Electronic Supplementary Material (ESI) for Chemical Communications

Electronic Supporting Information

Dramatic Reduction in Activation Barrier for Dinitrogen Splitting Using Amine-Borane as Hydrogen Carrier: Insights from DFT Study

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Contents:

S1. Computational Details:

Gas phase geometry optimization of all intermediates and transition states were done using the B3LYP hybrid functional. The effective core potential LANL2DZ along with LANL2DZ basis set was applied for tantalum and silicon atoms. For all other atoms Pople's 6-311++G(d,p) basis functions were employed. This basis set combination is called B1. Harmonic frequency analyses were performed at the same level of theory to characterize the nature of the stationary points as true intermediate or transition state. Furthermore, intrinsic reaction coordinate (IRC) analysis was carried out to confirm that all stationary points are connected to each other and constructs a smooth potential energy surface (PES). Following this single point calculations were executed at the same level of theory employing additional set of 6p functions and a set of f functions on Ta atom and a set of d functions on Si atoms in **gas phase**.[1] This basis set combination is called B2. To check the sensitivity of the predicted barriers on basis sets we have further optimized some crucial intermediates and transition states using B3LYP with basis set B2 with a set of additional p functions on all Si atoms[2] and the computed barriers showed variation less than 0.5 $kcalmol^{-1}$. The standard Gibbs free energies (G°) of all species were obtained by adding the free energy corrections (G_{Corr}) obtained from the frequency computations at B3LYP/B1 to the single point gas phase energies obtained at B3LYP/B2 on optimized geometries obtained at B3LYP/B1. The text in the manuscript discusses the stability in terms relative **gas phase** Gibbs free energy difference (ΔG) at 298 K and 1 atm pressure until and unless mentioned otherwise. All computations were done using Gaussian 09 suite of quantum chemistry programs.[3]

The reason behind choosing the B3LYP functional for computation for the present system is that the B3LYP functional was already used for describing the same silica supported tantalum surface in earlier theoretical reports.[4] Furthermore, B3LYP functional is routinely used for system containing tantalum metal.[5] To check whether B3LYP functional produces correct chemical trends or not, further single point computations using M06L,[6] TPSSH, and B3PW91 functional were performed employing the basis set B2 on optimized geometries obtained from B3LYP/B1. The results are provided in Table 1.

S2.

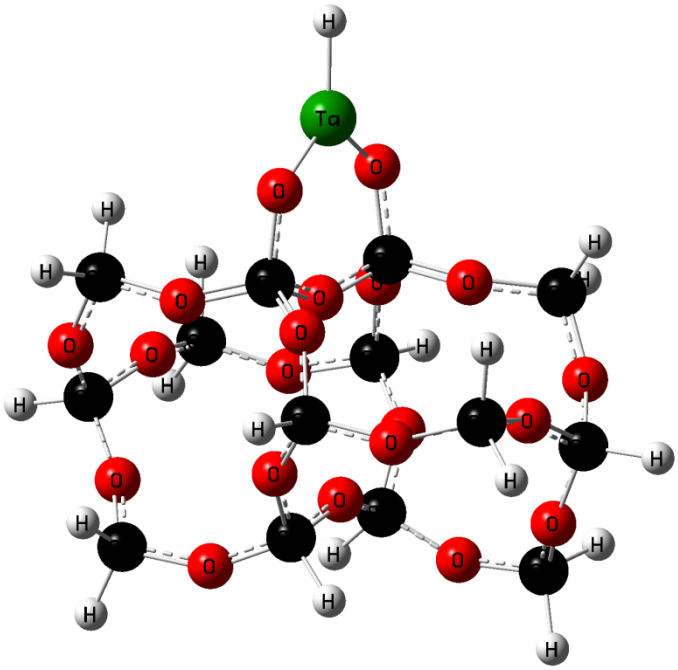
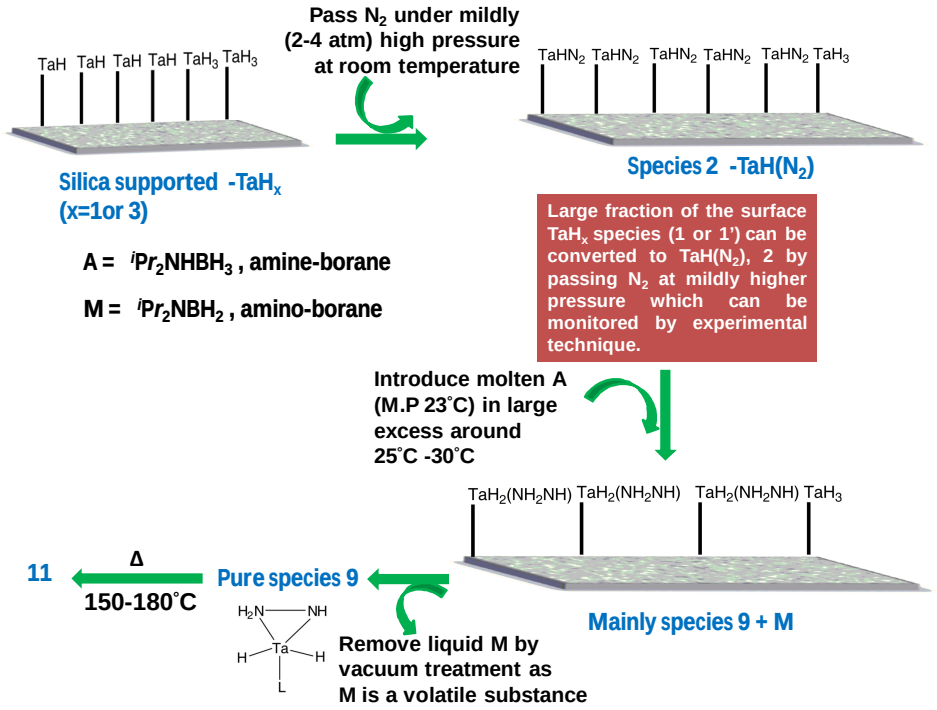
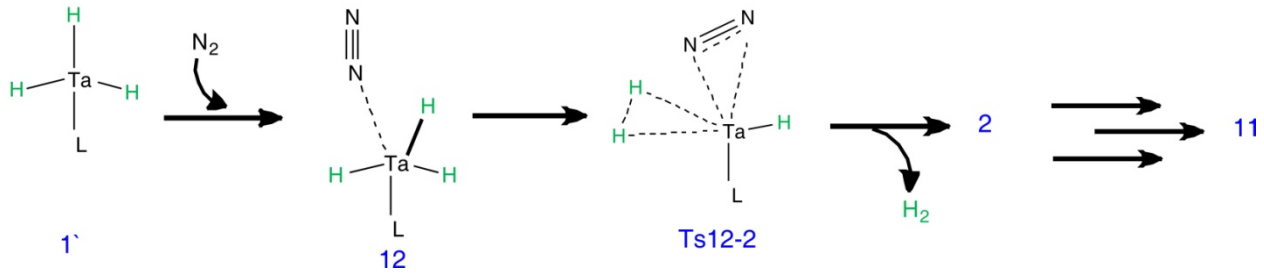


