top}B \ , \ U \in \mathbb{R}^{3N} \tag{10}$$

For the constraint optimization, the constraint vector, U_C, is formed by projecting the unit vector C corresponding to the constant primitive coordinates onto the full non-redundant subspace

$$U_C = \sum_{k=1}^{3N} \langle C|U_k\rangle U_k \tag{11}$$

The constraint vector, U_C, is normalized and the set V with 3N+1 vectors is formed by concatenating vectors U_k and the vector U_C

$$V = \{U_C, U_k; k = 1, \cdots, 3N\} \tag{12}$$

Schmidt orthonormalization is carried out to form a new set (V^*) with 3N-1 vectors U_k and the vector U_C

$$V_k^* = \alpha_k \left(V_k - \sum_{l=1}^{k-1} \langle V_k|V_l^*\rangle V_l^* \right) \tag{13}$$

where α_k is a normalization constant, V_k are the vectors from the set V, and vectors V_l^* compose the new orthonormal basis, V^*.[12,86]

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Hessian construction and update at each node

An initial diagonal Hessian in primitive coordinates is constructed from bonds, angles, and torsions and maintained to build a new non-redundant coordinates Hessian after each update and reparameterization step. This procedure is enforced because non-redundant coordinates change as reparameterization proceeds. The non-redundant coordinates Hessian, H, at each node is created by applying change of basis to the Hessian in primitive coordinates (H^{prim})

$$H = U^\top H^{prim} U \tag{14}$$

where U is the non-redundant coordinates matrix. Both Hessians are updated using the BFGS[106–109] scheme

$$\Delta H_{BFGS} = \frac{\Delta g \Delta g^\top}{\Delta g^\top \Delta x} - \frac{H_{i-1}\Delta x \Delta x^\top H_{i-1}}{\Delta x^\top H_{i-1} \Delta x} \tag{15}$$

where H_{i-1} is the Hessian of the previous step, and Δg and Δx are changes in current and previous gradient and coordinates, respectively. Note that Δg and Δx are in their respective non-redundant coordinate or primitive coordinate basis for each corresponding Hessian matrix.

Hessian construction and update at TS node

After completion of CI, the exact TS search starts by constructing a Hessian with desired eigenvalue structure from TS node's existing Hessian. The curvature, C, along the reaction path at the TS node is approximated using the two neighboring nodes to estimate the TS eigenvector[143]

$$C = \frac{2E_{TS-1}}{a(a+b)} - \frac{2E_{TS}}{ab} + \frac{2E_{TS+1}}{b(a+b)} \tag{16}$$

where E_{TS-1} and E_{TS+1} are the energies of the nodes prior to and following the TS node, E_{TS} is the energy of the TS node, a is the distance between the TS and the previous node, and b is the distance to the following node.

This modification is applied by subtracting the curvature along the reaction tangent from C, and multiplying it by a symmetric matrix with proper size, $U_C U_C^\top$,

$$\Delta H = \left(C - U_C^\top H U_C\right) U_C U_C^\top \tag{17}$$

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The new Hessian is updated using the Bofill[144] method, which allows negative eigenvalues

$$\Delta H_{Bofill} = \phi \Delta H_{MS} + (1-\phi)\Delta H_{PSB} \tag{18}$$

$$\Delta H_{MS} = \frac{(\Delta g - H_{i-1}\Delta x)(\Delta g - H_{i-1}\Delta x)^\top}{(\Delta g - H_{i-1}\Delta x)^\top \Delta x} \tag{19}$$

$$\Delta H_{PSB} = \frac{(\Delta g - H_{i-1}\Delta x)\Delta x^\top + \Delta x(\Delta g - H_{i-1}\Delta x)^\top}{\Delta x^\top \Delta x} - \frac{\Delta x^\top (\Delta g - H_{i-1}\Delta x)\Delta x \Delta x^\top}{(\Delta x \Delta x^\top)^2} \tag{20}$$

$$\phi = \frac{\left((\Delta g - H_{i-1}\Delta x)^\top \Delta x\right)^2}{|\Delta g - H_{i-1}\Delta x|^2 |\Delta x|^2} \tag{21}$$

where H_{i-1}, Δg, and Δx are the same variables as described for Equation (15).

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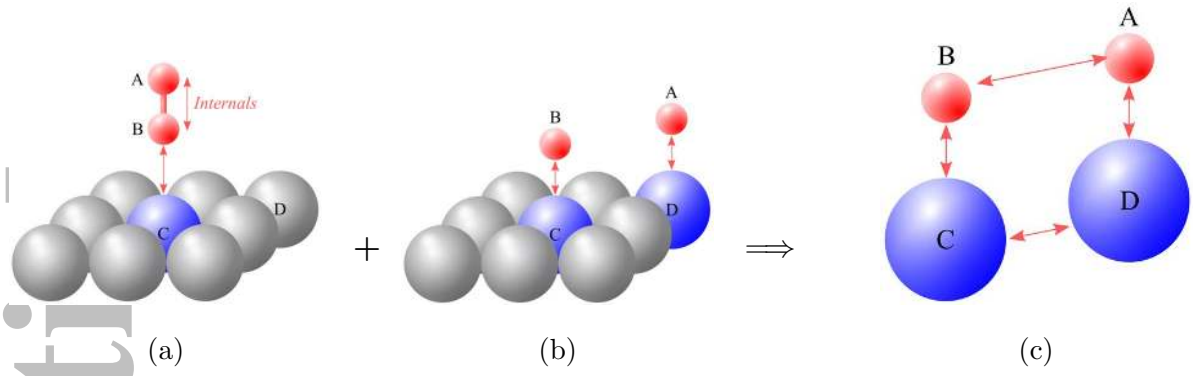


Figure 1: Illustration of the hybrid coordinate system for bonds. (a) ,(b), and (c) show bonds in reactant, product, and the union, respectively. Red and blue atoms indicate adsorbate and active surface species, respectively (red: IC only, blue: IC and Cartesians, grey: Cartesians only). Double arrows denote a bond between two atoms.

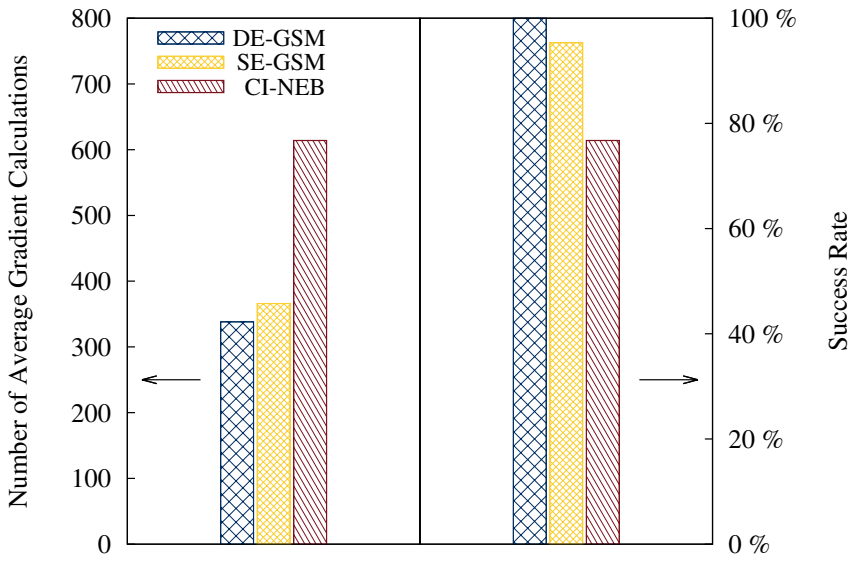


Figure 2: Average number of gradient calculations and success rate for each method. (Calculations with more than 1,800 gradient calculations are not included in the average gradient calculation).

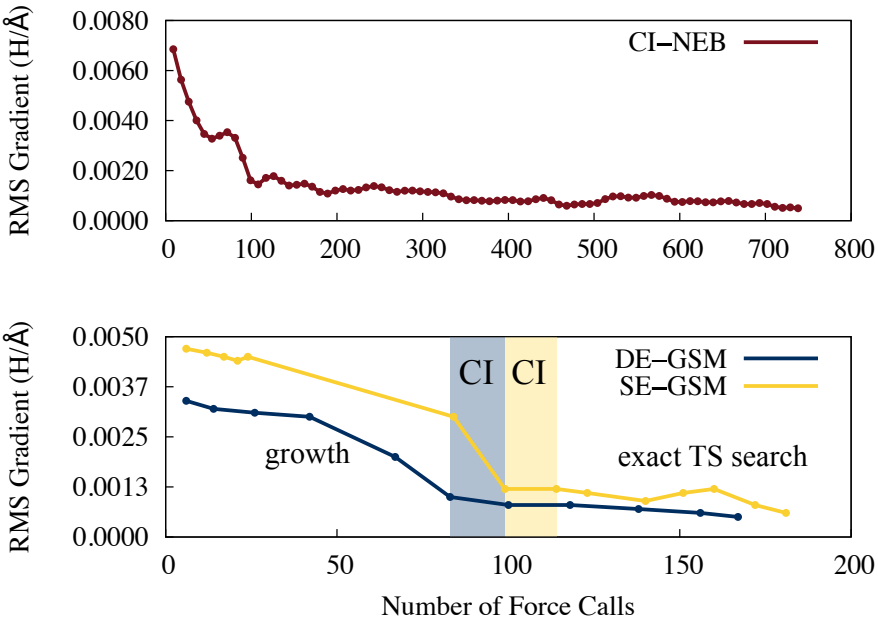


Figure 3: Convergence behavior of the methods plotted for reaction 8-b. CI-NEB has a higher initial RMS gradient compared to GSM in addition to larger RMSD of initial and final RPs, and therefore more force calls are required to reach convergence. The gradient calls required for each phase of GSM calculations are labeled in the bottom plot.

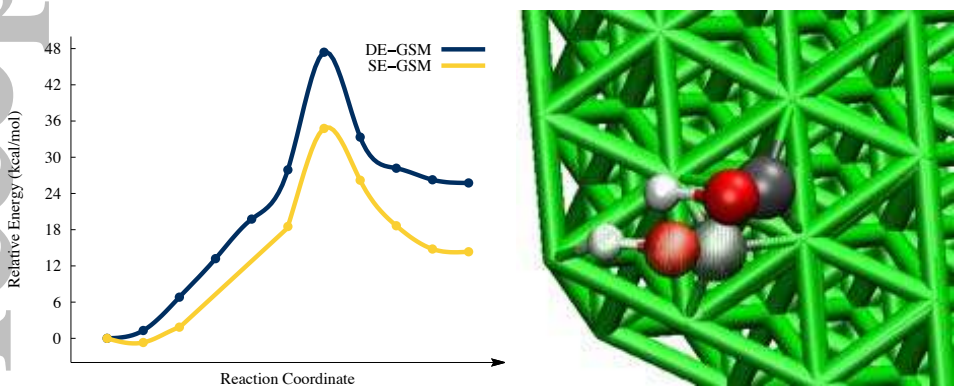
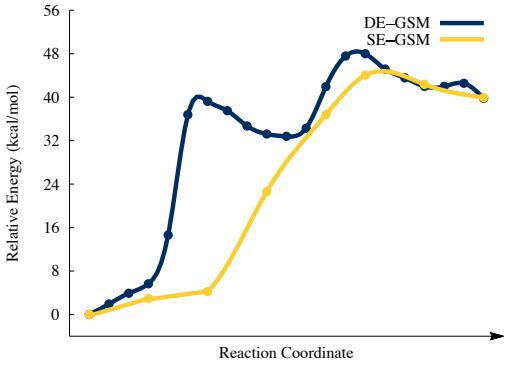
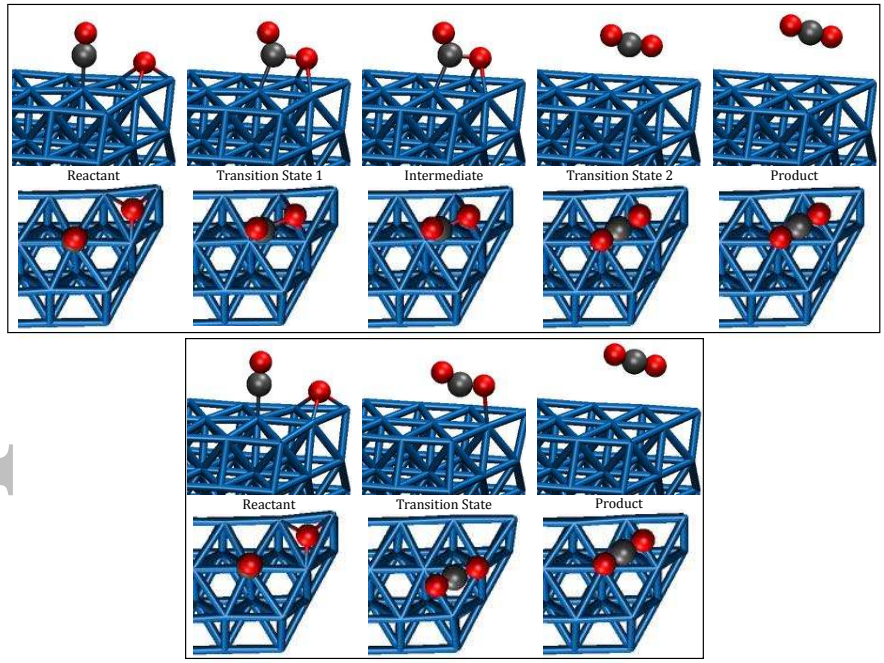


Figure 4: (a) Reaction path calculated by DE-GSM (blue) and SE-GSM (yellow) for COH formation on Ni(111). (b) TS structures calculated by DE-GSM (opaque) and SE-GSM (translucent). CO molecule is not stationary in the case of SE-GSM.



(a)



(b)

Figure 5: (a) Reaction path calculated by DE-GSM (blue) and SE-GSM (yellow) for CO_2 formation on Ru(0001). (b) Reactant, TS, and product structures for reaction (4) calculated by DE-GSM (top) and SE-GSM (bottom). Reaction proceeds in one and two elementary steps via SE-GSM and DE-GSM, respectively.

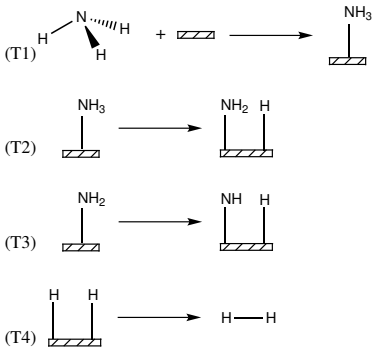


Figure 6: Proposed network of reactions for dehydrogenation of NH_3 on Cu(111).

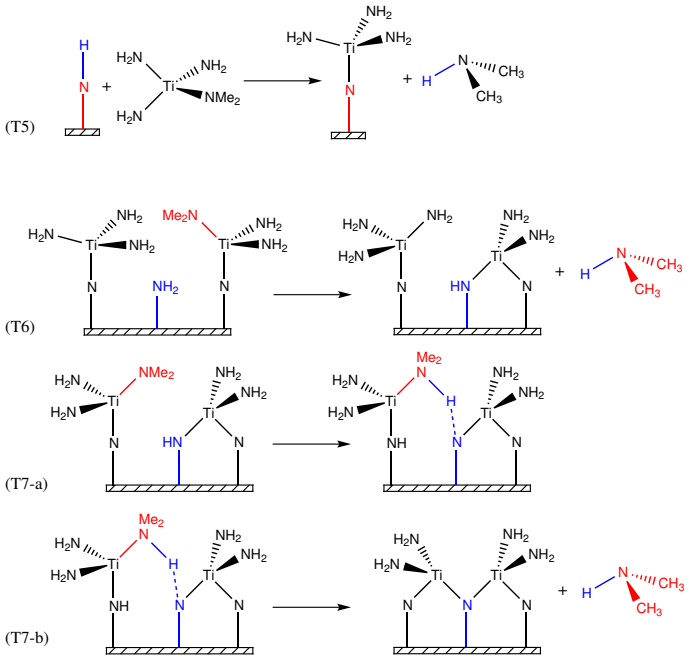


Figure 7: Proposed reactions during first TDMAT cycle.

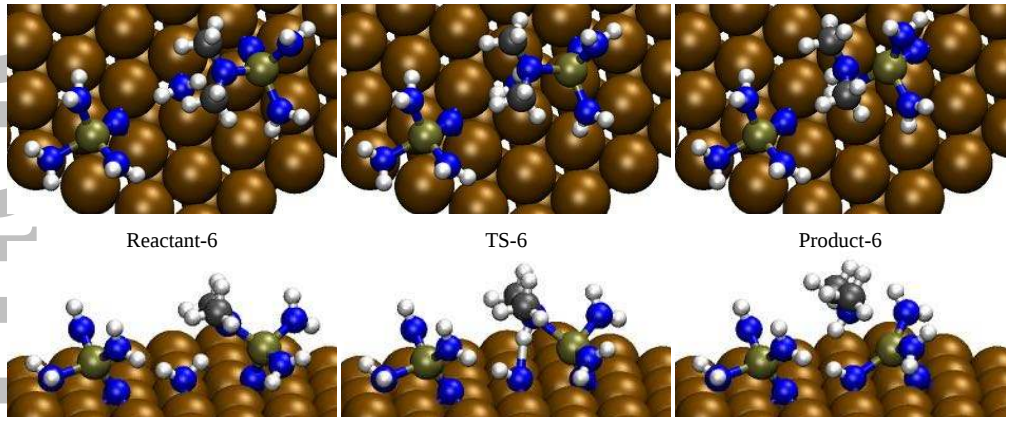


Figure 8: Reactants, TS, and products of Reaction (T6). After adsorption of two TDMAT molecules on surface, they connect by a bridging N* that comes from an NH_2 species adsorbed on surface. In this reaction, one of the adsorbed tris(dimethylamido)titanium species reacts with NH_2*. Atoms are N (blue), H (white), C (gray), Ti (tan green), and Cu (ochre).

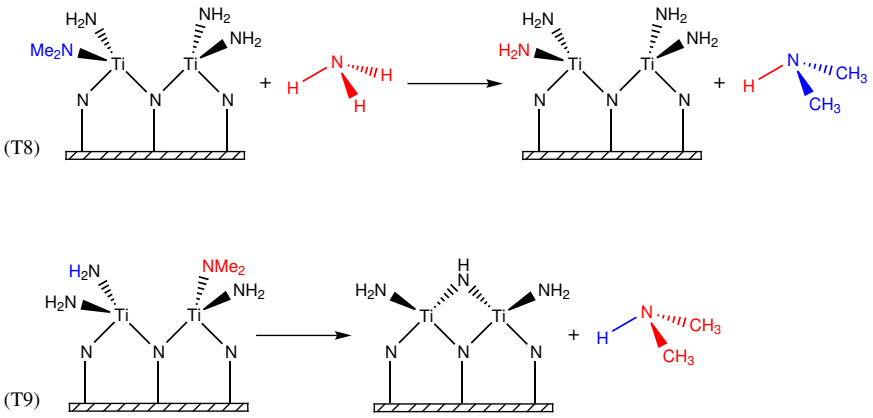


Figure 9: Second NH_3 cycle.

ID	Reaction	ID	Reaction
1	$Au(fcc) \xrightarrow{Pt(111)} Au(hcp)$	11-a	$OH^* + H^* \xrightarrow{Cu(100)} H_2O^*$
2	$CO(fcc) \xrightarrow{Pd(111)} CO(hcp)$	11-b	$CO^* + O^* \xrightarrow{Cu(100)} CO_2{}^*$
3-a	$CO + O \xrightarrow{Pd(111)} CO_2{}^*$	12-a	$OH^* + H^* \xrightarrow{Cu(111)} H_2O^*$
3-b	$CO_2{}^* \xrightarrow{Pd(111)} CO_2(g)$	12-b	$CO^* + O^* \xrightarrow{Cu(111)} CO_2{}^*$
4-a	$CO + O \xrightarrow{Ru(0001)} CO_2{}^*$	13-a	$OH^* + H^* \xrightarrow{Cu(110)} H_2O^*$
4-b	$CO_2{}^* \xrightarrow{Ru(0001)} CO_2(g)$	13-b	$CO^* + O^* \xrightarrow{Cu(110)} CO_2{}^*$
5-a	$H(fcc) \xrightarrow{Ni(111)} H(fcc)$	14-a	$H_2S^* \xrightarrow{W(111)} HS^* + H^*$
5-b	$H(fcc) \xrightarrow{Ni(111)} H(hcp)$	14-b	$HS^* \xrightarrow{W(111)} S^* + H^*$
5-c	$H(hcp) \xrightarrow{Ni(111)} H(fcc)$	14-c	$H^* + H^* \xrightarrow{W(111)} H_2(g)$
6-a	$Cu(bridge) \xrightarrow{Cu(110)} Cu(hollow)$	15-a	$H_2O^* \xrightarrow{W(111)} HO^* + H^*$
6-b	$Cu(hollow) \xrightarrow{Cu(110)} Cu(hollow)$	15-b	$HO^* \xrightarrow{W(111)} O^* + H^*$
6-c	$Cu \xrightarrow{Cu(110)} Cu(atom\ swap)$	16-a	$CH_2{=}CHCH_2OH^* + O^* \xrightarrow{Au(111)} CH_2{=}CHCH_2O^* + OH^*$
7-a	$CH_3CH_2COOH^* \xrightarrow{Pd(111)} CH_3CH_2CO^* + OH^*$	16-b	$CH_2{=}CHCH_2O^* + O^* \xrightarrow{Au(111)} CH_2{=}CHCH{=}O^* + OH^*$
7-b	$CH_3CH_2CO^* \xrightarrow{Pd(111)} CH_3CH_2{}^* + CO^*$	17-a	$CH_3OH^* \xrightarrow{Cu(110)} CH_3O^* + H^*$
8-a	$CH_2CH_2{}^* + H^* \xrightarrow{Pd(111)} CH_3CH_2{}^*$	17-b	$CH_3O^* \xrightarrow{Cu(110)} H_3C{=}O^* + H^*$
8-b	$CH_3CH_2{}^* + H^* \xrightarrow{Pd(111)} CH_3CH_3{}^*$	18-a	$CN^* + H^* \xrightarrow{Pt(111)} CNH^*$
9-a	$NH_3{}^* \xrightarrow{RuO_2(110)} NH_2{}^* + H^*$	18-b	$CNH^* + H^* \xrightarrow{Pt(111)} CNH_2{}^*$
9-b	$NH_2{}^* \xrightarrow{RuO_2(110)} NH^* + H^*$	19-a	$NH_3(g) \xrightarrow{Si(111)-Cl} NH_3{}^*$
9-c	$2\,N^* \xrightarrow{RuO_2(110)} N_2{}^*$	19-b	$NH_3{}^* \xrightarrow{Si(111)-Cl} NH_2{}^* + HCl(g)$
9-d	$N^* + O^* \xrightarrow{RuO_2(110)} NO^*$	20	$H_2O(g) \xrightarrow{Si(111)-H} OH^* + H_2(g)$
10-a	$CO^* + H^* \xrightarrow{Ni(111)} COH^*$	21	$CH_4(g) \xrightarrow{Ir(111)} CH_3{}^* + H^*$
10-b	$COH^* + H^* \xrightarrow{Ni(111)} C^* + H_2O(g)$		

Table 1: Elementary step test cases for GSM. Asterisks designate the surface species.

		DE-GSM		SE-GSM	
Bonds (Å) & angle	Reactant	Transition State	Product	Transition State	Product
C5-Ni1	2.037	1.965	1.892	1.940	1.884
C5-Ni2	2.082	1.939	1.949	3.287	3.187
C5-Ni3	1.856	1.800	1.803	1.870	1.849
C5-Ni4	3.114	2.974	2.991	1.880	1.863
C5-O6	1.189	1.273	1.339	1.280	1.348
O6-H7	3.557	1.349	0.981	1.311	0.983
∠C5-O6-H7	60.3	88.2	111.0	96.7	107.3

Table 2: Bond lengths and angles for the reactant, TSs, and products of Reaction 10-a calculated by DE-GSM and SE-GSM. Colored values indicate bonds and angles that are different in structures calculated by the methods. Both methods result in the same product while the product's position on the surface is different.

ID	E_a (kcal/mol)	$\Delta E_{reaction}$ (kcal/mol)
T1	-	-10.6
T2	31.4	16.8
T3	30.5	27.6
T4	22.6	5.4
T5	7.9	-13.5
T6	19.3	4.4
T7-a	24.0	22.8
T7-b	9.7	8.9
T8	29.9	10.0
T9	29.1	20.2

Table 3: Activation energies and heat of reactions for the elementary steps of ALD of TiN on Cu(111).

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SUPPORTING INFORMATION

Table of Contents

1 Additional Computational Details

The computational details for GSM are similar to those described in previous GSM papers.[50,51,86] There are slight differences in the convergence criteria for single-ended and double-ended GSMs during the growth phase. During the growth phase of SE-GSM, new nodes are optimized until the root mean square (RMS) gradient is below 10 times the convergence threshold (0.005 Hartree/Å), or 30 steps. In this method, the number of nodes is not specified in the input and is actively determined during the growth phase, so two criteria are used to determine whether to continue growing: (1) the frontier node is lower in energy than the previous node (by a threshold value), or (2) the frontier node's constraint gradient is positive. In DE-GSM, at most two nodes can be added during the growth phase, and each node undergoes two optimization steps per optimization iteration. The new nodes are added only when the perpendicular gradient magnitudes on the frontier nodes fall below 0.1 Hartree/Å. For double-ended methods (DE-GSM & CI-NEB), the number of nodes is predefined as part of the input parameters.

In both single-ended and double-ended GSM, the CI search commences after the sum of the perpendicular gradient magnitudes over all nodes, F, is converged to $F < 0.3$ Hartree/Å . The reaction path is considered converged when RMS gradient on the TS node is below 0.0005 Hartree/Å. The exact TS search is initiated when one of the three sets of conditions is met:

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1.) the total gradient is < 0.2 Hartree/Å, the TS node is converged to within 10 times the nodal convergence tolerance, and the constraint force is < 0.01 Hartree/Å, 2.) the total gradient is < 0.1 Hartree/Å, the TS node is converged to within 10 times the convergence tolerance and the constraint force is < 0.02 Hartree/Å, or 3.) the TS node is within five times the convergence tolerance. In SE-GSM, after completion of the exact TS search and string convergence, the last node on the string which is the predicted reaction product is optimized in all directions (without constraint) to a local minimum.

2 DE-GSM vs. CI-NEB RPs

RPs for Reaction 6-c is shown in Figure S5c in detail. As shown in the snapshots (4) to (8), the two swapping Cu atoms collide on the interpolated path which leads to CI-NEB's failure immediately after the initial interpolation for placing the nodes. This issue arises from linear interpolation in Cartesians and CI-NEB's strategy in node placement while the growing nature of DE-GSM prevents this problem. In the path calculated by DE-GSM (Figure S5b) the top left translucent Cu atom passes over the other moving Cu atom and avoids collision.

Similar to Reaction 6-c, Reaction 6-b has a problem with the initial interpolation in NEB, as shown in Figure S4c. Here, a Cu atom moves from within the surface to a hollow site on the top layer. Instead of moving upward then sideways, NEB's interpolation places the Cu atom between two surface Cu atoms, resulting in a problematic initial RP that never recovers to reach a realistic path. Specifically, optimization from this initial condition leads to deformation of the slab (Figure S4b, snapshots (3) and (5)), which is not desired or required for this reaction. Improvements to the interpolation algorithm in NEB, for instance linear and quadratic synchronous transit,[55,78,145] may be able to remedy these issues. DE-GSM, however, takes advantage of curvilinear interpolation for placing nodes and incremental node addition, and is able to refine path 6-c without a challenge (Figure S4a).

In Figure S3, the maximum difference in activation energies occurs for water dissociation on W(111) (15-a), which differs by 4.6 kcal/mol between DE-GSM and CI-NEB. To understand why the barriers are so different, the corresponding RPs are shown in Figure

S6b and the TS structures quantitatively compared in Table S2. While many aspects of the O−H dissociation are similar between DE-GSM and CI-NEB, two unique reaction paths were found. One proceeds by directly moving the transferring hydrogen to its final binding site and the other moves hydrogen in a half-circle before reaching its final location. The disagreement in activation barriers between DE-GSM and CI-NEB, therefore, is not due to failure of either method. In general, there is no guarantee that double-ended methods will converge to the same RP and TS, though it appears to be a relatively infrequent event in our test set.

A representative example of reactions that proceed through very different pathways when calculated by DE-GSM or CI-NEB is reaction 5-b (H diffusion in Ni(111) from fcc site to second layer) which is an example of hydrogen embrittlement in metals (Figure S7). Fracturing in metals due to hydrogen adsorption and then its diffusion into the bulk material is particularly important in high strength steels and nickel fabrication[146]. In this reaction, DE-GSM finds a path that involves diffusion of the H atom first directly into the surface (Figure S7b, snapshots (1) to (6)), and then its migration from fcc to hcp site underneath the top slab layer. The calculated TS for this reaction has an activation energy of 18.5 kcal/mol. The path calculated by CI-NEB first moves the H atom from fcc to hcp site over the top slab layer and then moves it in between the first and second layers to end up at the same product structure as DE-GSM. In cases with two distinct RPs from different methods, increasing the number of nodes in order to achieve a more converged path did not result in similar paths or activation barriers.

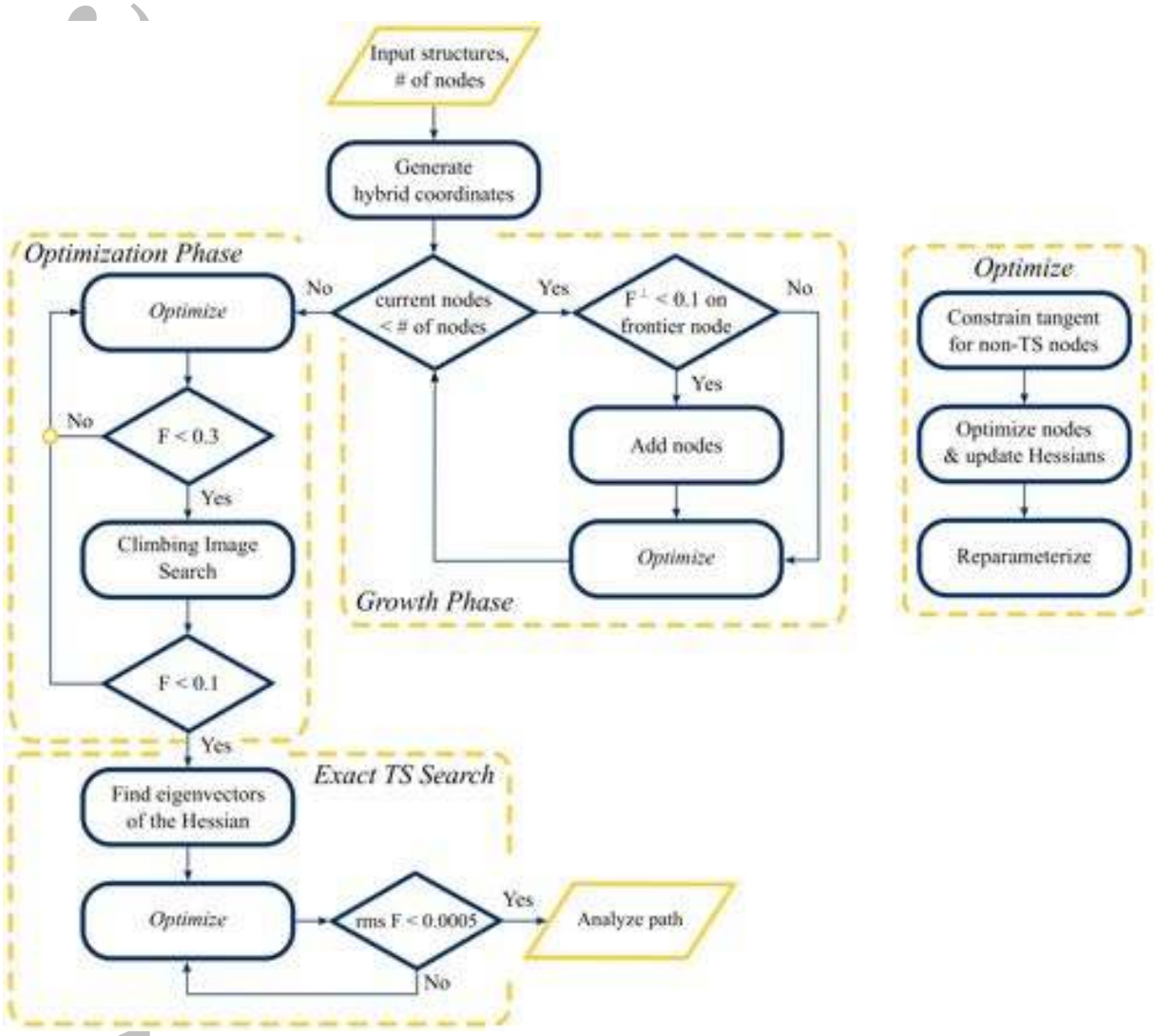


Figure S1: Process flow for DE-GSM.

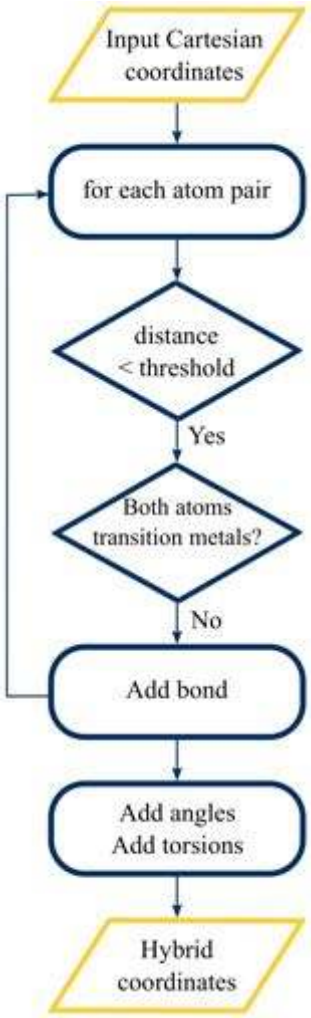


Figure S2: Process flow for generation of hybrid coordinate system. Threshold value is determined based on atomic radii of atoms.

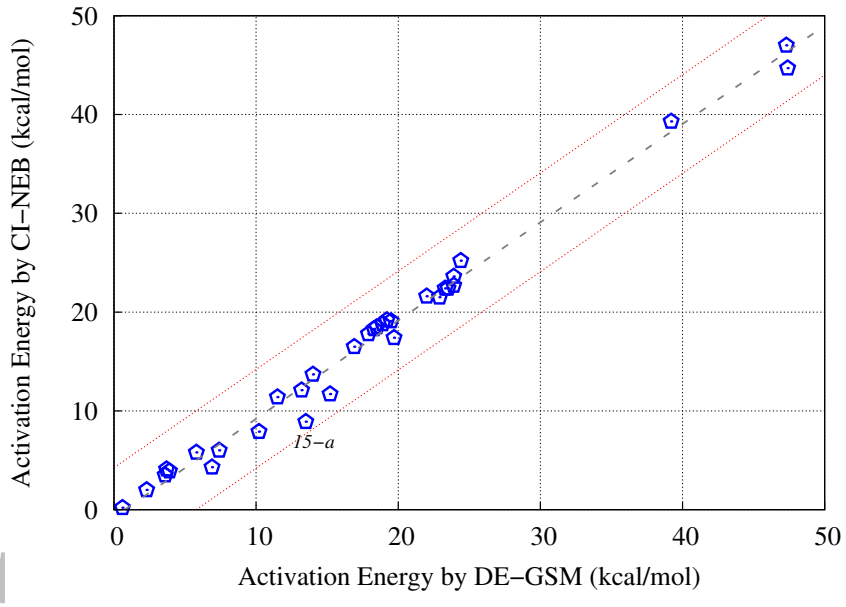
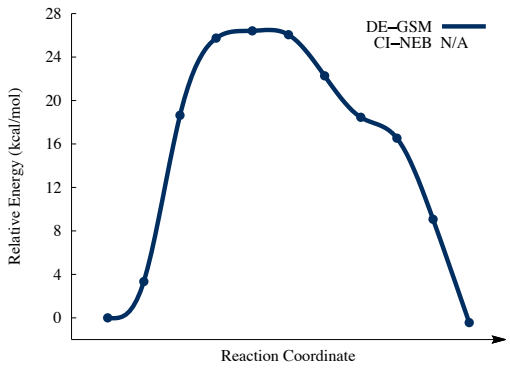
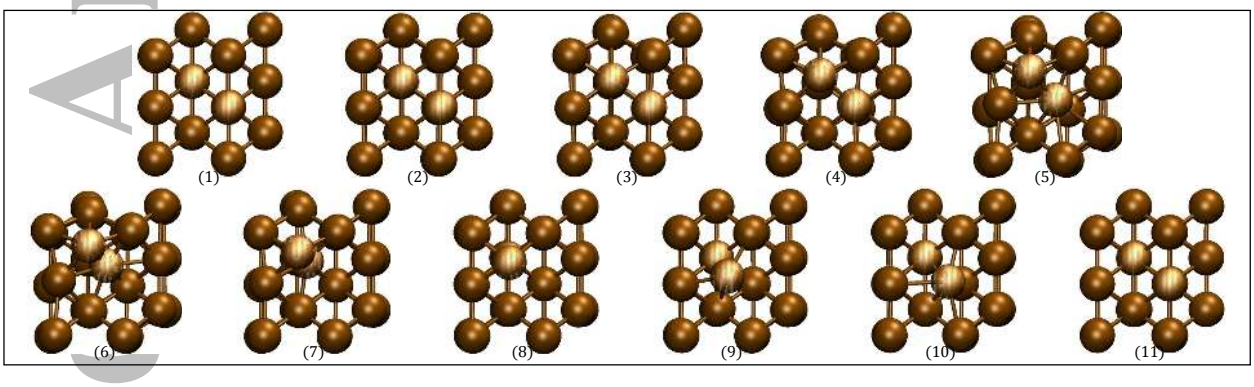


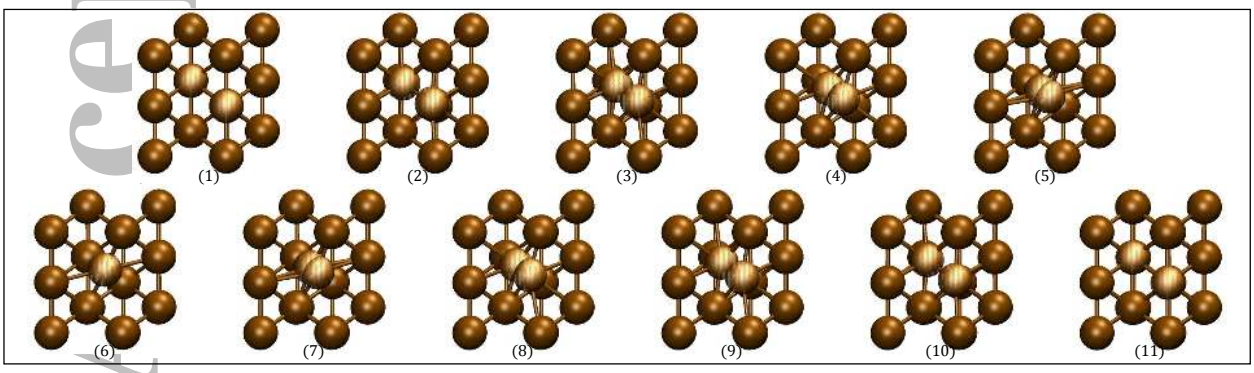
Figure S3: Comparison of the activation energies calculated by DE-GSM and CI-NEB methods. The area between the two dotted red lines confines ±5 kcal/mol deviation from the best fitted line ($R^2 = 0.989$ and $y = 0.995x - 0.75$).



(a) Reaction path calculated by DE-GSM (blue) for Cu atoms swapping on Cu(110).

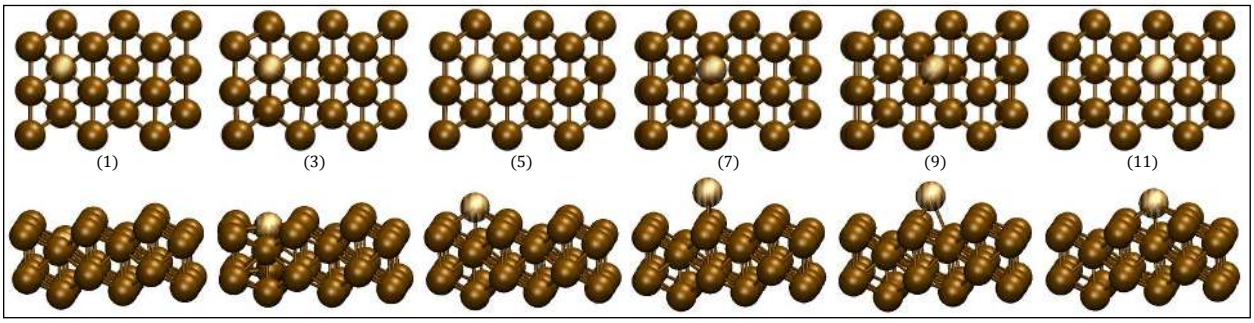


(b) Snapshots of Cu atoms swapping on Cu(110) calculated by DE-GSM. Number 5 is the transition state. The top left translucent atom moves over the other atom during the reaction.

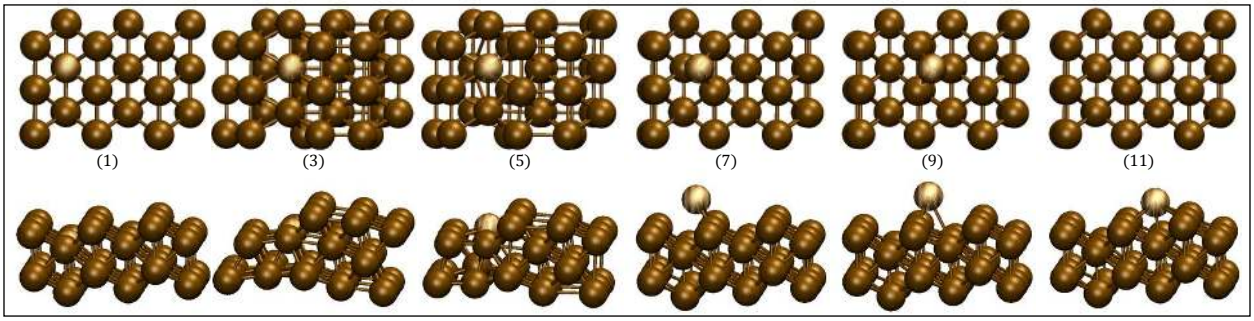


(c) Snapshots of Cu atoms swapping on Cu(110) calculated by CI-NEB. Calculation fails immediately after the initial interpolation due to the collision of the Cu atoms (image number (6)).

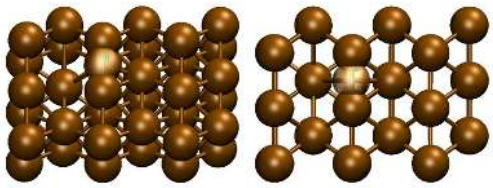
Figure S5: Reaction 6-c. Reaction paths for swapping of Cu atoms on Cu(110).



(a) Snapshots of a Cu atom moving on Cu(110) calculated by DE-GSM. Number 5 is the TS.

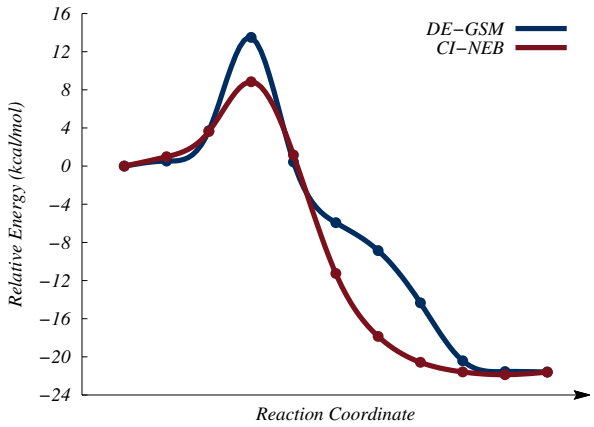


(b) Snapshots of a Cu atom moving on Cu(110) calculated by CI-NEB. The calculated path involves deformation of the slab.

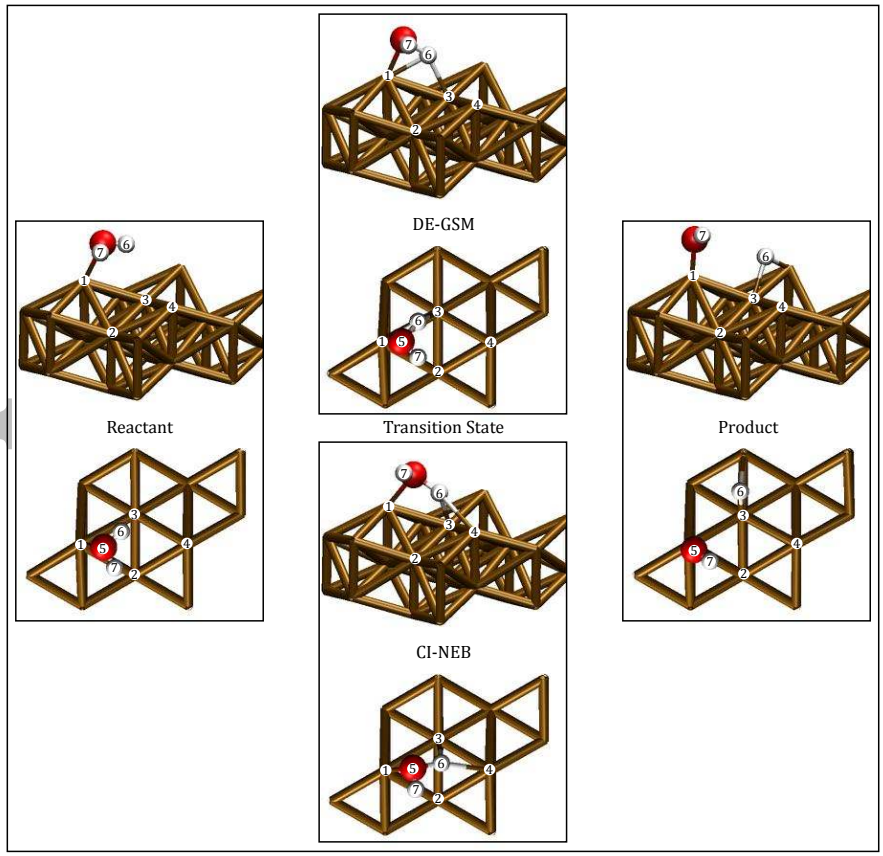


(c) Moving Cu atom intersects the bond between two other surface atoms in predicted TS along the initial interpolated path by CI-NEB.

Figure S4: Reaction 6-b. Reaction paths for a Cu atom diffusing to a hollow site on Cu(110).

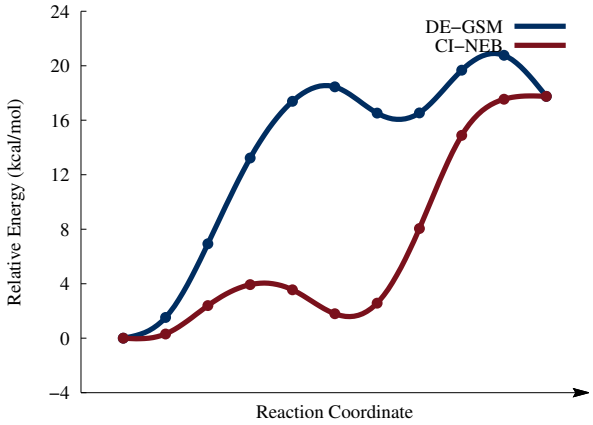


(a) Reaction paths calculated by DE-GSM (blue) and CI-NEB (red) for dissociation of H_2O atom on W(111).

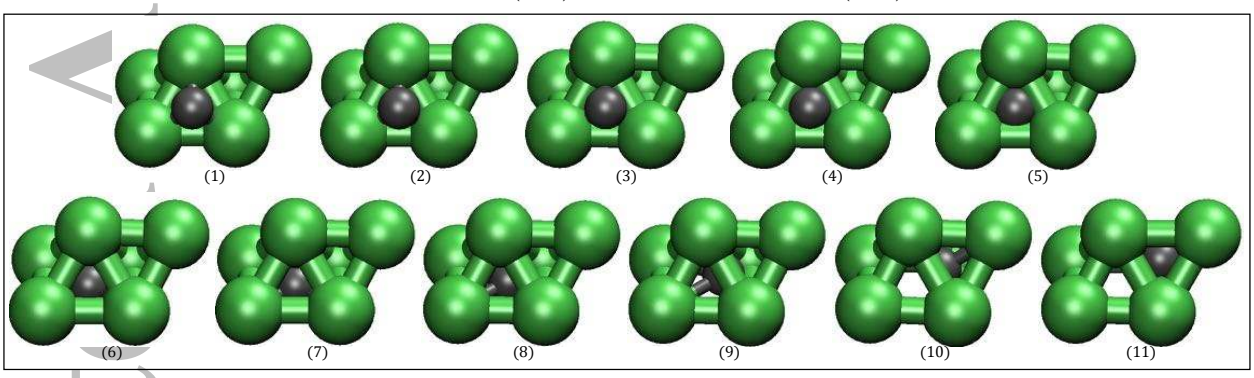


(b) Reactant, TS, and product structures for reaction 15-a calculated by DE-GSM (top) and CI-NEB (bottom).

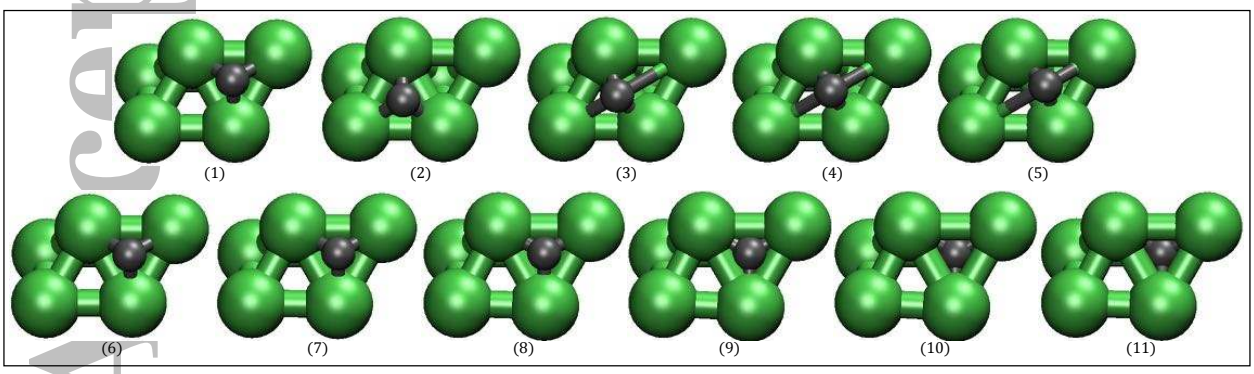
Figure S6: Reaction paths for dissociation of H_2O on W(111).



(a) Reaction paths calculated by DE-GSM (blue) and CI-NEB (red) for H diffusion in Ni(111).



(b) Snapshots of H (gray) diffusion in Ni(111) calculated by DE-GSM. There is a TS for diffusing from fcc to hcp site and another TS (node number 10) for diffusion beneath the first latyer.



(c) Snapshots of H (gray) diffusion in Ni(111) calculated by CI-NEB. The H atom first diffuses on the surface and there is no barrier for diffusion from hcp site to the layer below.

Figure S7: Reaction 5-b. Reaction paths for diffusion of H atom in Ni(111).

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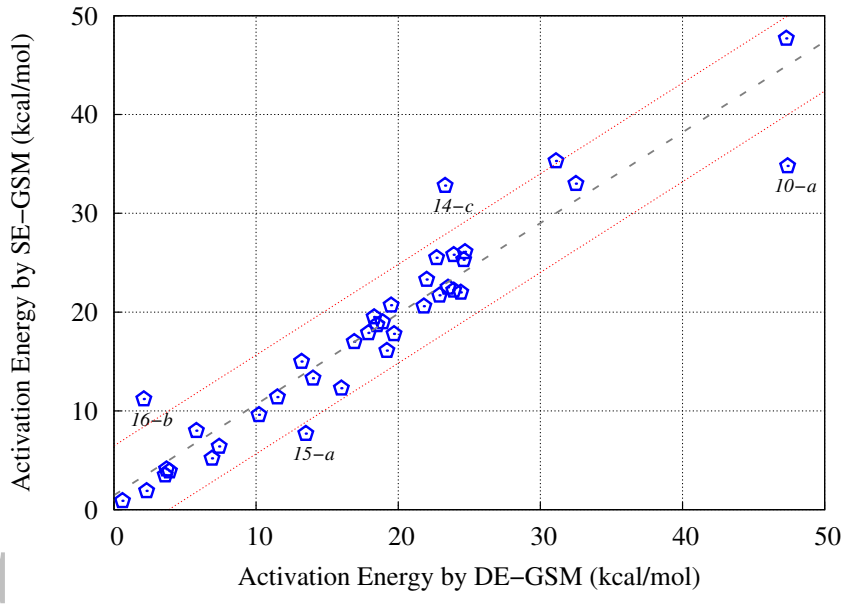

Figure S8: Comparison of the activation energies calculated by DE-GSM and SE-GSM methods. The area between the two dotted red lines confines ±5 kcal/mol deviation from the best fitted line ($R^2 = 0.875$ and $y = 0.899x + 1.92$).

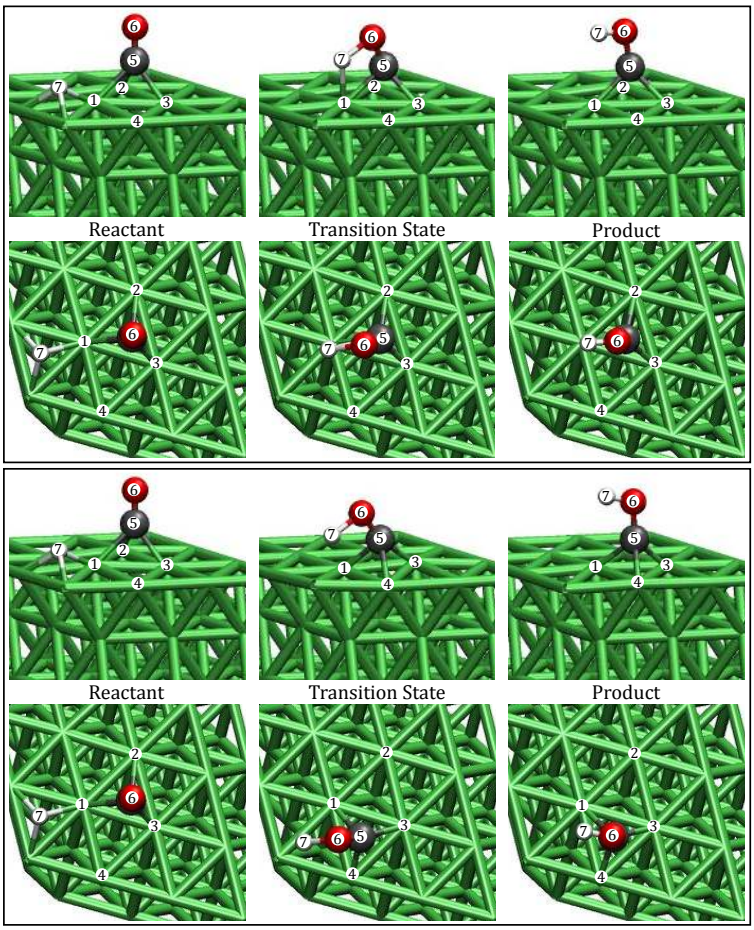

Figure S9: Reactant, TS, and product structures for reaction (10-a) calculated by DE-GSM (top) and SE-GSM (bottom). The CO molecule is not stationary in the case of SE-GSM.

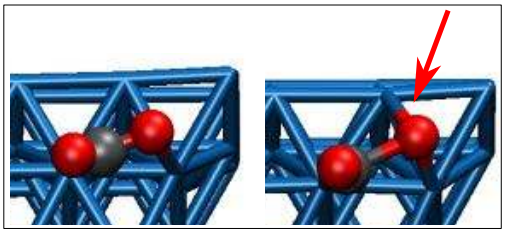

Figure S10: Complexes formed right before TS for SE-GSM (left) and DE-GSM (right). Note the asymmetric bond cleavage in SE-GSM case.

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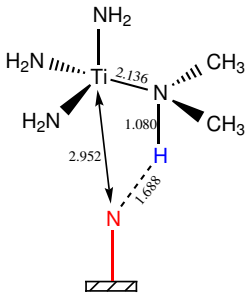

Figure S11: TS structure of reaction T5. Bond lengths are in Ångstroms.

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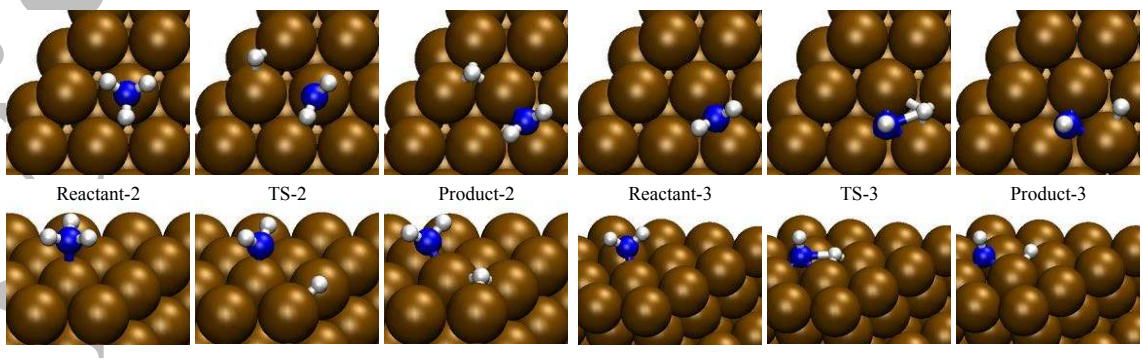
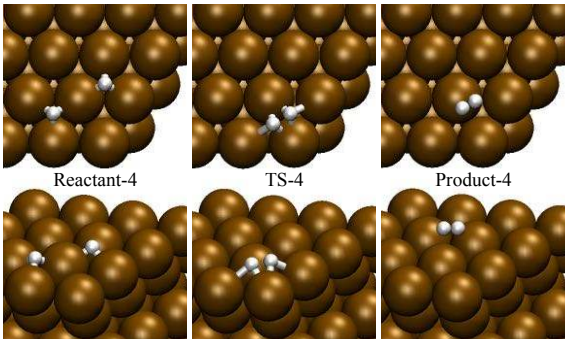


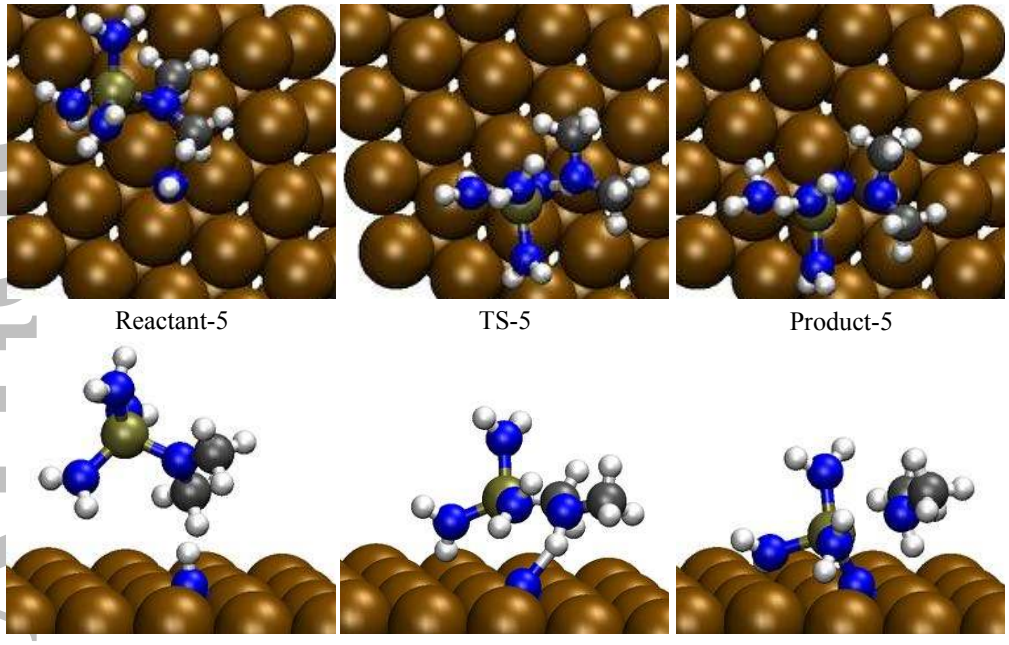
(a) Reaction-T2. Dissociation of NH_3.

(b) Reaction-T3. Dissociation of NH_2 to NH and H.

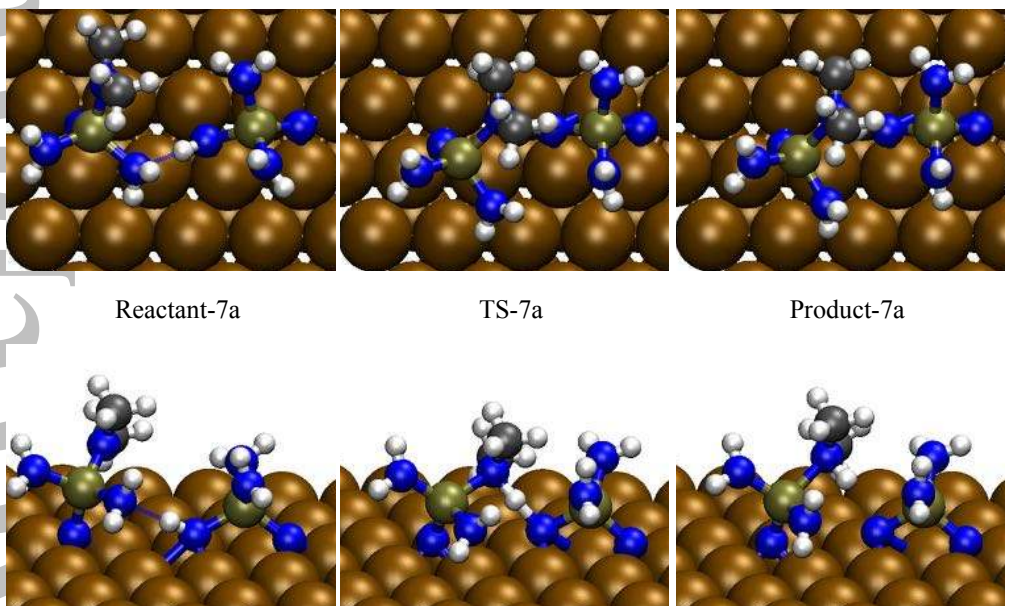


(c) Reaction-T4. Formation of H_2 from two H atoms.

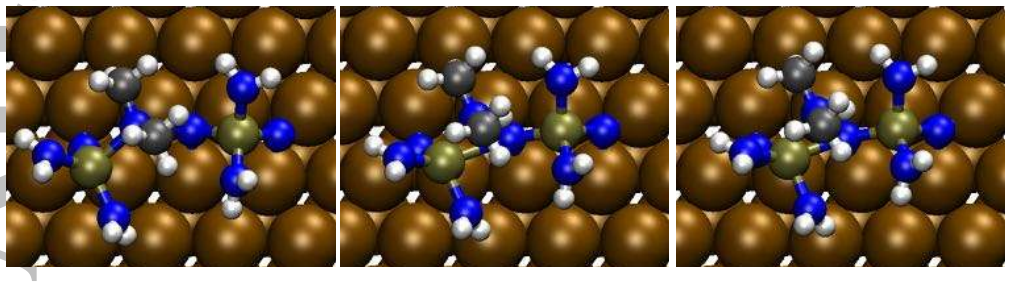
Figure S12: Reactants, TSs, and products of the first deposition cycle. Atoms are N (blue), H (white), C (gray), Ti (tan green), and Cu (ochre).



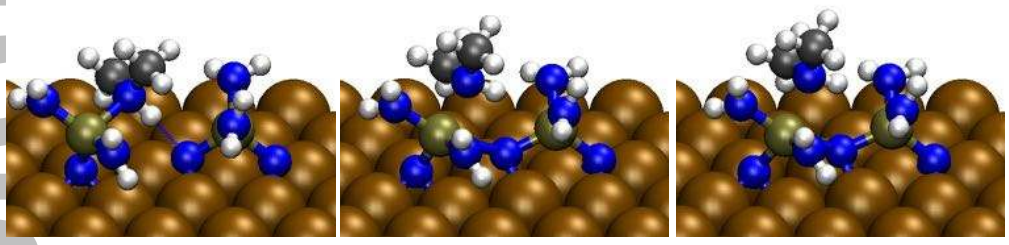
(a) Reaction-T5. Adsorption of first TDMAT molecule on the surface through ligand-exchange with NH*.



(b) Reaction-T7a. Following reaction T6, the second tris(dimethylamido)titanium species reacts with the remaining H on N to form a new atomic layer. This reaction takes place in two steps, the first step which is reaction (T7-a) proceeds through a hydrogen-transfer from NH_2* to dimethylamido ligand.

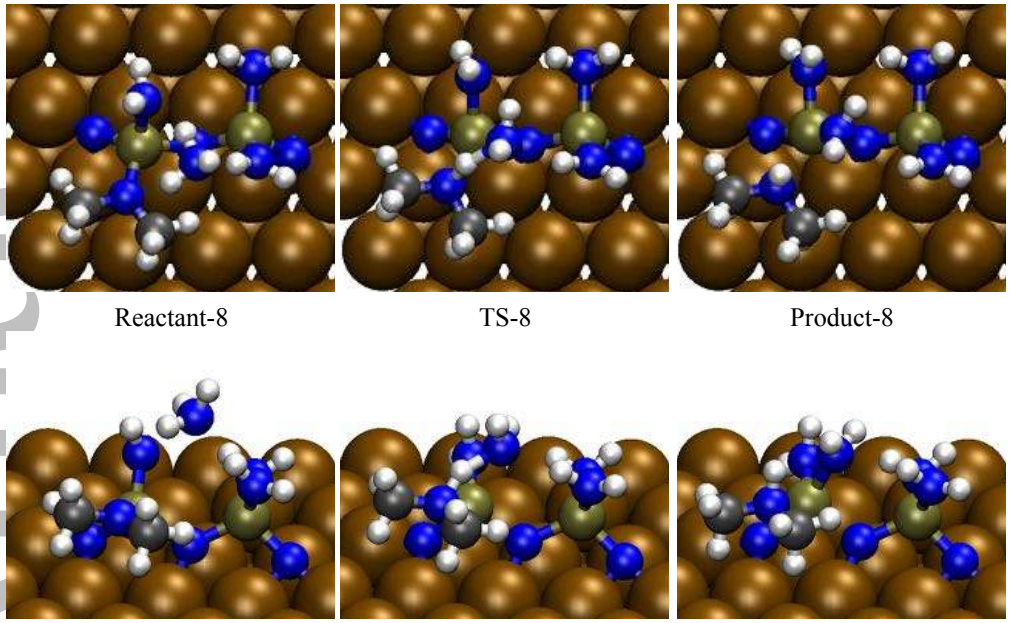


Reactant-7b TS-7b Product-7b

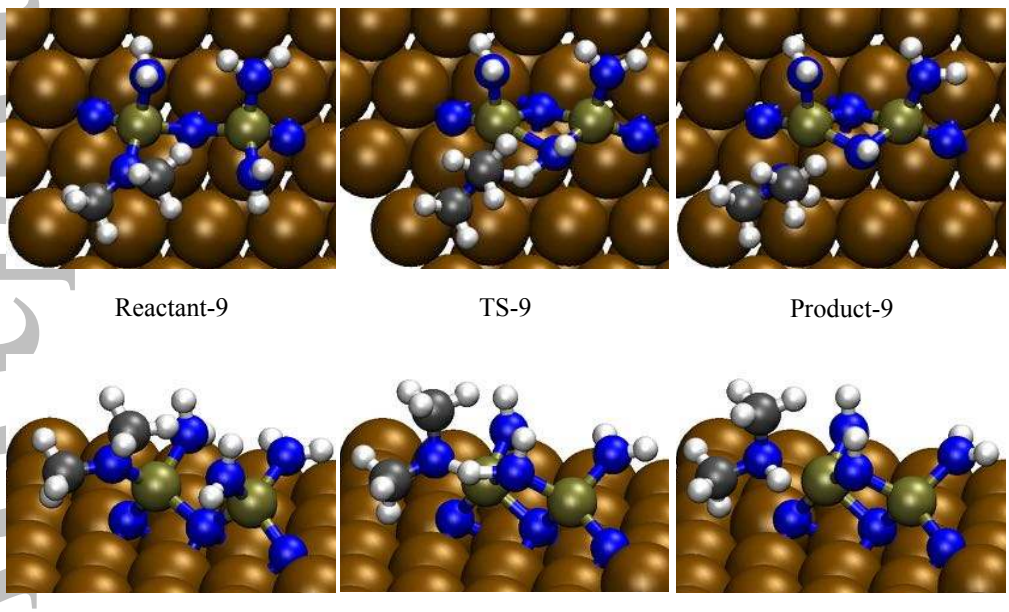


(c) Reaction-7b. In the second step of reaction (T7), dimethylamine desorbs from the surface while the second Ti connects to N* in an associative ligand-exchange reaction.

Figure S13: Reactants, TSs, and products of the second deposition cycle. Atoms are N (blue), H (white), C (gray), Ti (tan green), and Cu (ochre).

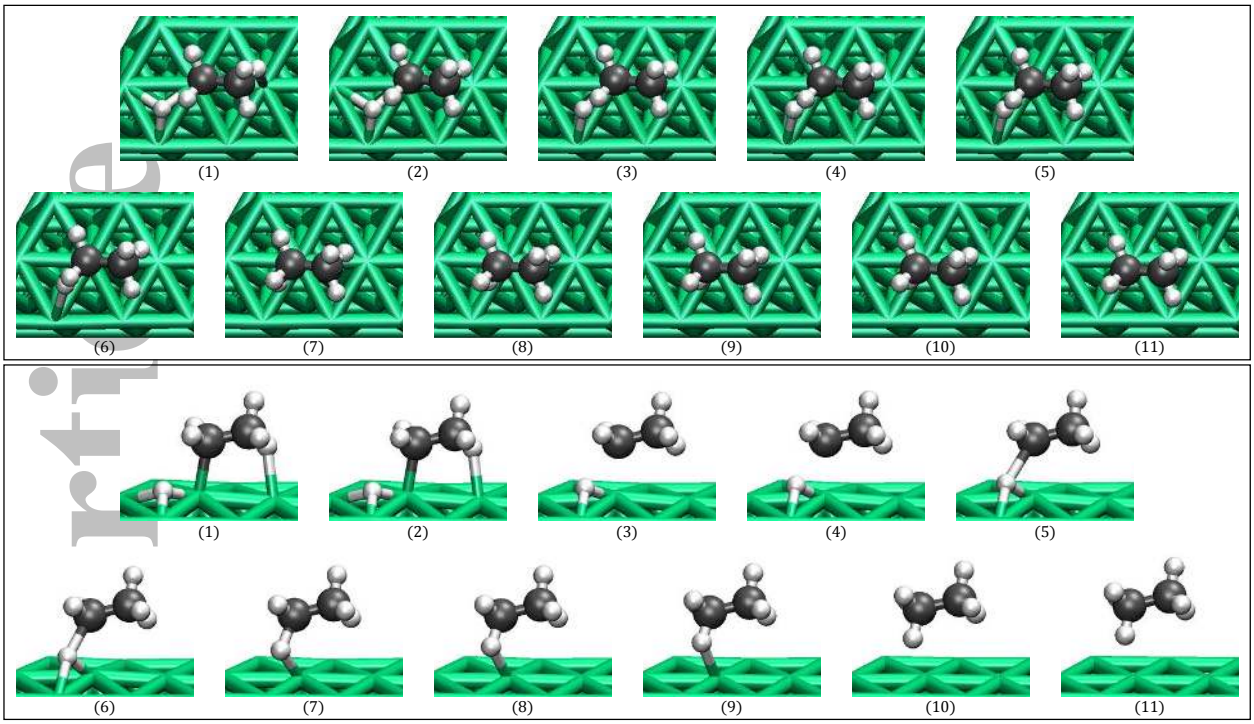


(a) Reaction-8. Hydrogen-transfer occurs between NH_3* and dimethylamido ligand of titanium while NH_2* connects to titanium through an associative process.

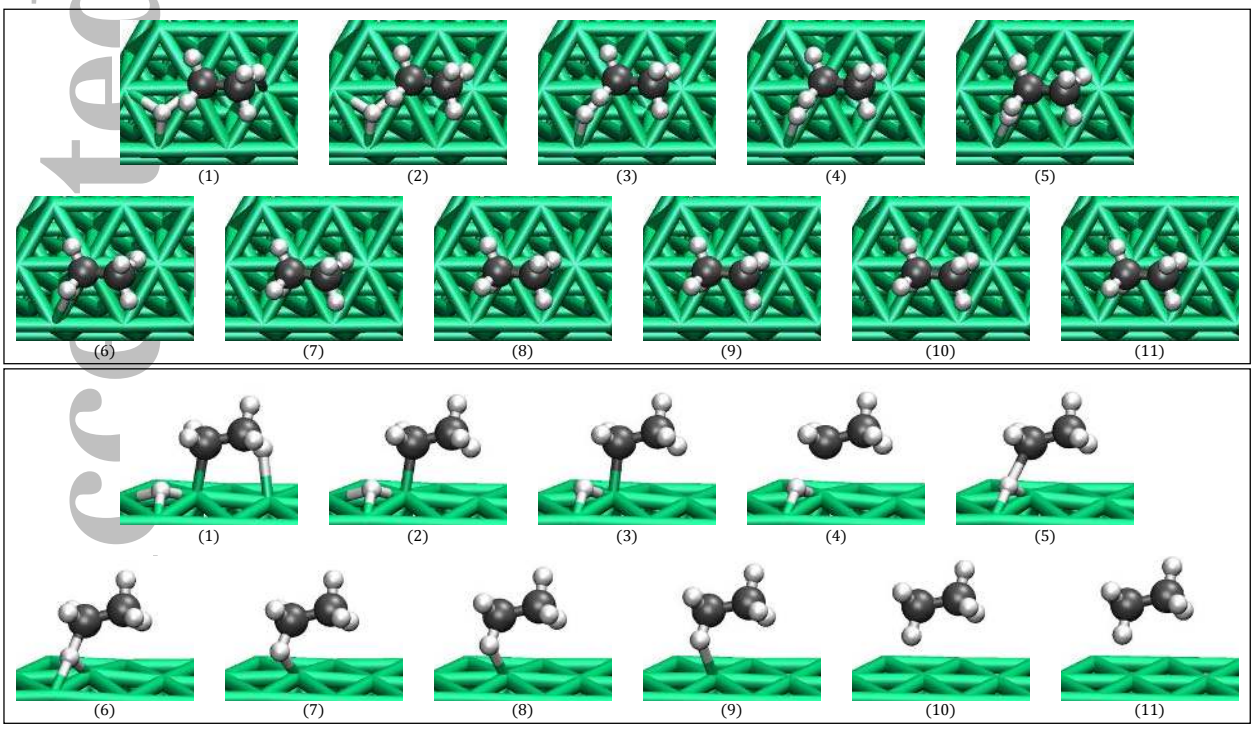


(b) Reaction-9. In this reaction, dimethylamido of one species reacts with amido of a nearby fragment which was replaced in reaction T8. The third atomic layer is formed and dimethylamine is released. The bridging NH can act as a binding site for the incoming TDMAT in the next TDMAT cycle.

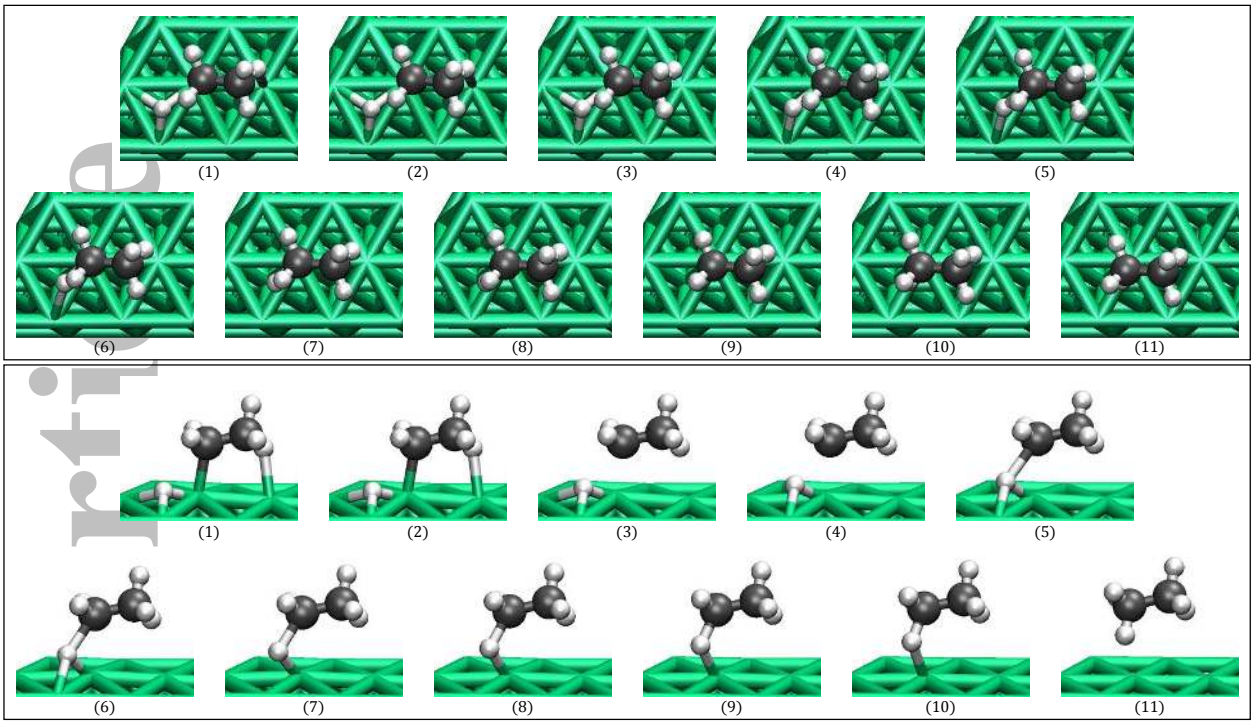
Figure S14: Reaction paths for ALD of TiN on Cu(111). Atoms are N (blue), H (white), C (gray), Ti (tan green), and Cu (ochre).



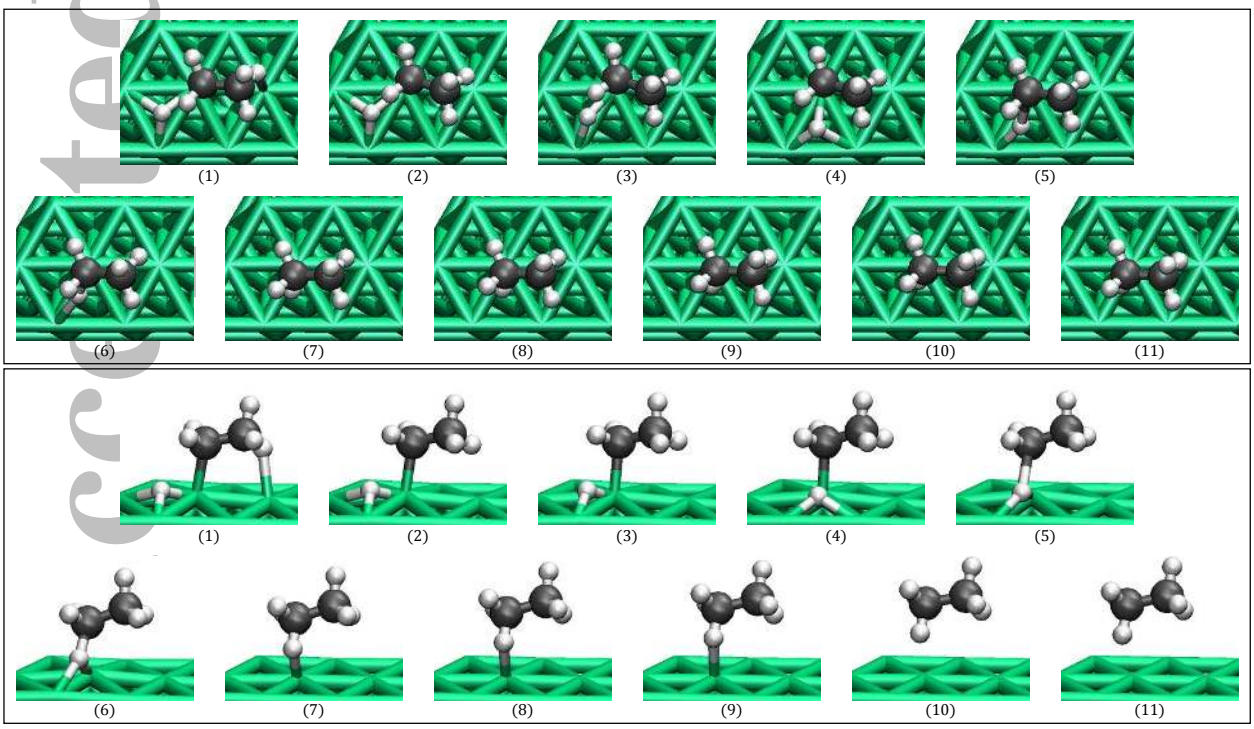
(a) Snapshots of the initial path of ethane formation on Pd(111) calculated by DE-GSM.



(b) Snapshots of the final converged path of ethane formation on Pd(111) calculated by DE-GSM.



(c) Snapshots of the initial path of ethane formation on Pd(111) calculated by CI-NEB.



(d) Snapshots of the final converged path of ethane formation on Pd(111) calculated by CI-NEB.

Figure S15: Reaction 8-b. Reaction paths for ethane formation on Pd(111) from ethyl and hydrogen.

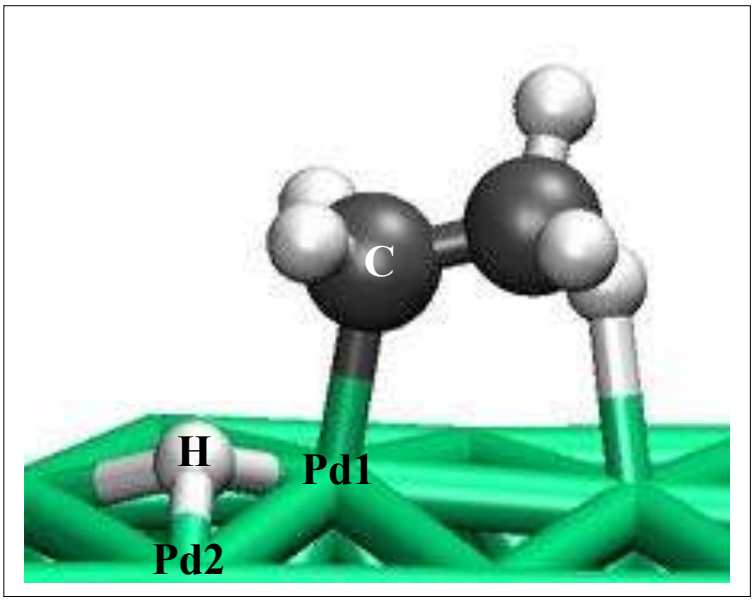


Figure S16: Atomic labels for Table S1.

	C-Pd1			H-Pd2		
Node	CI-NEB	DE-GSM	Diff. (GSM - NEB)	CI-NEB	DE-GSM	Diff. (GSM - NEB)
1	2.088	2.088	0.000	1.698	1.698	0.000
2	2.088	2.103	0.015	1.698	1.720	0.022
3	2.179	2.150	-0.029	1.776	1.767	-0.009
4	2.275	2.228	-0.047	1.864	1.846	-0.017
5	2.374	2.297	-0.077	1.959	1.917	-0.042
6	2.476	2.391	-0.084	2.061	2.023	-0.038
7	2.580	2.584	0.004	2.169	2.261	0.092
8	2.687	2.633	-0.054	2.282	2.377	0.095
9	2.795	2.782	-0.013	2.399	2.516	0.117
10	2.906	2.943	0.037	2.520	2.649	0.129
11	3.131	3.131	0.000	2.771	2.771	0.000

Table S1: Bond lengths for initial and final RPs of Reaction 8-b calculated by CI-NEB and DE-GSM. The difference is measured by subtracting CI-NEB's value from DE-GSM's. All values are in Ångstroms.

		DE-GSM	CI-NEB	
Bonds (Å) & angle	Reactant	Transition State	Transition State	Product
W1-O5	4.684	2.087	2.115	1.891
O5-H6	0.994	1.358	1.347	3.343
O5-H7	0.986	0.981	0.982	0.972
W3-H6	5.297	2.118	2.115	1.906
W4-H6	3.504	4.950	2.389	4.805
W2-H7	3.570	6.157	6.153	6.664
∠ O5-H6-W3	103.979	136.967	114.971	85.325
∠ O5-H6-W4	121.762	131.643	144.183	91.637
∠ H6-O5-H7	104.059	95.586	102.853	96.772

Table S2: Bond lengths and angles for the reactant, TSs, and product of Reaction 15-a calculated by DE-GSM and CI-NEB. Colored values indicate bonds and angles that are different in structures calculated by the methods.

	Reaction 4			
	TS1	Intermediate	TS2	Product
DE-GSM	39.2	32.8	48.0	39.8
SE-GSM	44.0	-	-	39.9

Table S3: Energies of TSs, intermediate, and products of Reaction 4. All the energies are in kcal/mol and referenced to the reactant structure of each reaction.

3 Tables of number of gradient calculations and activation energies

ID	DE-GSM	CI-NEB	SE-GSM
1	50	45	535
2	116	135	46
3-a	205	T	131
3-b	144	162	69
4-a	154	216	426
4-b	157	882	-
5-a	135	117	238
5-b	-	297	147
5-b-1	201	-	-
5-b-2	307	-	-
5-c	169	432	306
6-a	339	216	1282
6-b	-	F	F
6-b-1	277	-	-
6-b-2	180	-	-
6-c	639	F	F
7-a	826	T	1944
7-b	210	T	270
8-a	154	513	142
8-b	167	738	181
9-a	286	504	155
9-b	474	810	378
9-c	1572	459	336
9-d	1042	459	183
10-a	190	1422	257
10-b	932	1773	592
11-a	288	T	207
11-b	258	288	195
12-a	276	T	91
12-b	260	T	158
13-a	172	342	123
13-b	124	342	141
14-a	144	549	112

14-b	175	675	139
14-c	89	216	126
15-a	145	1548	120
25-b	182	513	263
16-a	152	477	494
16-b	512	T	92
17-a	255	882	184
17-b	166	558	183
18-a	181	585	167
18-b	222	477	340
19-a	518	1449	1133
19-b	757	549	1667
20	1158	T	884
21	258	1062	200

Table S4: Number of gradient calculations required by each method for the reactions in the test set. F and T stand for failed and terminated reactions. Terminated reactions are the ones that required more than 1,800 gradient calculations for 9 active images.

ID	DE-GSM	CI-NEB	SE-GSM
1	3.6	3.5	3.5
2	3.9	3.9	3.9
3-a	32.5	T	33.0
3-b	3.7	4.1	4.1
4-a	39.2	39.3	44.0
4-b	15.2	11.7	-
5-a	18.5	18.5	18.7
5-b	-	3.9	25.5
5-b-1	18.5	-	-
5-b-2	6.4	-	-
5-c	19.7	17.4	17.8
6-a	17.9	17.8	17.9
6-b	-	F	F
6-b-1	20.6	-	-
6-b-2	22.7	-	-
6-c	26.4	F	F
7-a	21.8	T	20.6
7-b	24.6	T	25.3
8-a	19.5	19.1	20.7
8-b	13.2	12.1	15.0
9-a	11.5	11.4	11.4
9-b	16.9	16.5	17.0
9-c	18.9	18.8	19.0
9-d	23.5	22.4	22.5
10-a	47.4	44.7	34.8
10-b	47.3	47.0	47.7
11-a	24.7	T	26.1
11-b	18.3	18.3	19.5
12-a	22.7	T	25.5
12-b	16.0	T	12.3
13-a	22.0	21.6	23.3
13-b	7.4	6.0	6.4
14-a	0.6	0.2	0.9
14-b	5.8	5.8	8.0

14-c	23.3	22.4	32.8
15-a	13.5	8.9	7.7
25-b	19.2	19.2	16.1
16-a	2.3	2.0	1.9
16-b	2.1	T	11.2
17-a	24.4	25.2	22.0
17-b	23.9	23.6	25.8
18-a	14.0	13.7	13.3
18-b	23.9	22.7	22.2
19-a	22.9	21.5	21.7
19-b	6.9	4.3	5.2
20	31.1	T	35.3
21	10.2	7.9	9.6

Table S5: Activation energies in kcal/mol calculated by each method for the reactions in the test set. F and T stand for failed and terminated reactions. Terminated reactions are the ones that required more than 1,800 gradient calculations for 9 active images.

4 Cartesian coordinates of the reactants, TSs, and products

reaction-1-reactant
65
-13.663661
Pt 0.000000 0.000000 10.000000
Pt 2.771859 0.000000 10.000000
Pt 5.543717 0.000000 10.000000
Pt 8.315576 0.000000 10.000000
Pt 1.385929 2.400500 10.000000
Pt 4.157788 2.400500 10.000000
Pt 6.929646 2.400500 10.000000
Pt 9.701505 2.400500 10.000000
Pt 2.771859 4.801000 10.000000
Pt 5.543717 4.801000 10.000000
Pt 8.315576 4.801000 10.000000
Pt 11.087434 4.801000 10.000000
Pt 4.157788 7.201500 10.000000
Pt 6.929646 7.201500 10.000000
Pt 9.701505 7.201500 10.000000
Pt 12.473364 7.201500 10.000000
Pt 1.385929 0.800167 12.263213
Pt 4.157788 0.800167 12.263213
Pt 6.929646 0.800167 12.263213
Pt 9.701505 0.800167 12.263213
Pt 2.771859 3.200667 12.263213
Pt 5.543717 3.200667 12.263213
Pt 8.315576 3.200667 12.263213
Pt 11.087434 3.200667 12.263213
Pt 4.157788 5.601167 12.263213
Pt 6.929646 5.601167 12.263213
Pt 9.701505 5.601167 12.263213
Pt 12.473364 5.601167 12.263213
Pt 5.543717 8.001666 12.263213
Pt 8.315576 8.001666 12.263213
Pt 11.087434 8.001666 12.263213
Pt 13.859293 8.001666 12.263213
Pt 0.002778 1.598729 14.586548
Pt 2.769081 1.598729 14.586548
Pt 5.544680 1.598754 14.585386
Pt 8.314613 1.598754 14.585386
Pt 1.385929 3.993662 14.602670
Pt 4.156902 4.002457 14.585386
Pt 6.929646 4.000833 14.580335
Pt 9.702391 4.002457 14.585386
Pt 2.770820 6.401932 14.581859
Pt 5.541868 6.401289 14.585386
Pt 8.317425 6.401289 14.585386
Pt 11.088472 6.401932 14.581859
Pt 4.163999 8.805419 14.602670
Pt 6.929646 8.805041 14.586548
Pt 9.695294 8.805419 14.602670
Pt 12.473364 8.800635 14.581859
Pt -0.063505 -0.036664 16.934816
Pt 2.835364 -0.036664 16.934816
Pt 5.568508 0.000088 16.946057
Pt 8.290785 0.000088 16.946057
Pt 1.385929 2.473830 16.934816
Pt 4.168057 2.406429 16.933787

Pt 6.929646 2.406192 16.942308
Pt 9.691236 2.406429 16.933787
Pt 2.784330 4.822425 16.946057
Pt 5.548647 4.798154 16.942308
Pt 8.310646 4.798154 16.942308
Pt 11.074962 4.822425 16.946057
Pt 4.145469 7.179986 16.946057
Pt 6.929646 7.189642 16.933787
Pt 9.713824 7.179986 16.946057
Pt 12.473364 7.201500 16.948982
Au 1.385929 0.800167 19.057047
reaction-1-product
65
-13.660690
Pt 0.000000 0.000000 10.000000
Pt 2.771859 0.000000 10.000000
Pt 5.543717 0.000000 10.000000
Pt 8.315576 0.000000 10.000000
Pt 1.385929 2.400500 10.000000
Pt 4.157788 2.400500 10.000000
Pt 6.929646 2.400500 10.000000
Pt 9.701505 2.400500 10.000000
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Pt 5.543717 4.801000 10.000000
Pt 8.315576 4.801000 10.000000
Pt 11.087434 4.801000 10.000000
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Pt 6.929646 7.201500 10.000000
Pt 9.701505 7.201500 10.000000
Pt 12.473364 7.201500 10.000000
Pt 1.385929 0.800167 12.263213
Pt 4.157788 0.800167 12.263213
Pt 6.929646 0.800167 12.263213
Pt 9.701505 0.800167 12.263213
Pt 2.771859 3.200667 12.263213
Pt 5.543717 3.200667 12.263213
Pt 8.315576 3.200667 12.263213
Pt 11.087434 3.200667 12.263213
Pt 4.157788 5.601167 12.263213
Pt 6.929646 5.601167 12.263213
Pt 9.701505 5.601167 12.263213
Pt 12.473364 5.601167 12.263213
Pt 5.543717 8.001666 12.263213
Pt 8.315576 8.001666 12.263213
Pt 11.087434 8.001666 12.263213
Pt 13.859293 8.001666 12.263213
Pt 0.002550 1.601595 14.592291
Pt 2.771859 1.600333 14.589651
Pt 5.541167 1.601595 14.592291
Pt 8.315576 1.598790 14.582130
Pt 1.386111 3.997994 14.592291
Pt 4.157606 3.997994 14.592291
Pt 6.932405 4.002426 14.586264
Pt 9.698746 4.002426 14.586264
Pt 2.771859 6.398810 14.585776
Pt 5.542380 6.402105 14.582130
Pt 8.315576 6.398147 14.586264
Pt 11.088771 6.402105 14.582130
Pt 4.159973 8.803095 14.585776
Pt 6.932014 8.803410 14.592291
Pt 9.699137 8.803410 14.592291
Pt 12.471178 8.803095 14.585776
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Pt 2.771859 -0.051919 16.943660
Pt 5.557124 -0.007741 16.941858
Pt 8.315576 -0.002112 16.945155
Pt 1.340966 2.426460 16.943660
Pt 4.202751 2.426460 16.943660
Pt 6.946663 2.399733 16.941404
Pt 9.684488 2.399733 16.941404
Pt 2.771859 4.816481 16.941858
Pt 5.551561 4.816120 16.941404
Pt 8.315576 4.801000 16.944699
Pt 11.079590 4.816120 16.941404
Pt 4.155959 7.202556 16.945155
Pt 6.920474 7.187147 16.941404
Pt 9.710678 7.187147 16.941404
Pt 12.475192 7.202556 16.945155
Au 2.771859 1.600333 19.103739
reaction-1-DE-GSM-TS
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Pt 5.543717 0.000000 10.000000
Pt 8.315576 0.000000 10.000000
Pt 1.385929 2.400500 10.000000
Pt 4.157788 2.400500 10.000000
Pt 6.929646 2.400500 10.000000
Pt 9.701505 2.400500 10.000000
Pt 2.771859 4.801000 10.000000
Pt 5.543717 4.801000 10.000000
Pt 8.315576 4.801000 10.000000
Pt 11.087434 4.801000 10.000000
Pt 4.157788 7.201500 10.000000
Pt 6.929646 7.201500 10.000000
Pt 9.701505 7.201500 10.000000
Pt 12.473364 7.201500 10.000000
Pt 1.385929 0.800167 12.263213
Pt 4.157788 0.800167 12.263213
Pt 6.929646 0.800167 12.263213
Pt 9.701505 0.800167 12.263213
Pt 2.771859 3.200667 12.263213
Pt 5.543717 3.200667 12.263213
Pt 8.315576 3.200667 12.263213
Pt 11.087434 3.200667 12.263213
Pt 4.157788 5.601167 12.263213
Pt 6.929646 5.601167 12.263213
Pt 9.701505 5.601167 12.263213
Pt 12.473364 5.601167 12.263213
Pt 5.543717 8.001666 12.263213
Pt 8.315576 8.001666 12.263213
Pt 11.087434 8.001666 12.263213
Pt 13.859293 8.001666 12.263213
Pt -0.001784 1.597632 14.586969
Pt 2.772395 1.600659 14.585152
Pt 5.541389 1.601093 14.590927
Pt 8.313797 1.598991 14.583881
Pt 1.383188 3.995629 14.596426
Pt 4.157312 3.998466 14.590952
Pt 6.930151 4.001165 14.585044
Pt 9.700424 4.001517 14.585933
Pt 2.771057 6.401519 14.584719
Pt 5.541652 6.400447 14.583914
Pt 8.315613 6.400054 14.585928
Pt 11.090150 6.402881 14.581469
Pt 4.161099 8.803713 14.593645
Pt 6.926370 8.801640 14.586931
Pt 9.695669 8.802059 14.596379
Pt 12.473096 8.801037 14.584703
Pt -0.016558 -0.009563 16.954229
Pt 2.815311 -0.057798 16.909762
Pt 5.566162 -0.003274 16.943440
Pt 8.310122 -0.001189 16.945782
Pt 1.357688 2.467067 16.909681

Pt 4.169981 2.407535 16.958073
Pt 6.933697 2.403080 16.942701
Pt 9.686160 2.401401 16.936057
Pt 2.780222 4.822134 16.943395
Pt 5.547975 4.803234 16.942595
Pt 8.311156 4.798438 16.944786
Pt 11.073698 4.825017 16.944029
Pt 4.154033 7.197371 16.945769
Pt 6.922754 7.187756 16.936061
Pt 9.715449 7.177585 16.944030
Pt 12.477344 7.203779 16.948043
Au 2.137998 1.234007 19.122193
reaction-1-SE-GSM-TS
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Pt 2.771859 0.000000 10.000000
Pt 5.543717 0.000000 10.000000
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Pt 1.385929 2.400500 10.000000
Pt 4.157788 2.400500 10.000000
Pt 6.929646 2.400500 10.000000
Pt 9.701505 2.400500 10.000000
Pt 2.771859 4.801000 10.000000
Pt 5.543717 4.801000 10.000000
Pt 8.315576 4.801000 10.000000
Pt 11.087434 4.801000 10.000000
Pt 4.157788 7.201500 10.000000
Pt 6.929646 7.201500 10.000000
Pt 9.701505 7.201500 10.000000
Pt 12.473364 7.201500 10.000000
Pt 1.385929 0.800167 12.263213
Pt 4.157788 0.800167 12.263213
Pt 6.929646 0.800167 12.263213
Pt 9.701505 0.800167 12.263213
Pt 2.771859 3.200667 12.263213
Pt 5.543717 3.200667 12.263213
Pt 8.315576 3.200667 12.263213
Pt 11.087434 3.200667 12.263213
Pt 4.157788 5.601167 12.263213
Pt 6.929646 5.601167 12.263213
Pt 9.701505 5.601167 12.263213
Pt 12.473364 5.601167 12.263213
Pt 5.543717 8.001666 12.263213
Pt 8.315576 8.001666 12.263213
Pt 11.087434 8.001666 12.263213
Pt 13.859293 8.001666 12.263213
Pt -0.018013 1.589951 14.584522
Pt 2.759365 1.593659 14.587900
Pt 5.518770 1.594281 14.604859
Pt 8.292341 1.592982 14.583688
Pt 1.367380 3.990407 14.592217
Pt 4.139662 3.983147 14.604925
Pt 6.911135 3.991069 14.588956
Pt 9.683103 3.993962 14.584270
Pt 2.758575 6.393207 14.585196
Pt 5.523969 6.386143 14.583277
Pt 8.299536 6.389642 14.584320
Pt 11.078008 6.395881 14.580271
Pt 4.146944 8.797075 14.595110
Pt 6.909878 8.791632 14.582698
Pt 9.683439 8.790774 14.590586
Pt 12.459366 8.795887 14.585807
Pt -0.034514 -0.018661 16.959233
Pt 2.782155 -0.080377 16.897960
Pt 5.537173 -0.021416 16.947097
Pt 8.287299 -0.014071 16.945441
Pt 1.323193 2.450902 16.904453
Pt 4.133349 2.387950 17.003803
Pt 6.897610 2.384661 16.951318
Pt 9.654042 2.385874 16.931392
Pt 2.748978 4.808713 16.947208
Pt 5.512520 4.783543 16.951309
Pt 8.275288 4.778543 16.945618
Pt 11.041600 4.810181 16.939483
Pt 4.128393 7.186473 16.944784
Pt 6.890441 7.167939 16.930944
Pt 9.685720 7.157262 16.939010
Pt 12.451178 7.190839 16.948274
Au 2.225007 1.276810 19.111423
reaction-1-SE-GSM-product
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Pt 8.315576 0.000000 10.000000
Pt 1.385929 2.400500 10.000000
Pt 4.157788 2.400500 10.000000
Pt 6.929646 2.400500 10.000000
Pt 9.701505 2.400500 10.000000
Pt 2.771859 4.801000 10.000000
Pt 5.543717 4.801000 10.000000
Pt 8.315576 4.801000 10.000000
Pt 11.087434 4.801000 10.000000
Pt 4.157788 7.201500 10.000000
Pt 6.929646 7.201500 10.000000
Pt 9.701505 7.201500 10.000000
Pt 12.473364 7.201500 10.000000
Pt 1.385929 0.800167 12.263213
Pt 4.157788 0.800167 12.263213
Pt 6.929646 0.800167 12.263213
Pt 9.701505 0.800167 12.263213
Pt 2.771859 3.200667 12.263213
Pt 5.543717 3.200667 12.263213
Pt 8.315576 3.200667 12.263213
Pt 11.087434 3.200667 12.263213
Pt 4.157788 5.601167 12.263213
Pt 6.929646 5.601167 12.263213
Pt 9.701505 5.601167 12.263213
Pt 12.473364 5.601167 12.263213
Pt 5.543717 8.001666 12.263213
Pt 8.315576 8.001666 12.263213
Pt 11.087434 8.001666 12.263213
Pt 13.859293 8.001666 12.263213
Pt -0.017150 1.593690 14.592702
Pt 2.750847 1.590984 14.593931
Pt 5.515364 1.592492 14.600713
Pt 8.291440 1.589408 14.582379
Pt 1.363387 3.984355 14.597832
Pt 4.135849 3.982549 14.601546
Pt 6.907163 3.990064 14.587032
Pt 9.677855 3.991430 14.584625
Pt 2.748950 6.387482 14.585289
Pt 5.518422 6.389001 14.581350
Pt 8.293848 6.388287 14.584810
Pt 11.068318 6.390783 14.582359
Pt 4.135364 8.792034 14.582135
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Pt 9.677294 8.791533 14.593330
Pt 12.447975 8.792911 14.586928
Pt -0.062077 -0.029244 16.932808
Pt 2.727708 -0.078110 16.930625
Pt 5.511722 -0.027847 16.948265
Pt 8.265695 -0.023113 16.943039

Pt 1.306960 2.404542 16.959795
Pt 4.139898 2.401917 16.974611
Pt 6.893202 2.379995 16.945042
Pt 9.641862 2.378646 16.936116
Pt 2.724974 4.797506 16.945843
Pt 5.503808 4.789968 16.945550
Pt 8.267636 4.776377 16.944039
Pt 11.032181 4.791769 16.940784
Pt 4.106113 7.179664 16.942486
Pt 6.872346 7.162438 16.935624
Pt 9.664013 7.161224 16.939793
Pt 12.428225 7.181439 16.946378
Au 2.679264 1.465937 19.132827
****
reaction-2-reactant
38
-7.112340
Pd 0.000000 0.000000 10.000000
Pd 2.750645 0.000000 10.000000
Pd 5.501291 0.000000 10.000000
Pd 1.375323 2.382129 10.000000
Pd 4.125968 2.382129 10.000000
Pd 6.876613 2.382129 10.000000
Pd 2.750645 4.764258 10.000000
Pd 5.501291 4.764258 10.000000
Pd 8.251936 4.764258 10.000000
Pd 1.375323 0.794043 12.245893
Pd 4.125968 0.794043 12.245893
Pd 6.876613 0.794043 12.245893
Pd 2.750645 3.176172 12.245893
Pd 5.501291 3.176172 12.245893
Pd 8.251936 3.176172 12.245893
Pd 4.125968 5.558300 12.245893
Pd 6.876613 5.558300 12.245893
Pd 9.627259 5.558300 12.245893
Pd 0.001542 1.590486 14.559731
Pd 2.750645 1.588086 14.578940
Pd 5.499748 1.590486 14.559731
Pd 1.374016 3.967679 14.559731
Pd 4.127275 3.967679 14.559731
Pd 6.876613 3.970215 14.552415
Pd 2.750645 6.352343 14.529421
Pd 5.504140 6.352479 14.559731
Pd 8.249087 6.352479 14.559731
Pd -0.016411 -0.009475 16.858214
Pd 2.750645 -0.012894 16.952545
Pd 5.517702 -0.009475 16.858214
Pd 1.364156 2.388576 16.952545
Pd 4.137135 2.388576 16.952545
Pd 6.876613 2.384391 16.875114
Pd 2.750645 4.783207 16.858214
Pd 5.503250 4.763126 16.875114
Pd 8.249977 4.763126 16.875114
C 2.750645 1.588086 18.256943
O 2.750645 1.588086 19.448024
reaction-2-product
38
-7.112960
Pd 0.000000 0.000000 10.000000
Pd 2.750645 0.000000 10.000000
Pd 5.501291 0.000000 10.000000
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Pd 4.125968 2.382129 10.000000
Pd 6.876613 2.382129 10.000000
Pd 2.750645 4.764258 10.000000
Pd 5.501291 4.764258 10.000000
Pd 8.251936 4.764258 10.000000
Pd 1.375323 0.794043 12.245893
Pd 4.125968 0.794043 12.245893
Pd 6.876613 0.794043 12.245893
Pd 2.750645 3.176172 12.245893
Pd 5.501291 3.176172 12.245893
Pd 8.251936 3.176172 12.245893
Pd 4.125968 5.558300 12.245893
Pd 6.876613 5.558300 12.245893
Pd 9.627259 5.558300 12.245893
Pd 0.001043 1.587484 14.565063
Pd 2.749602 1.587484 14.565063
Pd 5.501291 1.586298 14.542026
Pd 1.375323 3.966512 14.562592
Pd 4.124420 3.971108 14.542026
Pd 6.878161 3.971108 14.542026
Pd 2.753851 6.354195 14.562592
Pd 5.501291 6.353548 14.565063
Pd 8.248730 6.354195 14.562592
Pd -0.015982 -0.009227 16.944216
Pd 2.766628 -0.009227 16.944216
Pd 5.501291 0.000716 16.874256
Pd 1.375323 2.400583 16.944216
Pd 4.143105 2.392023 16.859439
Pd 6.859476 2.392023 16.859439
Pd 2.751266 4.763899 16.874256
Pd 5.501291 4.744469 16.859439
Pd 8.251316 4.763899 16.874256
C 1.375323 0.794043 18.246454
O 1.375323 0.794043 19.437395
reaction-2-DE-GSM-TS
38
-7.106049
Pd 0.000000 0.000000 10.000000
Pd 2.750645 0.000000 10.000000
Pd 5.501291 0.000000 10.000000
Pd 1.375323 2.382129 10.000000
Pd 4.125968 2.382129 10.000000
Pd 6.876613 2.382129 10.000000
Pd 2.750645 4.764258 10.000000
Pd 5.501291 4.764258 10.000000
Pd 8.251936 4.764258 10.000000
Pd 1.375323 0.794043 12.245893
Pd 4.125968 0.794043 12.245893
Pd 6.876613 0.794043 12.245893
Pd 2.750645 3.176172 12.245893
Pd 5.501291 3.176172 12.245893
Pd 8.251936 3.176172 12.245893
Pd 4.125968 5.558300 12.245893
Pd 6.876613 5.558300 12.245893
Pd 9.627259 5.558300 12.245893
Pd 0.000992 1.587533 14.564375
Pd 2.753144 1.588665 14.565366
Pd 5.500206 1.589550 14.551104
Pd 1.374206 3.964136 14.567794
Pd 4.125615 3.968171 14.550786
Pd 6.877577 3.969886 14.545006
Pd 2.753895 6.352770 14.545260
Pd 5.501214 6.354562 14.561633
Pd 8.246004 6.353959 14.566827
Pd -0.007213 -0.003921 16.900465
Pd 2.771513 -0.014619 16.954108
Pd 5.522030 -0.003021 16.864175
Pd 1.377951 2.405210 16.953629
Pd 4.142049 2.388591 16.903321
Pd 6.870821 2.387634 16.866705
Pd 2.760449 4.775740 16.871098
Pd 5.503082 4.758289 16.857117
Pd 8.258281 4.765363 16.869411

C 2.047646 1.183830 18.376952
O 2.053799 1.174812 19.557158
reaction-2-SE-GSM-TS
38
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Pd 2.750645 0.000000 10.000000
Pd 5.501291 0.000000 10.000000
Pd 1.375323 2.382129 10.000000
Pd 4.125968 2.382129 10.000000
Pd 6.876613 2.382129 10.000000
Pd 2.750645 4.764258 10.000000
Pd 5.501291 4.764258 10.000000
Pd 8.251936 4.764258 10.000000
Pd 1.375323 0.794043 12.245893
Pd 4.125968 0.794043 12.245893
Pd 6.876613 0.794043 12.245893
Pd 2.750645 3.176172 12.245893
Pd 5.501291 3.176172 12.245893
Pd 8.251936 3.176172 12.245893
Pd 4.125968 5.558300 12.245893
Pd 6.876613 5.558300 12.245893
Pd 9.627259 5.558300 12.245893
Pd -0.000972 1.587542 14.565797
Pd 2.747726 1.587396 14.559930
Pd 5.498741 1.587710 14.550488
Pd 1.373101 3.964177 14.570719
Pd 4.124936 3.969330 14.549539
Pd 6.875680 3.970294 14.549798
Pd 2.751077 6.353316 14.549966
Pd 5.498388 6.352676 14.568425
Pd 8.244575 6.354432 14.569447
Pd -0.025040 -0.015161 16.903970
Pd 2.764169 -0.010048 16.959178
Pd 5.508498 -0.000169 16.874333
Pd 1.371278 2.398448 16.960457
Pd 4.137279 2.391869 16.884004
Pd 6.867211 2.385051 16.869290
Pd 2.753597 4.771910 16.873785
Pd 5.498377 4.754845 16.869585
Pd 8.251332 4.764577 16.872121
C 2.024145 1.167999 18.389984
O 2.023508 1.165123 19.570197
reaction-2-SE-GSM-product
38
-7.112812
Pd 0.000000 0.000000 10.000000
Pd 2.750645 0.000000 10.000000
Pd 5.501291 0.000000 10.000000
Pd 1.375323 2.382129 10.000000
Pd 4.125968 2.382129 10.000000
Pd 6.876613 2.382129 10.000000
Pd 2.750645 4.764258 10.000000
Pd 5.501291 4.764258 10.000000
Pd 8.251936 4.764258 10.000000
Pd 1.375323 0.794043 12.245893
Pd 4.125968 0.794043 12.245893
Pd 6.876613 0.794043 12.245893
Pd 2.750645 3.176172 12.245893
Pd 5.501291 3.176172 12.245893
Pd 8.251936 3.176172 12.245893
Pd 4.125968 5.558300 12.245893
Pd 6.876613 5.558300 12.245893
Pd 9.627259 5.558300 12.245893
Pd -0.007084 1.585115 14.573419
Pd 2.737351 1.583321 14.546727
Pd 5.501464 1.586205 14.535581
Pd 1.372832 3.966538 14.567890
Pd 4.122518 3.976531 14.533379
Pd 6.875949 3.971484 14.550125
Pd 2.751814 6.355693 14.573849
Pd 5.494161 6.352082 14.577328
Pd 8.245201 6.356026 14.567602
Pd -0.019163 -0.014707 16.984554
Pd 2.762013 -0.007888 16.955157
Pd 5.500568 0.005639 16.879900
Pd 1.370381 2.395856 16.953194
Pd 4.124602 2.386969 16.810308
Pd 6.858846 2.391561 16.873869
Pd 2.752118 4.762912 16.879505
Pd 5.502936 4.739734 16.873258
Pd 8.254144 4.767678 16.878808
C 1.396498 0.807341 18.276899
O 1.405583 0.811301 19.467190
****
reaction-3-a-reactant
51
-9.376449
Pd 0.000000 0.000000 10.000000
Pd 2.750650 0.000000 10.000000
Pd 5.501290 0.000000 10.000000
Pd 8.251940 0.000000 10.000000
Pd 1.375320 2.382130 10.000000
Pd 4.125970 2.382130 10.000000
Pd 6.876610 2.382130 10.000000
Pd 9.627260 2.382130 10.000000
Pd 2.750650 4.764260 10.000000
Pd 5.501290 4.764260 10.000000
Pd 8.251940 4.764260 10.000000
Pd 11.002580 4.764260 10.000000
Pd 1.375320 0.794040 12.245890
Pd 4.125970 0.794040 12.245890
Pd 6.876610 0.794040 12.245890
Pd 9.627260 0.794040 12.245890
Pd 2.750650 3.176170 12.245890
Pd 5.501290 3.176170 12.245890
Pd 8.251940 3.176170 12.245890
Pd 11.002580 3.176170 12.245890
Pd 4.125970 5.558300 12.245890
Pd 6.876610 5.558300 12.245890
Pd 9.627260 5.558300 12.245890
Pd 12.377900 5.558300 12.245890
Pd -0.090756 1.662491 14.541882
Pd 2.691190 1.637092 14.527116
Pd 5.434385 1.662817 14.546988
Pd 8.146645 1.664281 14.565340
Pd 1.311301 4.012328 14.490317
Pd 4.068959 4.020792 14.516159
Pd 6.798877 4.028886 14.562748
Pd 9.542854 4.036766 14.535599
Pd 2.685746 6.422490 14.507902
Pd 5.416560 6.418452 14.546161
Pd 8.171379 6.384338 14.498169
Pd 10.944351 6.411716 14.480621
Pd -0.190919 0.166830 16.847442
Pd 2.556323 0.159943 16.774953
Pd 5.356985 0.091619 16.696701
Pd 8.103974 0.104500 16.774666
Pd 1.190167 2.537061 16.844181
Pd 3.893813 2.397306 16.917964
Pd 6.742650 2.407303 17.102515
Pd 9.500000 2.491781 16.892282
Pd 2.609909 4.892341 16.711325
Pd 5.383758 5.015407 16.888064
Pd 8.168714 4.920988 16.968102

Pd 10.897322 4.887373 16.768187
C 8.232495 3.373508 18.253826
O 8.296046 3.371276 19.445409
O 5.129906 3.452739 17.993615
reaction-3-a-product
51
-9.340962
Pd 0.000000 0.000000 10.000000
Pd 2.750650 0.000000 10.000000
Pd 5.501290 0.000000 10.000000
Pd 8.251940 0.000000 10.000000
Pd 1.375320 2.382130 10.000000
Pd 4.125970 2.382130 10.000000
Pd 6.876610 2.382130 10.000000
Pd 9.627260 2.382130 10.000000
Pd 2.750650 4.764260 10.000000
Pd 5.501290 4.764260 10.000000
Pd 8.251940 4.764260 10.000000
Pd 11.002580 4.764260 10.000000
Pd 1.375320 0.794040 12.245890
Pd 4.125970 0.794040 12.245890
Pd 6.876610 0.794040 12.245890
Pd 9.627260 0.794040 12.245890
Pd 2.750650 3.176170 12.245890
Pd 5.501290 3.176170 12.245890
Pd 8.251940 3.176170 12.245890
Pd 11.002580 3.176170 12.245890
Pd 4.125970 5.558300 12.245890
Pd 6.876610 5.558300 12.245890
Pd 9.627260 5.558300 12.245890
Pd 12.377900 5.558300 12.245890
Pd -0.087045 1.622927 14.503907
Pd 2.684127 1.631481 14.473290
Pd 5.436050 1.643925 14.511959
Pd 8.157076 1.646710 14.536132
Pd 1.310479 4.027507 14.510332
Pd 4.066847 4.025698 14.541490
Pd 6.807238 4.013148 14.571585
Pd 9.546169 4.021522 14.550073
Pd 2.668875 6.403540 14.519999
Pd 5.402923 6.375600 14.544609
Pd 8.164079 6.374079 14.500904
Pd 10.932999 6.396266 14.479785
Pd -0.224769 0.147588 16.837744
Pd 2.549666 0.157358 16.738794
Pd 5.318361 0.132584 16.679388
Pd 8.056081 0.142048 16.787580
Pd 1.144879 2.535191 16.717054
Pd 3.886058 2.513535 16.754929
Pd 6.665854 2.521778 16.961770
Pd 9.421722 2.507353 16.799729
Pd 2.535485 4.906618 16.833054
Pd 5.283021 4.933217 16.892543
Pd 8.068238 4.915873 16.972642
Pd 10.808975 4.908504 16.792750
C 7.057360 3.853969 18.616285
O 7.889078 3.368739 19.391226
O 5.955422 4.523384 18.834703
reaction-3-a-DE-GSM-TS
51
-9.324611
Pd 0.000000 0.000000 10.000000
Pd 2.750650 0.000000 10.000000
Pd 5.501290 0.000000 10.000000
Pd 8.251940 0.000000 10.000000
Pd 1.375320 2.382130 10.000000
Pd 4.125970 2.382130 10.000000
Pd 6.876610 2.382130 10.000000
Pd 9.627260 2.382130 10.000000
Pd 2.750650 4.764260 10.000000
Pd 5.501290 4.764260 10.000000
Pd 8.251940 4.764260 10.000000
Pd 11.002580 4.764260 10.000000
Pd 1.375320 0.794040 12.245890
Pd 4.125970 0.794040 12.245890
Pd 6.876610 0.794040 12.245890
Pd 9.627260 0.794040 12.245890
Pd 2.750650 3.176170 12.245890
Pd 5.501290 3.176170 12.245890
Pd 8.251940 3.176170 12.245890
Pd 11.002580 3.176170 12.245890
Pd 4.125970 5.558300 12.245890
Pd 6.876610 5.558300 12.245890
Pd 9.627260 5.558300 12.245890
Pd 12.377900 5.558300 12.245890
Pd -0.076375 1.645623 14.506832
Pd 2.699409 1.644166 14.539799
Pd 5.408574 1.638937 14.532162
Pd 8.157477 1.619401 14.512099
Pd 1.286286 4.010588 14.495147
Pd 4.056494 3.998573 14.521009
Pd 6.795134 4.017845 14.584876
Pd 9.510834 4.023765 14.540703
Pd 2.687689 6.404787 14.516743
Pd 5.415199 6.424217 14.545999
Pd 8.158549 6.361078 14.513648
Pd 10.932313 6.394184 14.487180
Pd -0.257144 0.214174 16.861717
Pd 2.534550 0.215816 16.769508
Pd 5.292499 0.034510 16.703552
Pd 8.053822 0.050900 16.819485
Pd 1.157016 2.564010 16.825016
Pd 3.999295 2.462292 17.055808
Pd 6.752277 2.337003 16.875346
Pd 9.440835 2.501587 16.768320
Pd 2.515984 4.887293 16.718336
Pd 5.241203 5.089784 16.788963
Pd 7.919788 4.874328 17.123283
Pd 10.741731 4.853713 16.773003
C 6.789434 3.598913 18.423946
O 7.105823 3.567317 19.573367
O 5.015552 3.786504 18.246840
reaction-3-a-SE-GSM-TS
51
-9.323881
Pd 0.000000 0.000000 10.000000
Pd 2.750650 0.000000 10.000000
Pd 5.501290 0.000000 10.000000
Pd 8.251940 0.000000 10.000000
Pd 1.375320 2.382130 10.000000
Pd 4.125970 2.382130 10.000000
Pd 6.876610 2.382130 10.000000
Pd 9.627260 2.382130 10.000000
Pd 2.750650 4.764260 10.000000
Pd 5.501290 4.764260 10.000000
Pd 8.251940 4.764260 10.000000
Pd 11.002580 4.764260 10.000000
Pd 1.375320 0.794040 12.245890
Pd 4.125970 0.794040 12.245890
Pd 6.876610 0.794040 12.245890
Pd 9.627260 0.794040 12.245890
Pd 2.750650 3.176170 12.245890
Pd 5.501290 3.176170 12.245890
Pd 8.251940 3.176170 12.245890
Pd 11.002580 3.176170 12.245890

Pd 4.125970 5.558300 12.245890
Pd 6.876610 5.558300 12.245890
Pd 9.627260 5.558300 12.245890
Pd 12.377900 5.558300 12.245890
Pd -0.105030 1.643137 14.511164
Pd 2.670556 1.639810 14.549365
Pd 5.373726 1.632251 14.540750
Pd 8.127981 1.614833 14.514505
Pd 1.251568 4.004688 14.501115
Pd 4.025878 3.989475 14.525080
Pd 6.762329 4.003482 14.587283
Pd 9.479641 4.019246 14.543207
Pd 2.668936 6.394208 14.511029
Pd 5.390214 6.416853 14.542739
Pd 8.131303 6.355177 14.506825
Pd 10.904347 6.382708 14.484966
Pd -0.303493 0.209949 16.856171
Pd 2.494304 0.201099 16.772569
Pd 5.242933 0.009649 16.704085
Pd 8.018246 0.020985 16.791030
Pd 1.093504 2.547356 16.839740
Pd 3.913685 2.457758 17.084946
Pd 6.676340 2.289257 16.892426
Pd 9.365277 2.485628 16.775304
Pd 2.465277 4.866946 16.719109
Pd 5.188146 5.084040 16.787491
Pd 7.857869 4.848945 17.099412
Pd 10.682783 4.830967 16.797418
C 6.798175 3.599756 18.410047
O 7.118543 3.554844 19.562664
O 5.059559 3.747903 18.232714
reaction-3-a-SE-GSM-product
51
-9.338004
Pd 0.000000 0.000000 10.000000
Pd 2.750650 0.000000 10.000000
Pd 5.501290 0.000000 10.000000
Pd 8.251940 0.000000 10.000000
Pd 1.375320 2.382130 10.000000
Pd 4.125970 2.382130 10.000000
Pd 6.876610 2.382130 10.000000
Pd 9.627260 2.382130 10.000000
Pd 2.750650 4.764260 10.000000
Pd 5.501290 4.764260 10.000000
Pd 8.251940 4.764260 10.000000
Pd 11.002580 4.764260 10.000000
Pd 1.375320 0.794040 12.245890
Pd 4.125970 0.794040 12.245890
Pd 6.876610 0.794040 12.245890
Pd 9.627260 0.794040 12.245890
Pd 2.750650 3.176170 12.245890
Pd 5.501290 3.176170 12.245890
Pd 8.251940 3.176170 12.245890
Pd 11.002580 3.176170 12.245890
Pd 4.125970 5.558300 12.245890
Pd 6.876610 5.558300 12.245890
Pd 9.627260 5.558300 12.245890
Pd 12.377900 5.558300 12.245890
Pd -0.072995 1.619735 14.500082
Pd 2.692158 1.636109 14.477973
Pd 5.435228 1.648537 14.500361
Pd 8.155548 1.649682 14.536051
Pd 1.303653 4.028852 14.507141
Pd 4.062101 4.024531 14.510119
Pd 6.814617 4.024168 14.576723
Pd 9.548795 4.033512 14.550455
Pd 2.676785 6.414171 14.519803
Pd 5.409674 6.370978 14.568793
Pd 8.168055 6.381959 14.515343
Pd 10.938627 6.396905 14.482464
Pd -0.207917 0.169216 16.856013
Pd 2.573159 0.184922 16.750054
Pd 5.337177 0.147154 16.680918
Pd 8.077322 0.127928 16.798145
Pd 1.178897 2.545044 16.725214
Pd 3.917449 2.544162 16.753900
Pd 6.732746 2.482608 16.917757
Pd 9.460944 2.521500 16.753862
Pd 2.547568 4.921750 16.797034
Pd 5.303393 4.979127 16.887745
Pd 8.058608 4.940423 17.027539
Pd 10.824900 4.906851 16.814147
C 7.124361 3.875441 18.580358
O 7.973718 3.654804 19.443869
O 5.819091 4.044792 18.696264
reaction-3-b-reactant: same as 3-a-product
reaction-3-b-product
51
-9.346676
Pd 0.000000 0.000000 10.000000
Pd 2.750650 0.000000 10.000000
Pd 5.501290 0.000000 10.000000
Pd 8.251940 0.000000 10.000000
Pd 1.375320 2.382130 10.000000
Pd 4.125970 2.382130 10.000000
Pd 6.876610 2.382130 10.000000
Pd 9.627260 2.382130 10.000000
Pd 2.750650 4.764260 10.000000
Pd 5.501290 4.764260 10.000000
Pd 8.251940 4.764260 10.000000
Pd 11.002580 4.764260 10.000000
Pd 1.375320 0.794040 12.245890
Pd 4.125970 0.794040 12.245890
Pd 6.876610 0.794040 12.245890
Pd 9.627260 0.794040 12.245890
Pd 2.750650 3.176170 12.245890
Pd 5.501290 3.176170 12.245890
Pd 8.251940 3.176170 12.245890
Pd 11.002580 3.176170 12.245890
Pd 4.125970 5.558300 12.245890
Pd 6.876610 5.558300 12.245890
Pd 9.627260 5.558300 12.245890
Pd 12.377900 5.558300 12.245890
Pd -0.084614 1.654752 14.510628
Pd 2.659036 1.655394 14.512518
Pd 5.411422 1.647437 14.505458
Pd 8.170502 1.652324 14.512562
Pd 1.290769 4.040281 14.517322
Pd 4.041260 4.038412 14.512337
Pd 6.790235 4.037225 14.509757
Pd 9.543086 4.034643 14.513638
Pd 2.664270 6.418506 14.515690
Pd 5.416398 6.416226 14.513742
Pd 8.166604 6.420922 14.509660
Pd 10.915409 6.418403 14.520137
Pd -0.225821 0.181996 16.778716
Pd 2.527751 0.172859 16.783912
Pd 5.271750 0.178185 16.797889
Pd 8.026913 0.166553 16.789148
Pd 1.146349 2.558907 16.780523
Pd 3.897521 2.559893 16.766964
Pd 6.651828 2.548199 16.751472
Pd 9.397535 2.557718 16.787703
Pd 2.523170 4.941627 16.792774

Pd 5.272123 4.944651 16.787862
Pd 8.025135 4.939568 16.767742
Pd 10.770750 4.940830 16.789124
C 7.119106 3.881620 20.083030
O 8.251708 3.638930 20.289954
O 5.983011 4.121536 19.884068
reaction-3-b-DE-GSM-TS
51
-9.335047
Pd 0.000000 0.000000 10.000000
Pd 2.750650 0.000000 10.000000
Pd 5.501290 0.000000 10.000000
Pd 8.251940 0.000000 10.000000
Pd 1.375320 2.382130 10.000000
Pd 4.125970 2.382130 10.000000
Pd 6.876610 2.382130 10.000000
Pd 9.627260 2.382130 10.000000
Pd 2.750650 4.764260 10.000000
Pd 5.501290 4.764260 10.000000
Pd 8.251940 4.764260 10.000000
Pd 11.002580 4.764260 10.000000
Pd 1.375320 0.794040 12.245890
Pd 4.125970 0.794040 12.245890
Pd 6.876610 0.794040 12.245890
Pd 9.627260 0.794040 12.245890
Pd 2.750650 3.176170 12.245890
Pd 5.501290 3.176170 12.245890
Pd 8.251940 3.176170 12.245890
Pd 11.002580 3.176170 12.245890
Pd 4.125970 5.558300 12.245890
Pd 6.876610 5.558300 12.245890
Pd 9.627260 5.558300 12.245890
Pd 12.377900 5.558300 12.245890
Pd -0.088145 1.634046 14.507616
Pd 2.676619 1.637698 14.490810
Pd 5.430979 1.652851 14.515563
Pd 8.159892 1.652189 14.531499
Pd 1.302587 4.029177 14.510059
Pd 4.058994 4.029877 14.526771
Pd 6.800811 4.021465 14.551293
Pd 9.545325 4.026214 14.541838
Pd 2.666282 6.409674 14.514890
Pd 5.407687 6.383563 14.535017
Pd 8.162580 6.384532 14.506805
Pd 10.927202 6.405608 14.490219
Pd -0.225749 0.159582 16.808678
Pd 2.544579 0.166409 16.748788
Pd 5.302621 0.148945 16.702464
Pd 8.045222 0.152425 16.789245
Pd 1.142661 2.539745 16.739593
Pd 3.892148 2.524192 16.755847
Pd 6.670513 2.543726 16.896980
Pd 9.400172 2.533817 16.796978
Pd 2.528448 4.920715 16.800367
Pd 5.283220 4.936645 16.875244
Pd 8.045700 4.920322 16.909943
Pd 10.795719 4.915898 16.787120
C 6.942191 3.900876 19.003813
O 7.881158 3.410539 19.572142
O 5.860604 4.484551 19.043388
reaction-3-b-SE-GSM-TS
51
-9.338359
Pd 0.000000 0.000000 10.000000
Pd 2.750650 0.000000 10.000000
Pd 5.501290 0.000000 10.000000
Pd 8.251940 0.000000 10.000000
Pd 1.375320 2.382130 10.000000
Pd 4.125970 2.382130 10.000000
Pd 6.876610 2.382130 10.000000
Pd 9.627260 2.382130 10.000000
Pd 2.750650 4.764260 10.000000
Pd 5.501290 4.764260 10.000000
Pd 8.251940 4.764260 10.000000
Pd 11.002580 4.764260 10.000000
Pd 1.375320 0.794040 12.245890
Pd 4.125970 0.794040 12.245890
Pd 6.876610 0.794040 12.245890
Pd 9.627260 0.794040 12.245890
Pd 2.750650 3.176170 12.245890
Pd 5.501290 3.176170 12.245890
Pd 8.251940 3.176170 12.245890
Pd 11.002580 3.176170 12.245890
Pd 4.125970 5.558300 12.245890
Pd 6.876610 5.558300 12.245890
Pd 9.627260 5.558300 12.245890
Pd 12.377900 5.558300 12.245890
Pd -0.093696 1.634112 14.494175
Pd 2.656162 1.634709 14.493310
Pd 5.405179 1.641208 14.494566
Pd 8.150553 1.639048 14.495375
Pd 1.287145 4.028807 14.521596
Pd 4.057476 4.037456 14.537100
Pd 6.807056 4.042172 14.562406
Pd 9.532483 4.044601 14.556992
Pd 2.658077 6.406502 14.515111
Pd 5.400841 6.376522 14.538341
Pd 8.153285 6.385153 14.521232
Pd 10.917731 6.398922 14.501233
Pd -0.221674 0.151845 16.791600
Pd 2.538038 0.137468 16.751020
Pd 5.296440 0.144426 16.735542
Pd 8.044348 0.140386 16.789001
Pd 1.107068 2.541894 16.748147
Pd 3.863762 2.518555 16.736446
Pd 6.623173 2.537143 16.741868
Pd 9.376953 2.525174 16.732763
Pd 2.491715 4.905779 16.809695
Pd 5.226791 4.923426 16.924740
Pd 8.000534 4.893901 17.026444
Pd 10.744382 4.932959 16.843846
C 7.279531 4.717094 19.298345
O 8.420860 4.767080 19.659437
O 6.082091 4.657444 19.384888
reaction-3-b-SE-GSM-product
51
-9.344124
Pd 0.000000 0.000000 10.000000
Pd 2.750650 0.000000 10.000000
Pd 5.501290 0.000000 10.000000
Pd 8.251940 0.000000 10.000000
Pd 1.375320 2.382130 10.000000
Pd 4.125970 2.382130 10.000000
Pd 6.876610 2.382130 10.000000
Pd 9.627260 2.382130 10.000000
Pd 2.750650 4.764260 10.000000
Pd 5.501290 4.764260 10.000000
Pd 8.251940 4.764260 10.000000
Pd 11.002580 4.764260 10.000000
Pd 1.375320 0.794040 12.245890
Pd 4.125970 0.794040 12.245890
Pd 6.876610 0.794040 12.245890
Pd 9.627260 0.794040 12.245890
Pd 2.750650 3.176170 12.245890
Pd 5.501290 3.176170 12.245890

Pd 8.251940 3.176170 12.245890
Pd 11.002580 3.176170 12.245890
Pd 4.125970 5.558300 12.245890
Pd 6.876610 5.558300 12.245890
Pd 9.627260 5.558300 12.245890
Pd 12.377900 5.558300 12.245890
Pd -0.080255 1.636631 14.509692
Pd 2.666979 1.640954 14.502377
Pd 5.418002 1.647393 14.501958
Pd 8.164752 1.651811 14.510851
Pd 1.299925 4.029241 14.510756
Pd 4.053368 4.039499 14.525123
Pd 6.795731 4.041144 14.531305
Pd 9.545810 4.034280 14.518777
Pd 2.667276 6.417061 14.518632
Pd 5.414776 6.395081 14.530129
Pd 8.170225 6.409133 14.507564
Pd 10.930914 6.414676 14.507233
Pd -0.208107 0.159474 16.808648
Pd 2.541753 0.165923 16.773070
Pd 5.307695 0.159044 16.763486
Pd 8.052152 0.169119 16.802169
Pd 1.148391 2.548389 16.760732
Pd 3.898186 2.541535 16.745304
Pd 6.644732 2.565223 16.756025
Pd 9.406035 2.544636 16.767193
Pd 2.527842 4.931845 16.792126
Pd 5.272957 4.932442 16.872282
Pd 8.053200 4.946979 16.823034
Pd 10.791753 4.926447 16.778096
C 7.145361 3.924844 19.977299
O 8.238062 3.608023 20.273864
O 6.000161 4.109973 19.768961
****
reaction-4-a-reactant
51
-15.917148
Ru 0.058490 1.523390 10.080360
Ru 2.758490 1.523390 10.080360
Ru 5.458490 1.523390 10.080360
Ru 8.158490 1.523390 10.080360
Ru 1.408490 3.861660 10.080360
Ru 4.108490 3.861660 10.080360
Ru 6.808490 3.861660 10.080360
Ru 9.508490 3.861660 10.080360
Ru 2.758490 6.199930 10.080360
Ru 5.458490 6.199930 10.080360
Ru 8.158490 6.199930 10.080360
Ru 10.858490 6.199930 10.080360
Ru 0.001690 0.006150 12.127120
Ru 2.701690 0.006150 12.127120
Ru 5.401690 0.006150 12.127120
Ru 8.101690 0.006150 12.127120
Ru 1.351690 2.344420 12.127120
Ru 4.051690 2.344420 12.127120
Ru 6.751690 2.344420 12.127120
Ru 9.451690 2.344420 12.127120
Ru 2.701690 4.682680 12.127120
Ru 5.401690 4.682680 12.127120
Ru 8.101690 4.682680 12.127120
Ru 10.801690 4.682680 12.127120
Ru 0.032130 1.547842 14.296208
Ru 2.705591 1.576005 14.252694
Ru 5.410176 1.532041 14.244113
Ru 8.141277 1.527612 14.324459
Ru 1.353169 3.836573 14.277141
Ru 4.036853 3.869096 14.263883
Ru 6.725636 3.879087 14.283358
Ru 9.425038 3.882811 14.306553
Ru 2.689293 6.254020 14.285508
Ru 5.390089 6.206439 14.319068
Ru 8.109317 6.239375 14.269403
Ru 10.778166 6.242776 14.302285
Ru 0.043014 -0.156565 16.447080
Ru 2.615863 0.053644 16.378559
Ru 5.270703 0.078100 16.325782
Ru 8.022760 -0.016917 16.317483
Ru 1.361760 2.466228 16.594043
Ru 4.150376 2.340961 16.578230
Ru 6.822558 2.317770 16.347086
Ru 9.318116 2.478215 16.371589
Ru 2.557290 4.740676 16.320240
Ru 5.320294 4.647544 16.336289
Ru 7.882601 4.757279 16.307464
Ru 10.852605 4.609206 16.300083
O 4.016551 2.169844 19.625330
C 4.086058 2.251418 18.463559
O 1.246489 0.844022 17.695811
reaction-4-a-product
51
-15.864914
Ru 0.058490 1.523390 10.080360
Ru 2.758490 1.523390 10.080360
Ru 5.458490 1.523390 10.080360
Ru 8.158490 1.523390 10.080360
Ru 1.408490 3.861660 10.080360
Ru 4.108490 3.861660 10.080360
Ru 6.808490 3.861660 10.080360
Ru 9.508490 3.861660 10.080360
Ru 2.758490 6.199930 10.080360
Ru 5.458490 6.199930 10.080360
Ru 8.158490 6.199930 10.080360
Ru 10.858490 6.199930 10.080360
Ru 0.001690 0.006150 12.127120
Ru 2.701690 0.006150 12.127120
Ru 5.401690 0.006150 12.127120
Ru 8.101690 0.006150 12.127120
Ru 1.351690 2.344420 12.127120
Ru 4.051690 2.344420 12.127120
Ru 6.751690 2.344420 12.127120
Ru 9.451690 2.344420 12.127120
Ru 2.701690 4.682680 12.127120
Ru 5.401690 4.682680 12.127120
Ru 8.101690 4.682680 12.127120
Ru 10.801690 4.682680 12.127120
Ru 0.032181 1.548777 14.332706
Ru 2.731963 1.588902 14.294562
Ru 5.407140 1.534471 14.246889
Ru 8.124015 1.537185 14.293860
Ru 1.327171 3.866185 14.289452
Ru 4.064022 3.868526 14.257189
Ru 6.735301 3.896178 14.286828
Ru 9.439370 3.892174 14.295289
Ru 2.695093 6.241844 14.286273
Ru 5.389501 6.207020 14.296540
Ru 8.093644 6.235297 14.315086
Ru 10.794163 6.200934 14.306329
Ru -0.032172 -0.081151 16.318612
Ru 2.555784 0.069749 16.354904
Ru 5.345802 0.057553 16.327150
Ru 7.992935 0.005984 16.310038
Ru 1.424312 2.370388 16.393178
Ru 4.093615 2.297069 16.424290
Ru 6.782713 2.336703 16.334255
Ru 9.321283 2.442680 16.343934

Ru 2.517152 4.782609 16.368436
Ru 5.389958 4.683534 16.356612
Ru 7.960847 4.704629 16.344910
Ru 10.822916 4.630789 16.358538
O 3.901783 1.962978 19.364979
C 3.337314 1.789548 18.304252
O 2.079587 1.205895 18.160470
reaction-4-a-DE-GSM-TS
51
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Ru 0.058490 1.523390 10.080360
Ru 2.758490 1.523390 10.080360
Ru 5.458490 1.523390 10.080360
Ru 8.158490 1.523390 10.080360
Ru 1.408490 3.861660 10.080360
Ru 4.108490 3.861660 10.080360
Ru 6.808490 3.861660 10.080360
Ru 9.508490 3.861660 10.080360
Ru 2.758490 6.199930 10.080360
Ru 5.458490 6.199930 10.080360
Ru 8.158490 6.199930 10.080360
Ru 10.858490 6.199930 10.080360
Ru 0.001690 0.006150 12.127120
Ru 2.701690 0.006150 12.127120
Ru 5.401690 0.006150 12.127120
Ru 8.101690 0.006150 12.127120
Ru 1.351690 2.344420 12.127120
Ru 4.051690 2.344420 12.127120
Ru 6.751690 2.344420 12.127120
Ru 9.451690 2.344420 12.127120
Ru 2.701690 4.682680 12.127120
Ru 5.401690 4.682680 12.127120
Ru 8.101690 4.682680 12.127120
Ru 10.801690 4.682680 12.127120
Ru 0.032751 1.560914 14.324045
Ru 2.721577 1.590171 14.271792
Ru 5.408892 1.539753 14.253455
Ru 8.119699 1.537813 14.305284
Ru 1.334075 3.870012 14.255064
Ru 4.057933 3.861832 14.279545
Ru 6.726573 3.890986 14.298645
Ru 9.440232 3.887780 14.298485
Ru 2.696532 6.249430 14.306912
Ru 5.396814 6.206468 14.301332
Ru 8.101540 6.232538 14.283996
Ru 10.795750 6.210191 14.296621
Ru -0.003289 -0.077947 16.325931
Ru 2.575923 0.065764 16.353876
Ru 5.334086 0.046992 16.320175
Ru 7.994796 0.000012 16.320948
Ru 1.400931 2.390718 16.448605
Ru 4.095390 2.281758 16.465409
Ru 6.773757 2.342457 16.342984
Ru 9.311700 2.450909 16.353331
Ru 2.529896 4.767488 16.356020
Ru 5.357815 4.683213 16.357979
Ru 7.937072 4.724330 16.322389
Ru 10.847222 4.601668 16.331763
O 3.704782 1.732065 19.503569
C 3.437419 1.803871 18.355100
O 1.859237 1.120858 17.977082
reaction-4-SE-GSM-TS
51
-15.846966
Ru 0.058490 1.523390 10.080360
Ru 2.758490 1.523390 10.080360
Ru 5.458490 1.523390 10.080360
Ru 8.158490 1.523390 10.080360
Ru 1.408490 3.861660 10.080360
Ru 4.108490 3.861660 10.080360
Ru 6.808490 3.861660 10.080360
Ru 9.508490 3.861660 10.080360
Ru 2.758490 6.199930 10.080360
Ru 5.458490 6.199930 10.080360
Ru 8.158490 6.199930 10.080360
Ru 10.858490 6.199930 10.080360
Ru 0.001690 0.006150 12.127120
Ru 2.701690 0.006150 12.127120
Ru 5.401690 0.006150 12.127120
Ru 8.101690 0.006150 12.127120
Ru 1.351690 2.344420 12.127120
Ru 4.051690 2.344420 12.127120
Ru 6.751690 2.344420 12.127120
Ru 9.451690 2.344420 12.127120
Ru 2.701690 4.682680 12.127120
Ru 5.401690 4.682680 12.127120
Ru 8.101690 4.682680 12.127120
Ru 10.801690 4.682680 12.127120
Ru 0.031568 1.560936 14.301460
Ru 2.726544 1.540452 14.311756
Ru 5.422179 1.554164 14.280094
Ru 8.130844 1.540412 14.301366
Ru 1.368180 3.878577 14.289292
Ru 4.058841 3.889937 14.288945
Ru 6.773444 3.873645 14.270177
Ru 9.462686 3.889036 14.282665
Ru 2.645851 6.205183 14.304517
Ru 5.375820 6.243752 14.288055
Ru 8.049232 6.214926 14.315877
Ru 10.771318 6.225849 14.301397
Ru -0.241464 0.047213 16.349026
Ru 2.649784 -0.001420 16.347939
Ru 5.199485 0.063065 16.348343
Ru 7.982114 0.053261 16.332635
Ru 1.349330 2.339407 16.376581
Ru 4.126757 2.389011 16.362147
Ru 6.725241 2.354553 16.333007
Ru 9.516762 2.351151 16.337642
Ru 2.805392 4.669688 16.366453
Ru 5.289264 4.763942 16.352856
Ru 8.115752 4.676341 16.354789
Ru 10.628006 4.749940 16.355234
O 3.506952 3.218049 19.527185
C 2.654894 2.841066 18.781159
O 1.523549 2.381188 18.613682
reaction-4-DE-GSM-product
51
-15.853514
Ru 0.058490 1.523390 10.080360
Ru 2.758490 1.523390 10.080360
Ru 5.458490 1.523390 10.080360
Ru 8.158490 1.523390 10.080360
Ru 1.408490 3.861660 10.080360
Ru 4.108490 3.861660 10.080360
Ru 6.808490 3.861660 10.080360
Ru 9.508490 3.861660 10.080360
Ru 2.758490 6.199930 10.080360
Ru 5.458490 6.199930 10.080360
Ru 8.158490 6.199930 10.080360
Ru 10.858490 6.199930 10.080360
Ru 0.001690 0.006150 12.127120
Ru 2.701690 0.006150 12.127120
Ru 5.401690 0.006150 12.127120
Ru 8.101690 0.006150 12.127120
Ru 1.351690 2.344420 12.127120

Ru 4.051690 2.344420 12.127120
Ru 6.751690 2.344420 12.127120
Ru 9.451690 2.344420 12.127120
Ru 2.701690 4.682680 12.127120
Ru 5.401690 4.682680 12.127120
Ru 8.101690 4.682680 12.127120
Ru 10.801690 4.682680 12.127120
Ru 0.005040 1.553492 14.280898
Ru 2.688347 1.560278 14.281144
Ru 5.393379 1.559410 14.277434
Ru 8.103464 1.533882 14.286009
Ru 1.333789 3.858996 14.298270
Ru 4.050545 3.889353 14.303874
Ru 6.726575 3.893775 14.312580
Ru 9.438575 3.907157 14.298968
Ru 2.714844 6.247185 14.283270
Ru 5.409838 6.221932 14.272016
Ru 8.121050 6.215318 14.297348
Ru 10.818817 6.218894 14.313853
Ru -0.039590 0.003040 16.339411
Ru 2.776932 -0.021487 16.351725
Ru 5.280023 0.123624 16.336365
Ru 8.145502 0.043211 16.339155
Ru 1.274783 2.394228 16.353778
Ru 3.902773 2.364921 16.329403
Ru 6.792265 2.285555 16.343983
Ru 9.274807 2.440029 16.362457
Ru 2.605113 4.720373 16.334384
Ru 5.270263 4.808311 16.337467
Ru 7.988524 4.712255 16.339787
Ru 10.806611 4.617582 16.352595
O 3.621755 1.949348 20.337904
C 2.689134 1.439297 19.838290
O 1.766008 0.904588 19.336738
reaction-4-b-reactant: same as product of 4-a
reaction-4-b-product
51
-15.853708
Ru 0.058490 1.523390 10.080360
Ru 2.758490 1.523390 10.080360
Ru 5.458490 1.523390 10.080360
Ru 8.158490 1.523390 10.080360
Ru 1.408490 3.861660 10.080360
Ru 4.108490 3.861660 10.080360
Ru 6.808490 3.861660 10.080360
Ru 9.508490 3.861660 10.080360
Ru 2.758490 6.199930 10.080360
Ru 5.458490 6.199930 10.080360
Ru 8.158490 6.199930 10.080360
Ru 10.858490 6.199930 10.080360
Ru 0.001690 0.006150 12.127120
Ru 2.701690 0.006150 12.127120
Ru 5.401690 0.006150 12.127120
Ru 8.101690 0.006150 12.127120
Ru 1.351690 2.344420 12.127120
Ru 4.051690 2.344420 12.127120
Ru 6.751690 2.344420 12.127120
Ru 9.451690 2.344420 12.127120
Ru 2.701690 4.682680 12.127120
Ru 5.401690 4.682680 12.127120
Ru 8.101690 4.682680 12.127120
Ru 10.801690 4.682680 12.127120
Ru 0.004391 1.549329 14.278678
Ru 2.689708 1.560847 14.281628
Ru 5.389218 1.561567 14.275929
Ru 8.100632 1.534090 14.285823
Ru 1.331201 3.863047 14.297670
Ru 4.048283 3.884963 14.305927
Ru 6.726711 3.891720 14.315276
Ru 9.439371 3.909539 14.299913
Ru 2.715105 6.248532 14.284558
Ru 5.409480 6.219630 14.271576
Ru 8.122030 6.214162 14.299190
Ru 10.822449 6.218805 14.316649
Ru -0.036331 0.002180 16.339408
Ru 2.775827 -0.022933 16.349029
Ru 5.277122 0.125692 16.337597
Ru 8.151681 0.045690 16.342966
Ru 1.274161 2.392738 16.345550
Ru 3.896991 2.364899 16.336880
Ru 6.789461 2.283952 16.346086
Ru 9.273117 2.439720 16.359734
Ru 2.604265 4.721222 16.337120
Ru 5.270204 4.804674 16.336852
Ru 7.992642 4.709823 16.339899
Ru 10.804405 4.618447 16.354715
O 3.629768 1.958180 20.308437
C 2.692664 1.428850 19.837240
O 1.749597 0.902164 19.363556
reaction-4-b-DE-GSM-TS
51
-15.840660
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Ru 2.758490 1.523390 10.080360
Ru 5.458490 1.523390 10.080360
Ru 8.158490 1.523390 10.080360
Ru 1.408490 3.861660 10.080360
Ru 4.108490 3.861660 10.080360
Ru 6.808490 3.861660 10.080360
Ru 9.508490 3.861660 10.080360
Ru 2.758490 6.199930 10.080360
Ru 5.458490 6.199930 10.080360
Ru 8.158490 6.199930 10.080360
Ru 10.858490 6.199930 10.080360
Ru 0.001690 0.006150 12.127120
Ru 2.701690 0.006150 12.127120
Ru 5.401690 0.006150 12.127120
Ru 8.101690 0.006150 12.127120
Ru 1.351690 2.344420 12.127120
Ru 4.051690 2.344420 12.127120
Ru 6.751690 2.344420 12.127120
Ru 9.451690 2.344420 12.127120
Ru 2.701690 4.682680 12.127120
Ru 5.401690 4.682680 12.127120
Ru 8.101690 4.682680 12.127120
Ru 10.801690 4.682680 12.127120
Ru 0.029209 1.539103 14.302017
Ru 2.718011 1.580072 14.286653
Ru 5.405321 1.543185 14.261435
Ru 8.124331 1.535739 14.280726
Ru 1.323486 3.859456 14.306586
Ru 4.050524 3.882244 14.275029
Ru 6.730316 3.893910 14.284790
Ru 9.429507 3.908533 14.294277
Ru 2.711446 6.240562 14.292485
Ru 5.395413 6.202364 14.285121
Ru 8.104346 6.219344 14.321907
Ru 10.799037 6.216420 14.317515
Ru -0.010317 -0.076926 16.330463
Ru 2.672284 0.021822 16.337675
Ru 5.290488 0.126390 16.333229
Ru 8.081338 0.031602 16.316715
Ru 1.380755 2.383836 16.359987
Ru 4.026807 2.353753 16.347124

Ru 6.809520 2.302734 16.340009
Ru 9.297457 2.454871 16.348165
Ru 2.518506 4.765717 16.357308
Ru 5.301040 4.736844 16.354169
Ru 7.940222 4.688040 16.349333
Ru 10.805181 4.627711 16.362307
O 3.967716 2.284487 19.554133
C 3.123271 1.765978 18.905182
O 2.114593 1.140041 18.656122
****
reaction-5-a-reactant
19
-3.365740
Ni 0.004790 1.434268 7.036460
Ni 2.484226 1.434268 7.036460
Ni 4.978032 1.436981 7.016164
Ni 1.244508 3.579928 7.033422
Ni 3.733477 3.592612 7.016164
Ni 6.222586 3.592612 7.016164
Ni 2.499977 5.754464 7.033422
Ni 4.978032 5.753667 7.036460
Ni 7.456087 5.754464 7.033422
Ni -0.007597 -0.004386 9.058379
Ni 2.496613 -0.004386 9.058379
Ni 4.978032 -0.000150 9.008529
Ni 1.244508 2.164323 9.058379
Ni 3.740031 2.159308 9.002170
Ni 6.216032 2.159308 9.002170
Ni 2.488886 4.311177 9.008529
Ni 4.978032 4.303588 9.002170
Ni 7.467177 4.311177 9.008529
H 1.244508 0.718517 9.957356
reaction-5-a-product
19
-3.342668
Ni -0.035808 1.456802 6.981816
Ni 2.504616 1.453833 6.980922
Ni 4.966446 1.446152 7.005789
Ni 1.236843 3.602377 6.996481
Ni 3.723492 3.598627 7.004558
Ni 6.206708 3.596475 7.004919
Ni 2.475752 5.749819 6.996853
Ni 4.970534 5.725549 6.980574
Ni 7.463544 5.750355 7.002551
Ni -0.033081 -0.011475 9.034332
Ni 2.512138 -0.014913 9.038534
Ni 4.972425 0.004813 8.988821
Ni 1.236955 2.190197 9.033630
Ni 3.731002 2.161845 9.003185
Ni 6.208215 2.164550 9.003100
Ni 2.482317 4.313787 8.992521
Ni 4.971891 4.309938 9.005092
Ni 7.459608 4.312386 8.986964
H 1.240042 0.721024 8.027559
reaction-5-a-DE-GSM-TS
19
-3.336227
Ni -0.013119 1.448999 7.027741
Ni 2.494160 1.444883 7.015720
Ni 4.975646 1.447552 7.012098
Ni 1.241253 3.601310 6.974384
Ni 3.727536 3.601362 7.004200
Ni 6.216435 3.606156 7.011481
Ni 2.482289 5.758847 7.001145
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Ni 2.530933 0.046126 8.828487
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reaction-6-a-SE-GSM-product
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reaction-6-b-reactant
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Cu 1.747985 6.397693 6.990351
Cu 5.452103 6.379037 7.059559
Cu 8.903296 6.380570 7.094618
Cu -0.078121 0.001438 8.159771
Cu 3.595797 0.001315 8.123379
Cu 7.168888 -0.000648 8.322794
Cu -0.076897 2.550593 8.142475
Cu 3.595516 2.550824 8.117313
Cu 7.182423 2.558470 8.286679
Cu -0.077148 5.109453 8.138803
Cu 3.595095 5.110557 8.116611
Cu 7.184999 5.101251 8.284315
Cu 1.779781 1.302804 9.433844
Cu 5.348303 1.263797 9.616714
Cu 8.986438 1.273980 9.663135
Cu 5.280714 3.833312 11.887313
Cu 5.339866 3.830699 9.497027
Cu 9.004781 3.828747 9.605751
Cu 1.776824 6.357867 9.432458
Cu 5.349888 6.396299 9.616198
Cu 8.988396 6.383832 9.663142
Cu 0.058879 -0.000033 10.674387
Cu 3.470203 0.000027 10.665821
Cu 7.171469 -0.000340 10.826453
Cu 0.057800 2.561009 10.643120
Cu 3.489241 2.567902 10.692946
Cu 7.151048 2.563604 10.805206
Cu 0.059000 5.092389 10.640682
Cu 3.487737 5.093185 10.689303
Cu 7.152355 5.093717 10.802564
reaction-6-b-DE-GSM-TS
36
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Cu 5.486222 1.283651 7.011124
Cu 8.911382 1.279954 7.053814
Cu 1.782363 3.829562 9.211397
Cu 5.479429 3.829044 7.005317
Cu 8.910679 3.829170 6.988272
Cu 1.751329 6.381773 6.949484
Cu 5.485984 6.374837 7.010425
Cu 8.911236 6.378322 7.052730
Cu -0.073645 -0.000175 8.113495
Cu 3.612407 0.000536 8.038644
Cu 7.199278 0.000188 8.303087
Cu -0.087127 2.547319 8.131290
Cu 3.627872 2.544019 8.102261
Cu 7.197413 2.557054 8.261763
Cu -0.087312 5.110853 8.130872
Cu 3.628391 5.114767 8.102388
Cu 7.197545 5.101602 8.260457
Cu 1.775972 1.291611 9.373797
Cu 5.355611 1.274092 9.552612
Cu 9.024402 1.270506 9.644415
Cu 3.455143 3.830203 12.622874
Cu 5.338112 3.829458 9.552625
Cu 9.022039 3.828985 9.590782
Cu 1.775814 6.366901 9.374219
Cu 5.355832 6.385868 9.551525
Cu 9.024332 6.387806 9.643834
Cu 0.090419 0.000147 10.654674
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Cu 3.466380 5.115403 10.650248
Cu 7.165340 5.101873 10.730640
reaction-6-c-reactant
36
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Cu 5.415000 1.276328 7.063855
Cu 9.025000 1.276328 7.063855
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Cu 0.000000 0.000000 8.219827
Cu 3.610000 0.000000 8.219827
Cu 7.220000 0.000000 8.219827
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Cu 3.610000 2.552655 8.219827
Cu 7.220000 2.552655 8.219827
Cu 0.000000 5.105311 8.219827
Cu 3.610000 5.105311 8.219827
Cu 7.220000 5.105311 8.219827
Cu 1.805000 1.276328 9.609157

Cu 5.415000 1.276328 9.609157
Cu 9.025000 1.276328 9.609157
Cu 1.805000 3.828983 9.609157
Cu 5.415000 3.828983 9.609157
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Cu 7.220000 5.105311 10.765128
reaction-6-c-product
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Cu 5.473452 1.239554 7.180655
Cu 9.027380 1.234387 7.149216
Cu 1.891613 3.789335 7.154831
Cu 5.467126 3.794033 7.178439
Cu 9.031640 3.785166 7.152243
Cu 1.886930 6.341551 7.143107
Cu 5.476599 6.344629 7.180887
Cu 9.023438 6.338914 7.152330
Cu 0.044267 -0.039079 8.269086
Cu 3.680087 -0.040686 8.339588
Cu 7.253836 -0.038229 8.353813
Cu 0.047193 2.507827 8.264510
Cu 3.680948 2.512327 8.346805
Cu 7.250012 2.513839 8.358665
Cu 0.046410 5.064821 8.267345
Cu 3.676093 5.068127 8.332974
Cu 7.253134 5.060491 8.354402
Cu 1.840368 1.240017 9.666343
Cu 5.464883 1.238158 9.750539
Cu 9.080070 1.238497 9.669682
Cu 3.628352 2.518155 10.870250
Cu 5.455075 3.797878 9.745095
Cu 9.084471 3.792528 9.667555
Cu 1.844675 6.348472 9.660440
Cu 5.460423 6.344917 9.747241
Cu 9.092773 6.343861 9.669828
Cu 0.052169 -0.032267 10.828585
Cu 3.618542 -0.028073 10.864459
Cu 7.304624 -0.042377 10.871811
Cu 0.048574 2.518822 10.819677
Cu 1.848075 3.789617 9.666196
Cu 7.295630 2.517592 10.875204
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Cu 3.612475 5.072738 10.864643
Cu 7.303230 5.066162 10.869601
reaction-6-c-DE-GSM-TS
36
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Cu 5.625791 1.179451 6.958038
Cu 8.981404 1.195121 7.016533
Cu 1.810544 3.732924 7.708780
Cu 5.601542 3.752679 6.973476
Cu 9.027762 3.764694 7.076752
Cu 1.798892 6.239616 7.229026
Cu 5.585353 6.304042 6.994987
Cu 9.006306 6.309548 7.073226
Cu -0.031611 -0.090356 8.177198
Cu 3.697936 -0.093619 8.057412
Cu 7.288167 -0.030066 8.293653
Cu -0.098454 2.409982 8.219808
Cu 3.771482 2.410476 7.961471
Cu 7.287106 2.485606 8.262600
Cu -0.095242 5.046706 8.378546
Cu 3.785113 5.025214 8.199585
Cu 7.283561 5.043978 8.282152
Cu 1.867375 1.153634 9.297373
Cu 5.351574 1.292417 9.552827
Cu 9.098868 1.254597 9.710709
Cu 1.899220 4.367272 11.804053
Cu 5.446284 3.767067 9.530534
Cu 9.044484 3.764811 9.681803
Cu 1.907962 5.990968 9.700901
Cu 5.474007 6.413102 9.506655
Cu 9.000166 6.386805 9.669197
Cu 0.194397 -0.009755 10.644586
Cu 3.557055 -0.000253 10.616231
Cu 7.164988 0.002319 10.789004
Cu 0.445210 2.733420 10.599181
Cu 3.175150 2.918645 10.311400
Cu 7.196624 2.515397 10.748894
Cu -0.141554 5.160005 10.901888
Cu 3.965432 5.194367 10.900116
Cu 7.166681 5.076970 10.783302
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reaction-7-a-reactant
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Pd 2.728164 1.567755 14.914830
Pd 5.452295 1.569923 14.918894
Pd 8.224124 1.556551 14.836690
Pd 1.339114 3.944579 14.892606
Pd 4.091405 3.922838 14.917225
Pd 6.850347 3.941011 14.852047
Pd 9.598893 3.942516 14.850942
Pd 2.724913 6.318650 14.872044
Pd 5.473499 6.322624 14.857689
Pd 8.220682 6.324629 14.871891
Pd 10.969228 6.330146 14.865080
Pd -0.013180 -0.009209 17.201008
Pd 2.731406 -0.021009 17.199588
Pd 5.494600 -0.024780 17.206692
Pd 8.240333 -0.005970 17.187065
Pd 1.346253 2.374964 17.206730
Pd 4.119242 2.373056 17.324244
Pd 6.886210 2.371343 17.171828
Pd 9.617722 2.374770 17.176724
Pd 2.731582 4.769766 17.216311
Pd 5.498701 4.762855 17.181633
Pd 8.242767 4.751456 17.186326
Pd 10.984013 4.758295 17.206434
H 6.429914 3.251675 22.550127
O 3.988989 2.406772 21.817555
H 3.014764 2.383537 21.691246
H 6.307835 3.339486 19.987426
C 4.539291 2.395971 20.582250
C 6.732353 2.401076 21.922773
O 3.802181 2.361205 19.590948
C 6.037166 2.436195 20.566558
H 7.820501 2.446014 21.782903
H 6.493693 1.479223 22.471063
H 6.355578 1.599496 19.915477
reaction-7-a-product

35
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Pd 5.655749 1.573075 14.989808
Pd 8.438909 1.560894 15.008692
Pd 1.547117 3.949841 15.036676
Pd 4.280603 3.933012 15.070488
Pd 7.034843 3.962724 14.929947
Pd 9.795865 3.943890 14.951800
Pd 2.926865 6.286455 15.160092
Pd 5.691649 6.350499 15.058662
Pd 8.425921 6.346821 14.940945
Pd 11.166373 6.354364 15.017999
Pd 0.072751 0.008790 17.444409
Pd 2.792961 -0.051214 17.321798
Pd 5.626681 0.018843 17.406228
Pd 8.346755 0.048347 17.387798
Pd 1.438411 2.392191 17.439814
Pd 4.283094 2.335190 17.421774
Pd 7.011699 2.415384 17.260323
Pd 9.712060 2.411663 17.357923
Pd 2.832252 4.795621 17.473504
Pd 5.599352 4.735028 17.325471
Pd 8.364715 4.775903 17.228399
Pd 11.074862 4.802675 17.279167
H 4.015489 2.874752 20.920734
O 2.243623 3.524978 19.081573
H 1.478481 3.974307 19.500907
H 6.192854 2.216532 19.738503
C 4.615487 0.957053 18.985015
C 4.637624 2.041832 21.275845
O 3.551153 0.333424 19.280301
C 5.480498 1.472856 20.131716
H 5.296599 2.403434 22.075739
H 3.971023 1.272176 21.685322
H 6.083753 0.611080 20.472548
reaction-7-a-DE-GSM-TS
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Pd 5.561120 1.664774 15.079056
Pd 8.332377 1.638207 15.002126
Pd 1.459733 4.032748 15.024939
Pd 4.191054 4.018984 15.092864
Pd 6.952425 4.029719 14.963279
Pd 9.706544 4.029263 14.976988
Pd 2.827965 6.367852 15.104524
Pd 5.580218 6.414661 14.981160
Pd 8.327908 6.424795 14.991685
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Pd 2.838952 0.111711 17.322019
Pd 5.581864 0.102277 17.346561
Pd 8.315554 0.124743 17.349283
Pd 1.422286 2.484473 17.308004
Pd 4.203837 2.495439 17.613337
Pd 6.964264 2.495528 17.323363
Pd 9.706077 2.485755 17.306223
Pd 2.821334 4.880495 17.501488
Pd 5.602498 4.872959 17.287848
Pd 8.338689 4.867524 17.287113
Pd 11.069779 4.870703 17.317805
H 4.403703 3.952291 22.181702
O 2.935507 4.446085 19.508615
H 2.065086 4.034728 19.701769
H 5.438699 4.282879 19.886338
C 4.035701 2.674834 19.665898
C 5.215526 3.301414 21.831760
O 3.283277 1.856618 20.144709
C 5.277503 3.276645 20.303879
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reaction-7-a-SE-GSM-TS
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Pd 5.488993 1.591941 14.863570
Pd 8.250811 1.573487 14.836611
Pd 1.377198 3.954628 14.887580
Pd 4.101269 3.972926 14.944097
Pd 6.856094 3.958664 14.895949
Pd 9.622085 3.955617 14.812241
Pd 2.745183 6.330009 14.893887
Pd 5.487141 6.308247 14.955440
Pd 8.242554 6.349206 14.846191
Pd 11.002555 6.344799 14.821313
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Pd 2.724641 -0.022082 17.209083
Pd 5.487089 0.001688 17.148379
Pd 8.233944 0.017560 17.168710
Pd 1.347134 2.396488 17.213773
Pd 4.101213 2.374705 17.290290
Pd 6.906217 2.365274 17.175561
Pd 9.614450 2.408855 17.168481
Pd 2.703805 4.807468 17.332476
Pd 5.492558 4.732058 17.384696
Pd 8.256204 4.775953 17.161815
Pd 10.966818 4.774972 17.134543
H 4.401429 5.728584 21.064029
O 2.420117 4.983599 19.308835
H 1.453086 5.155202 19.432677
H 6.679124 5.479680 19.930805
C 5.396993 3.926511 19.179766
C 5.154053 5.021843 21.437570
O 4.683728 2.942427 19.367077
C 6.121796 4.617699 20.319862
H 5.716767 5.499068 22.251966
H 4.626287 4.145093 21.834307
H 6.864227 3.882394 20.681853
reaction-7-a-SE-GSM-product
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Pd 5.480793 1.560803 14.801617
Pd 8.223500 1.544201 14.905213
Pd 1.364192 3.916010 14.862441
Pd 4.105479 3.933481 14.902073
Pd 6.834481 3.927136 14.861804
Pd 9.599153 3.903765 14.796869
Pd 2.730650 6.267572 14.991912
Pd 5.476318 6.288159 14.930912
Pd 8.227197 6.314351 14.780241
Pd 10.990352 6.318627 14.778120
Pd -0.064860 -0.009914 17.272587
Pd 2.690152 -0.041732 17.177080
Pd 5.454059 -0.007143 17.081154
Pd 8.178707 0.024514 17.217278
Pd 1.270434 2.372388 17.327946
Pd 4.066826 2.310817 17.191291
Pd 6.831928 2.405067 17.269729

Pd 9.545163 2.400390 17.228713
Pd 2.655639 4.793726 17.303557
Pd 5.463668 4.741121 17.345926
Pd 8.217118 4.775199 17.099858
Pd 10.906881 4.789718 17.070566
H 5.750462 5.667960 20.509031
O 1.999817 3.578153 18.923998
H 1.198603 4.013234 19.288658
H 7.684115 4.340529 19.542977
C 5.866029 3.373585 18.885401
C 6.113535 4.753933 20.999527
O 4.832545 2.713869 19.195486
C 6.812806 3.835590 19.993002
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H 5.257224 4.246053 21.463932
H 7.173791 2.917231 20.492087
reaction-7-b-reactant
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Pd 8.430471 1.579620 14.950793
Pd 1.544022 3.973479 14.987445
Pd 4.296045 3.948010 15.049882
Pd 7.055647 3.976067 14.962300
Pd 9.806322 3.971823 14.962885
Pd 2.925831 6.341644 14.995541
Pd 5.709316 6.363302 15.013686
Pd 8.439583 6.366615 14.994097
Pd 11.159442 6.363912 15.050769
Pd 0.129860 0.001124 17.308039
Pd 2.839417 -0.037192 17.321933
Pd 5.670082 0.034908 17.496353
Pd 8.418094 0.027307 17.325017
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Pd 4.290833 2.361994 17.486205
Pd 7.073670 2.405311 17.278868
Pd 9.796813 2.393497 17.266103
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Pd 5.645781 4.737355 17.315132
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Pd 11.169102 4.782459 17.324968
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C 4.509071 2.009685 21.368686
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H 5.975693 0.590350 20.599204
reaction-7-b-product
33
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Pd 5.455178 1.506278 14.830483
Pd 8.179332 1.505260 14.807816
Pd 1.318249 3.883585 14.704273
Pd 4.067108 3.867961 14.756540
Pd 6.820005 3.868302 14.765537
Pd 9.569976 3.878145 14.714612
Pd 2.690294 6.267885 14.743549
Pd 5.458641 6.270502 14.736338
Pd 8.201184 6.267597 14.760505
Pd 10.936027 6.279212 14.757069
Pd -0.054145 -0.060770 17.057828
Pd 2.675387 -0.064910 17.141026
Pd 5.474935 -0.056892 17.165502
Pd 8.200254 -0.048981 17.091862
Pd 1.302228 2.332532 17.022937
Pd 4.063004 2.350369 17.154533
Pd 6.867263 2.365363 17.348931
Pd 9.587687 2.310876 17.045881
Pd 2.685351 4.712614 17.052601
Pd 5.438873 4.711933 17.038718
Pd 8.205626 4.688569 17.025917
Pd 10.954646 4.703606 17.029166
H 8.270222 4.397063 19.481532
H 5.943846 3.320476 19.527831
C 4.055639 0.744340 18.443480
C 8.084787 3.407188 19.943161
O 4.048530 0.725403 19.638673
C 6.859204 2.724295 19.392962
H 8.997163 2.800022 19.844362
H 7.932525 3.605003 21.023842
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reaction-7-b-DE-GSM-TS
33
-6.004210
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Pd 5.532475 1.598930 14.933063
Pd 8.265612 1.582084 14.902353
Pd 1.415386 3.962396 14.813637
Pd 4.157892 3.940323 14.808802
Pd 6.915404 3.952873 14.754240
Pd 9.669708 3.949480 14.755176
Pd 2.790025 6.345973 14.837670
Pd 5.552959 6.368537 14.736151
Pd 8.301020 6.358577 14.747958
Pd 11.031423 6.361463 14.837929
Pd 0.008934 0.003480 17.133194
Pd 2.724125 -0.038200 17.139193
Pd 5.529791 -0.062065 17.204849
Pd 8.285317 -0.034245 17.191413
Pd 1.402798 2.384052 17.180857
Pd 4.164086 2.345551 17.620284
Pd 6.998470 2.383253 17.286146
Pd 9.680470 2.370384 17.131085
Pd 2.758270 4.736446 17.143206
Pd 5.480477 4.803651 16.991730
Pd 8.287311 4.740480 17.026419
Pd 11.028712 4.737586 17.100070
H 5.884788 4.469323 20.337524
H 5.736269 3.442409 18.280939
C 4.039932 0.371468 18.571167
C 5.882461 3.378904 20.461490
O 4.015673 0.162907 19.749378
C 5.832517 2.646607 19.161016
H 6.780765 3.071994 21.023486
H 5.014110 3.101413 21.085367
H 6.033456 1.574361 19.228429
reaction-7-b-SE-GSM-TS
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Pd 2.718226 1.602033 14.912729
Pd 5.435661 1.590516 14.783378
Pd 8.203768 1.584030 14.739825
Pd 1.342838 3.976884 14.879978
Pd 4.068450 3.967777 14.856968
Pd 6.800035 3.969854 14.829664
Pd 9.572883 3.966362 14.784912

Pd 2.700880 6.342204 14.805432
Pd 5.440081 6.319541 14.893821
Pd 8.185371 6.354122 14.802719
Pd 10.949360 6.345876 14.765670
Pd -0.066080 0.048029 17.129022
Pd 2.676187 -0.007178 17.173072
Pd 5.437480 0.004892 17.085726
Pd 8.183440 0.034157 17.081344
Pd 1.278150 2.401456 17.177207
Pd 4.072352 2.371241 17.232334
Pd 6.850386 2.375015 17.063932
Pd 9.555715 2.417301 17.104074
Pd 2.644354 4.826185 17.239893
Pd 5.402704 4.747134 17.349706
Pd 8.178935 4.784942 17.117447
Pd 10.914486 4.792848 17.128951
H 4.810557 6.743198 20.305947
O 2.878916 4.935024 19.246953
H 2.779584 5.876428 19.498678
H 6.749252 5.258271 19.780712
C 5.100427 4.087451 19.213156
C 5.112519 5.955187 21.012045
O 4.695175 2.930529 19.335329
C 5.868187 4.839848 20.292869
H 5.776479 6.413363 21.759288
H 4.220676 5.569374 21.522802
H 6.206371 4.066798 21.004100
reaction-7-b-SE-GSM-product
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Pd 5.474903 1.583352 14.741821
Pd 8.215120 1.578344 14.847682
Pd 1.356813 3.939506 14.777620
Pd 4.095799 3.953092 14.831626
Pd 6.820578 3.951294 14.822107
Pd 9.588188 3.937619 14.730700
Pd 2.723877 6.294177 14.921708
Pd 5.460781 6.307426 14.901607
Pd 8.214450 6.338357 14.730414
Pd 10.985002 6.346752 14.704916
Pd -0.082218 0.021597 17.225358
Pd 2.669754 -0.023569 17.138268
Pd 5.444570 0.012147 17.013925
Pd 8.162942 0.051999 17.146499
Pd 1.250851 2.405507 17.266742
Pd 4.043709 2.321935 17.127726
Pd 6.814618 2.430857 17.234769
Pd 9.525507 2.431795 17.168388
Pd 2.641772 4.826094 17.210034
Pd 5.429397 4.749673 17.308412
Pd 8.195291 4.798999 17.053280
Pd 10.896274 4.812740 16.994565
H 5.440314 5.607394 20.536745
O 2.049095 3.618336 18.830791
H 1.287526 4.056560 19.264058
H 7.499969 4.492339 19.559558
C 5.800919 3.372429 18.840997
C 5.869089 4.707203 21.000376
O 4.805354 2.643721 19.131022
C 6.674650 3.896025 19.979506
H 6.526524 5.024124 21.822579
H 5.048104 4.107951 21.415836
H 7.122343 3.004552 20.454289
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reaction-8-a-reactant
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Pd 5.759420 -0.208030 13.955320
Pd 8.510060 -0.208030 13.955320
Pd 1.633450 2.174100 13.955320
Pd 4.384090 2.174100 13.955320
Pd 7.134740 2.174100 13.955320
Pd 9.885380 2.174100 13.955320
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Pd 5.759420 4.556230 13.955320
Pd 8.510060 4.556230 13.955320
Pd 11.260710 4.556230 13.955320
Pd 1.443790 0.733900 16.231780
Pd 4.194430 0.733900 16.231780
Pd 6.945080 0.733900 16.231780
Pd 9.695730 0.733900 16.231780
Pd 2.819110 3.116030 16.231780
Pd 5.569760 3.116030 16.231780
Pd 8.320400 3.116030 16.231780
Pd 11.071050 3.116030 16.231780
Pd 4.194430 5.498160 16.231780
Pd 6.945080 5.498160 16.231780
Pd 9.695730 5.498160 16.231780
Pd 12.446370 5.498160 16.231780
Pd -0.046333 1.635832 18.510089
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Pd 5.454305 1.657859 18.539467
Pd 8.171250 1.654027 18.557837
Pd 1.317617 4.011487 18.496375
Pd 4.055882 4.007008 18.518474
Pd 6.809276 4.006484 18.534277
Pd 9.566297 4.010967 18.505448
Pd 2.679591 6.400459 18.484334
Pd 5.431531 6.388991 18.475515
Pd 8.179375 6.390117 18.469685
Pd 10.931708 6.399156 18.477259
Pd -0.252827 0.171782 20.753792
Pd 2.479336 0.184748 20.695622
Pd 5.250125 0.195791 20.695861
Pd 8.025006 0.143621 20.753786
Pd 1.136897 2.565315 20.818786
Pd 3.898561 2.545816 21.069839
Pd 6.603358 2.498179 21.131056
Pd 9.428098 2.521792 20.841965
Pd 2.547326 4.917961 20.777033
Pd 5.289623 4.937486 20.763718
Pd 8.096385 4.980998 20.812417
Pd 10.823477 4.941868 20.770479
H 3.911610 1.765565 23.431605
C 4.452408 2.671775 23.105990
H 3.979011 3.624129 23.402372
C 5.896654 2.625480 23.161273
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reaction-8-a-product
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Pd 3.008770 -0.208030 13.955320
Pd 5.759420 -0.208030 13.955320
Pd 8.510060 -0.208030 13.955320
Pd 1.633450 2.174100 13.955320
Pd 4.384090 2.174100 13.955320
Pd 7.134740 2.174100 13.955320
Pd 9.885380 2.174100 13.955320

Pd 3.008770 4.556230 13.955320
Pd 5.759420 4.556230 13.955320
Pd 8.510060 4.556230 13.955320
Pd 11.260710 4.556230 13.955320
Pd 1.443790 0.733900 16.231780
Pd 4.194430 0.733900 16.231780
Pd 6.945080 0.733900 16.231780
Pd 9.695730 0.733900 16.231780
Pd 2.819110 3.116030 16.231780
Pd 5.569760 3.116030 16.231780
Pd 8.320400 3.116030 16.231780
Pd 11.071050 3.116030 16.231780
Pd 4.194430 5.498160 16.231780
Pd 6.945080 5.498160 16.231780
Pd 9.695730 5.498160 16.231780
Pd 12.446370 5.498160 16.231780
Pd -0.050639 1.635141 18.501053
Pd 2.716279 1.648438 18.540534
Pd 5.442664 1.658533 18.551210
Pd 8.176964 1.636589 18.521997
Pd 1.307494 4.011851 18.515989
Pd 4.036507 4.002408 18.525723
Pd 6.807445 4.001351 18.501734
Pd 9.573223 4.016323 18.490096
Pd 2.686957 6.390675 18.497183
Pd 5.440231 6.399673 18.474501
Pd 8.182954 6.398746 18.489256
Pd 10.927507 6.401931 18.496444
Pd -0.257537 0.184785 20.752153
Pd 2.493273 0.188033 20.747113
Pd 5.262617 0.180403 20.755561
Pd 8.013266 0.166704 20.772562
Pd 1.125442 2.565919 20.825300
Pd 3.903451 2.549098 21.054293
Pd 6.621445 2.574992 20.930454
Pd 9.378882 2.555666 20.750123
Pd 2.500648 4.926190 20.801306
Pd 5.261235 4.956867 20.726779
Pd 8.025236 4.944035 20.732458
Pd 10.758937 4.946395 20.798439
H 3.496077 1.896642 23.441480
C 4.136183 2.731912 23.097438
H 3.667351 3.708691 23.325352
C 5.567528 2.630236 23.555832
H 5.908932 1.589953 23.696258
H 5.745202 3.192742 24.500192
H 6.296319 3.155609 22.841228
reaction-8-a-DE-GSM-TS
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Pd 3.008770 -0.208030 13.955320
Pd 5.759420 -0.208030 13.955320
Pd 8.510060 -0.208030 13.955320
Pd 1.633450 2.174100 13.955320
Pd 4.384090 2.174100 13.955320
Pd 7.134740 2.174100 13.955320
Pd 9.885380 2.174100 13.955320
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Pd 8.510060 4.556230 13.955320
Pd 11.260710 4.556230 13.955320
Pd 1.443790 0.733900 16.231780
Pd 4.194430 0.733900 16.231780
Pd 6.945080 0.733900 16.231780
Pd 9.695730 0.733900 16.231780
Pd 2.819110 3.116030 16.231780
Pd 5.569760 3.116030 16.231780
Pd 8.320400 3.116030 16.231780
Pd 11.071050 3.116030 16.231780
Pd 4.194430 5.498160 16.231780
Pd 6.945080 5.498160 16.231780
Pd 9.695730 5.498160 16.231780
Pd 12.446370 5.498160 16.231780
Pd -0.051903 1.627723 18.505029
Pd 2.732855 1.644761 18.544300
Pd 5.458649 1.645790 18.544215
Pd 8.167285 1.636530 18.528920
Pd 1.304196 4.004920 18.502705
Pd 4.040244 3.989674 18.502458
Pd 6.810192 4.014776 18.514293
Pd 9.563205 4.015441 18.518153
Pd 2.690758 6.396443 18.495957
Pd 5.429092 6.394696 18.466179
Pd 8.167534 6.375867 18.480760
Pd 10.936146 6.387421 18.481270
Pd -0.257136 0.180712 20.790101
Pd 2.491597 0.169465 20.717535
Pd 5.262938 0.132840 20.692842
Pd 8.036677 0.134076 20.775987
Pd 1.141770 2.557044 20.812879
Pd 3.931854 2.525754 21.083498
Pd 6.609044 2.526455 20.954242
Pd 9.394278 2.527421 20.752268
Pd 2.501225 4.909051 20.765222
Pd 5.236602 4.963236 20.708136
Pd 8.030301 4.926714 20.873264
Pd 10.764417 4.925576 20.804903
H 4.217015 2.064032 23.458446
C 4.697515 2.943767 22.985381
H 4.203953 3.895713 23.253382
C 6.174300 2.961096 23.148181
H 6.626644 2.012693 23.482953
H 6.531730 3.801291 23.775806
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reaction-8-a-SE-GSM-TS
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Pd 5.759420 -0.208030 13.955320
Pd 8.510060 -0.208030 13.955320
Pd 1.633450 2.174100 13.955320
Pd 4.384090 2.174100 13.955320
Pd 7.134740 2.174100 13.955320
Pd 9.885380 2.174100 13.955320
Pd 3.008770 4.556230 13.955320
Pd 5.759420 4.556230 13.955320
Pd 8.510060 4.556230 13.955320
Pd 11.260710 4.556230 13.955320
Pd 1.443790 0.733900 16.231780
Pd 4.194430 0.733900 16.231780
Pd 6.945080 0.733900 16.231780
Pd 9.695730 0.733900 16.231780
Pd 2.819110 3.116030 16.231780
Pd 5.569760 3.116030 16.231780
Pd 8.320400 3.116030 16.231780
Pd 11.071050 3.116030 16.231780
Pd 4.194430 5.498160 16.231780
Pd 6.945080 5.498160 16.231780
Pd 9.695730 5.498160 16.231780
Pd 12.446370 5.498160 16.231780
Pd -0.045759 1.606019 18.512917
Pd 2.736702 1.627003 18.568018
Pd 5.456462 1.630341 18.570331

Pd 8.165861 1.613711 18.529432
Pd 1.296475 3.982001 18.514348
Pd 4.031953 3.969641 18.508982
Pd 6.805517 3.989058 18.508997
Pd 9.559770 3.990425 18.522012
Pd 2.685227 6.368952 18.491111
Pd 5.432193 6.369402 18.465518
Pd 8.166143 6.357565 18.476261
Pd 10.925795 6.362209 18.484209
Pd -0.261190 0.125110 20.765954
Pd 2.484433 0.126238 20.722986
Pd 5.248365 0.082248 20.709064
Pd 8.022152 0.088856 20.758599
Pd 1.127485 2.515655 20.845925
Pd 3.923740 2.474923 21.157394
Pd 6.585665 2.485002 20.968331
Pd 9.383143 2.473234 20.766504
Pd 2.495797 4.860246 20.787278
Pd 5.233927 4.909737 20.714247
Pd 8.030974 4.874932 20.853505
Pd 10.757453 4.876007 20.824045
H 4.360933 2.002609 23.484557
C 4.790617 2.909780 23.012945
H 4.267504 3.835238 23.309664
C 6.274946 2.979524 23.158771
H 6.726826 2.089358 23.623527
H 6.590582 3.905663 23.674233
H 7.234056 3.377841 22.205349
reaction-8-a-SE-GSM-product
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Pd 8.510060 -0.208030 13.955320
Pd 1.633450 2.174100 13.955320
Pd 4.384090 2.174100 13.955320
Pd 7.134740 2.174100 13.955320
Pd 9.885380 2.174100 13.955320
Pd 3.008770 4.556230 13.955320
Pd 5.759420 4.556230 13.955320
Pd 8.510060 4.556230 13.955320
Pd 11.260710 4.556230 13.955320
Pd 1.443790 0.733900 16.231780
Pd 4.194430 0.733900 16.231780
Pd 6.945080 0.733900 16.231780
Pd 9.695730 0.733900 16.231780
Pd 2.819110 3.116030 16.231780
Pd 5.569760 3.116030 16.231780
Pd 8.320400 3.116030 16.231780
Pd 11.071050 3.116030 16.231780
Pd 4.194430 5.498160 16.231780
Pd 6.945080 5.498160 16.231780
Pd 9.695730 5.498160 16.231780
Pd 12.446370 5.498160 16.231780
Pd -0.049896 1.606187 18.495663
Pd 2.718757 1.616783 18.540469
Pd 5.434701 1.631450 18.547040
Pd 8.168732 1.604885 18.511003
Pd 1.307110 3.975945 18.504841
Pd 4.038485 3.977832 18.520249
Pd 6.809660 3.975597 18.503527
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Pd 2.679635 6.365056 18.491672
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Pd 10.929012 6.371985 18.485739
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Pd 5.259741 0.110879 20.728281
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Pd 1.118882 2.505428 20.825809
Pd 3.910077 2.486783 21.059931
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H 3.598864 1.806504 23.433881
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H 3.654201 3.628363 23.317684
C 5.609907 2.668657 23.578470
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H 5.844836 3.513551 24.253041
H 6.402308 2.827542 22.733873
reaction-8-b-reactant
56
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Pd 8.510060 -0.208030 13.955320
Pd 1.633450 2.174100 13.955320
Pd 4.384090 2.174100 13.955320
Pd 7.134740 2.174100 13.955320
Pd 9.885380 2.174100 13.955320
Pd 3.008770 4.556230 13.955320
Pd 5.759420 4.556230 13.955320
Pd 8.510060 4.556230 13.955320
Pd 11.260710 4.556230 13.955320
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Pd 4.194430 0.733900 16.231780
Pd 6.945080 0.733900 16.231780
Pd 9.695730 0.733900 16.231780
Pd 2.819110 3.116030 16.231780
Pd 5.569760 3.116030 16.231780
Pd 8.320400 3.116030 16.231780
Pd 11.071050 3.116030 16.231780
Pd 4.194430 5.498160 16.231780
Pd 6.945080 5.498160 16.231780
Pd 9.695730 5.498160 16.231780
Pd 12.446370 5.498160 16.231780
Pd -0.058170 1.638827 18.514543
Pd 2.688190 1.634724 18.568780
Pd 5.425580 1.648922 18.561533
Pd 8.171605 1.633239 18.522227
Pd 1.291010 3.997366 18.515308
Pd 4.021063 3.991023 18.507513
Pd 6.790893 3.988109 18.486243
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Pd 2.662910 6.394400 18.485513
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Pd 10.906688 6.396188 18.492802
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Pd 5.205272 0.159279 20.780068
Pd 7.930888 0.173587 20.758903
Pd 1.075957 2.582240 20.917168
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Pd 6.633307 2.543270 20.931684
Pd 9.366907 2.542990 20.788551
Pd 2.475782 4.958169 20.756265
Pd 5.259262 4.922298 20.674811

Pd 8.005909 4.928244 20.718855
Pd 10.738691 4.922618 20.781246
H 3.574269 2.001646 23.584519
C 4.213100 2.797137 23.164245
H 3.787419 3.795811 23.374717
C 5.653674 2.657813 23.570603
H 5.977205 1.606798 23.659860
H 5.848611 3.168764 24.540790
H 6.369453 3.206369 22.866857
H 2.577525 1.611880 21.617871
reaction-8-b-product
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Pd 5.759420 -0.208030 13.955320
Pd 8.510060 -0.208030 13.955320
Pd 1.633450 2.174100 13.955320
Pd 4.384090 2.174100 13.955320
Pd 7.134740 2.174100 13.955320
Pd 9.885380 2.174100 13.955320
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Pd 8.510060 4.556230 13.955320
Pd 11.260710 4.556230 13.955320
Pd 1.443790 0.733900 16.231780
Pd 4.194430 0.733900 16.231780
Pd 6.945080 0.733900 16.231780
Pd 9.695730 0.733900 16.231780
Pd 2.819110 3.116030 16.231780
Pd 5.569760 3.116030 16.231780
Pd 8.320400 3.116030 16.231780
Pd 11.071050 3.116030 16.231780
Pd 4.194430 5.498160 16.231780
Pd 6.945080 5.498160 16.231780
Pd 9.695730 5.498160 16.231780
Pd 12.446370 5.498160 16.231780
Pd -0.106031 1.642360 18.501983
Pd 2.650121 1.644350 18.495904
Pd 5.400377 1.650577 18.501737
Pd 8.145362 1.650151 18.501666
Pd 1.271477 4.029273 18.499022
Pd 4.020278 4.020280 18.504426
Pd 6.770636 4.030847 18.505434
Pd 9.523255 4.029787 18.502503
Pd 2.651235 6.410966 18.499146
Pd 5.397855 6.414226 18.503963
Pd 8.147540 6.408266 18.499839
Pd 10.902202 6.408264 18.495277
Pd -0.343653 0.215069 20.788936
Pd 2.407533 0.212573 20.777074
Pd 5.166524 0.209853 20.756919
Pd 7.914479 0.211438 20.768725
Pd 1.019752 2.599880 20.765687
Pd 3.778175 2.599745 20.794073
Pd 6.534895 2.598965 20.787740
Pd 9.277204 2.596804 20.778281
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reaction-8-b-DE-GSM-TS
56
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Pd 4.384090 2.174100 13.955320
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Pd 6.945080 0.733900 16.231780
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Pd 4.194430 5.498160 16.231780
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reaction-8-b-SE-GSM-TS
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Ru 3.237941 3.135177 16.347575

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39
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Cu 5.507066 3.704624 10.093048
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Cu 5.434694 3.833858 12.542222
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Cu 9.009015 6.375670 12.613391
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Cu 9.056650 3.815465 15.107170
Cu 1.817037 6.379706 15.155494
Cu 5.419940 6.360775 15.115436
Cu 9.043471 6.372338 15.112268
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S 8.866372 3.723466 15.807524
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reaction-14-a-SE-GSM-product
57
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W 6.638097 3.861937 14.507196
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W 8.925334 7.732448 14.218466
W 13.399698 7.724199 14.222663
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reaction-14-b-DE-GSM-TS
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reaction-14-b-SE-GSM-TS
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H 9.919916 2.855188 15.215683
reaction-14-b-SE-GSM-product
57
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reaction-14-c-reactant
57
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H 11.113031 5.532100 15.238211
reaction-14-c-product
57
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reaction-14-c-DE-GSM-TS
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W 4.468910 7.740390 11.692830
W 8.937830 7.740390 11.692830
W 13.406740 7.740390 11.692830
W 2.235704 1.289673 12.872158
W 6.716339 1.295898 12.885339
W 11.188615 1.284102 12.853404
W 4.471483 5.132381 12.850625
W 8.936074 5.160972 12.791526
W 13.418785 5.148979 12.852674
W 6.728653 9.041268 12.850813
W 11.173138 9.017308 12.885110
W 15.645573 9.027201 12.869420
W -0.005832 2.583503 13.524084
W 4.481275 2.574597 13.540399
W 8.960386 2.588320 13.552036
W 2.230421 6.432700 13.519881
W 6.606119 6.505738 13.534592
W 11.176531 6.426289 13.553192
W 4.482351 10.331598 13.519917
W 8.948539 10.312725 13.540256
W 13.412893 10.316836 13.520940
W 0.007403 0.016786 14.235367
W 4.476374 -0.004013 14.227628
W 8.932718 -0.022529 14.244961
W 2.222497 3.855323 14.235337
W 6.700197 3.872822 14.283679
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W 4.399448 7.780047 14.248314
W 8.932526 7.741695 14.283756
W 13.423093 7.756854 14.244896
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S 7.993433 5.705581 15.369041
H 10.608590 4.924012 15.671696
reaction-14-c-SE-GSM-TS
57
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W 8.901737 5.148012 12.851988
W 13.401153 5.174009 12.867758
W 6.697045 9.035649 12.884656
W 11.182382 9.025397 12.866898
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W 6.696418 6.427499 13.538986
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W 4.456915 10.327256 13.522002
W 8.943968 10.316441 13.524628
W 13.399083 10.338521 13.521986
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W 4.459540 -0.000662 14.231714
W 8.911178 -0.029619 14.231082
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W 8.931910 7.747972 14.230387
W 13.405454 7.738565 14.225670
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reaction-14-c-SE-GSM-product
57
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W 8.937830 2.580130 11.011410
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W 6.703370 6.450320 11.011410
W 11.172290 6.450320 11.011410
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W 8.937830 10.320520 11.011410
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W 8.937830 0.000000 11.692830
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W 15.633007 9.022723 12.866953
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W 4.501798 2.595359 13.543235
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W 8.947541 10.314793 13.524606
W 13.411927 10.337254 13.525414
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W 2.237888 3.874846 14.230503
W 6.720343 3.863359 14.546805
W 11.183671 3.878259 14.240675
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W 8.949276 7.738213 14.229293
W 13.410706 7.738452 14.223832
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H 10.473468 3.284966 16.972400
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reaction-15-a-reactant
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W 2.254936 1.280385 12.794823
W 6.705019 1.293463 12.809832

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W 8.937962 5.155528 12.812771
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W 4.468577 2.572590 13.532608
W 2.254469 6.444181 13.540451
W 6.709694 6.440551 13.543233
W 0.030400 -0.018192 14.173655
W 4.499870 -0.015434 14.175521
W 2.269713 3.844164 14.171118
W 6.817745 3.849319 14.234927
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O 5.800069 3.971480 16.281952
H 5.064696 3.305440 16.214565
reaction-15-a-product
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W 6.702022 1.303288 12.799090
W 4.489332 5.162149 12.805600
W 8.947128 5.150755 12.818854
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W 6.790892 3.888078 14.451764
H 5.868036 4.552420 16.821638
O 6.553524 4.082723 16.317649
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W 8.965370 5.164418 12.824102
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W 6.719413 6.416994 13.550779
W 0.070780 0.000896 14.170876
W 4.509590 -0.028422 14.176729
W 2.260440 3.847961 14.164098
W 6.843764 3.844362 14.328748
H 5.331370 4.485219 16.393001
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W 8.944925 5.155251 12.792216
W -0.002472 2.602078 13.541297
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W 2.245993 6.464041 13.545696
W 6.718990 6.440677 13.539935
W 0.023405 0.017784 14.165996
W 4.519663 0.040985 14.189523
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W 6.787246 3.922971 14.246282
H 5.156375 3.494036 16.314186
O 5.856179 2.945259 15.895139
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reaction-15-a-SE-GSM-product
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W 6.703370 6.450320 11.001150
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W 8.950660 5.151346 12.815315
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W 4.465618 0.021000 14.187209
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W 6.786120 3.888463 14.455323
H 5.689701 4.256250 16.760626
O 6.466617 3.865833 16.323565
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reaction-15-b-reactant
27

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W 2.234460 6.450320 11.001150
W 6.703370 6.450320 11.001150
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W 2.264621 1.293064 12.808007
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W 4.489332 5.162149 12.805600
W 8.947128 5.150755 12.818854
W -0.036990 2.609301 13.553450
W 4.524752 2.606167 13.583402
W 2.251787 6.453484 13.529889
W 6.710646 6.412737 13.555406
W 0.082686 0.017889 14.157849
W 4.458128 0.021778 14.186256
W 2.225217 3.820823 14.161274
W 6.790892 3.888078 14.451764
H 5.868036 4.552420 16.821638
O 6.553524 4.082723 16.317649
H 4.599537 1.608218 15.205864
reaction-15-b-product
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W 4.514506 2.635869 13.599785
W 2.220756 6.458701 13.527807
W 6.680437 6.387080 13.600293
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W 4.337031 0.078858 14.200556
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W 6.701863 3.875234 14.612047
H 7.500085 6.941360 15.222434
O 6.773205 3.840161 16.338043
H 4.410743 1.656750 15.220285
reaction-15-b-DE-GSM-TS
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W 2.171006 3.878623 14.172934
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H 5.827756 6.299146 15.356901
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reaction-15-b-SE-GSM-product
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W 6.703370 6.450320 11.001150
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W 6.685607 1.306078 12.801121

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W 8.934215 5.145657 12.817683
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W 6.676030 6.403248 13.595041
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W 4.371408 0.071325 14.181734
W 2.159122 3.819371 14.165705
W 6.722468 3.855170 14.640343
H 5.659645 6.649619 15.168178
O 6.732128 3.805849 16.363197
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Au 11.528910 0.005450 13.806570
Au 1.431420 2.503930 13.806570
Au 4.316420 2.503930 13.806570
Au 7.201410 2.503930 13.806570
Au 10.086410 2.503930 13.806570
Au 12.971400 2.503930 13.806570
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Au 5.758920 5.002410 13.806570
Au 8.643910 5.002410 13.806570
Au 11.528910 5.002410 13.806570
Au 14.413900 5.002410 13.806570
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Au 7.201410 7.500890 13.806570
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Au 15.856400 7.500890 13.806570
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Au 7.169110 0.844330 16.301670
Au 10.054110 0.844330 16.301670
Au 12.939100 0.844330 16.301670
Au 2.841620 3.342810 16.301670
Au 5.726610 3.342810 16.301670
Au 8.611610 3.342810 16.301670
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Au 7.169110 5.841290 16.301670
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Au 8.611610 8.339770 16.301670
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Au 14.381600 8.339770 16.301670
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Au 8.769374 1.711588 18.744958
Au 11.679682 1.686633 18.794663
Au 1.563482 4.211858 18.795377
Au 4.416572 4.222764 18.766130
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Au 16.034743 7.397185 21.262118
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O 8.925136 5.169030 23.481352
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H 8.068472 3.340412 24.125160
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H 9.391144 1.235802 23.992442
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Au 11.528910 5.002410 13.806570
Au 14.413900 5.002410 13.806570
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Cu 5.409823 3.828777 17.582211
Cu 9.024622 3.831465 17.587959
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reaction-17-a-DE-GSM-TS
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Cu 3.610000 0.000000 16.276328
Cu 7.220000 0.000000 16.276328
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Cu 7.220000 2.552655 16.276328
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Cu 1.804148 1.258274 17.548515
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Cu 5.411160 3.821547 17.560223
Cu 9.031373 3.831827 17.575022
Cu 1.812049 6.362593 17.600568
Cu 5.411599 6.355765 17.587849
Cu 9.028721 6.370755 17.584847
Cu 0.001547 0.001336 18.740990
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Cu 7.223260 -0.014233 18.736200
Cu -0.006086 2.556794 18.759128
Cu 3.618305 2.511788 18.794777
Cu 7.247076 2.539130 18.737972
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reaction-17-a-SE-GSM-TS
42
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Cu 5.415000 1.276328 15.000000
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Cu 9.025000 3.828983 15.000000
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Cu 9.025000 6.381639 15.000000
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Cu 7.220000 2.552655 16.276328
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Cu 0.003346 0.011013 18.729659
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reaction-17-a-SE-GSM-product
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reaction-17-b-reactant
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Cu 5.415000 6.381639 15.000000
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O 3.678678 1.291375 20.268369

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reaction-17-b-product
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Cu 5.426868 3.820059 17.552100
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Cu 3.623531 2.557641 18.899773
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Cu -0.022575 5.089892 18.750224
Cu 3.622220 5.062750 18.835516
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C 3.237782 1.625286 20.940134
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reaction-17-b-DE-GSM-TS
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H 3.599452 2.739389 21.780349
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H 2.090513 2.247442 20.765151
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reaction-17-b-SE-GSM-TS
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Cu 9.025000 3.828983 15.000000
Cu 1.805000 6.381639 15.000000
Cu 5.415000 6.381639 15.000000
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Cu 3.610000 2.552655 16.276328
Cu 7.220000 2.552655 16.276328
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Cu 7.220000 5.105311 16.276328
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C 2.942360 2.160909 20.765340
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reaction-17-b-SE-GSM-product
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reaction-18-a-reactant
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reaction-18-a-product
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Pt 7.968850 1.802540 9.907410
Pt 10.740710 1.802540 9.907410
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reaction-18-a-SE-GSM-product
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Pt 7.968850 1.802540 9.907410
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reaction-18-b-SE-GSM-product
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Pt 3.811060 4.203040 9.907410
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Pt 9.354780 4.203040 9.907410
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Pt 10.051350 0.598690 12.251600
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reaction-19-a-product
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