Fig 1: Cluster model system of the silica supported mono tantalum hydride species (**1**) used for computation. Si atoms are represented by black balls.

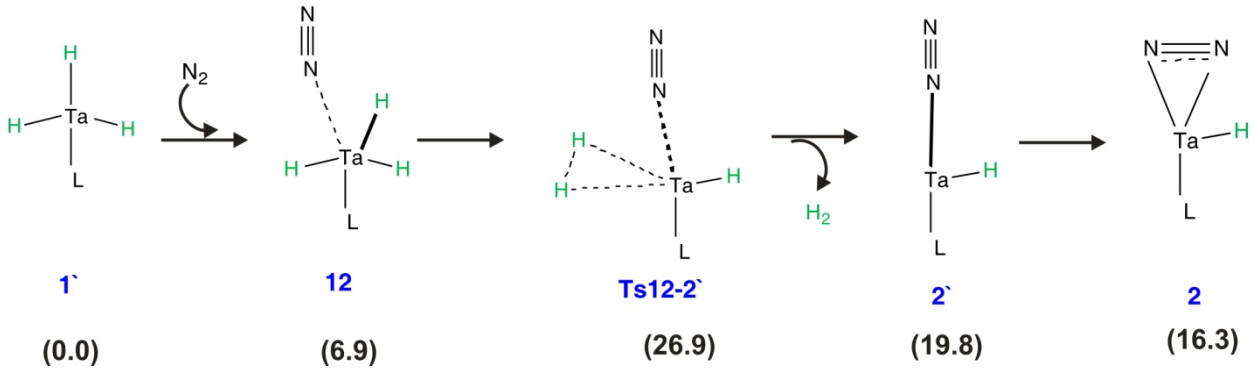
S3. Schematic representation of proposed experimental strategy.



S4. N_2 splitting by the trihydride species $[(\equiv Si\text{-}O)_2TaH_3]$(1') in presence of N_2 and $^{i}Pr_2NHBH_3$ (A) as hydrogen carrier.



Scheme 1: Formation of intermediate **11** from Tantalum trihydride species.



Scheme 2: Alternative low barrier channel of formation of **2** from **1'** and N_2. The relative Gibbs free energy values (in kcalmol^{-1}) are given in parenthesis.

Since the manufacturing process of silica supported tantalum hydrides having general formula $[(\equiv Si\text{-}O)_2TaH_x]$ from the precursor yielded the mono hydride(i.e x=1) as the major product,[7] we consider the silica supported tantalum monohydride $[(\equiv Si\text{-}O)_2TaH]$(**1**) as the most abundant reactive species and the generation of final tantalum amido imido product,$[(\equiv Si\text{-}O)_2Ta(=NH)(NH_2)]$ (**11**) by using ($^{i}Pr_2NHBH_3$) (**A**) as a hydrogen carrier instead of direct molecular H_2 has been discussed in the main manuscript. As the trihydride species $[(\equiv Si\text{-}O)_2TaH_3]$(**1'**) is another possible reactive species which may be present in the reaction system, we conducted computation for the transformation of **1'** into **11** in presence of N_2 and **A**. We found **1'** is free energetically 27.1 kcalmol^{-1} stable compared to isolated **1** and H_2. **1'** can convert to **2** by displacement of H_2 by N_2. We found two different routes for this process (see **Scheme 1** and **Scheme 2** above). One operates at an overall free energy activation barrier of 35.8 kcal/mol and the other at only 26.9 kcal/mol. Formation of **2** from isolated **1'** and N_2 is endoergic by 16.3 kcalmol^{-1}. The route shown in Scheme 1 is in excellent agreement with the previous theoretical study.[4] However, route shown in Scheme 2 is in satisfactory agreement (but not Scheme 1) with the experimental findings of Basset et al.[8] The mechanistic route for transformation of **2** into **11** in presence of **A** has been described in details in the manuscript.

The free energy profile for the overall reaction represented by the equation: **1'**+N_2+*2***A** = **11**+*2***M**+*2*H_2 is given below.

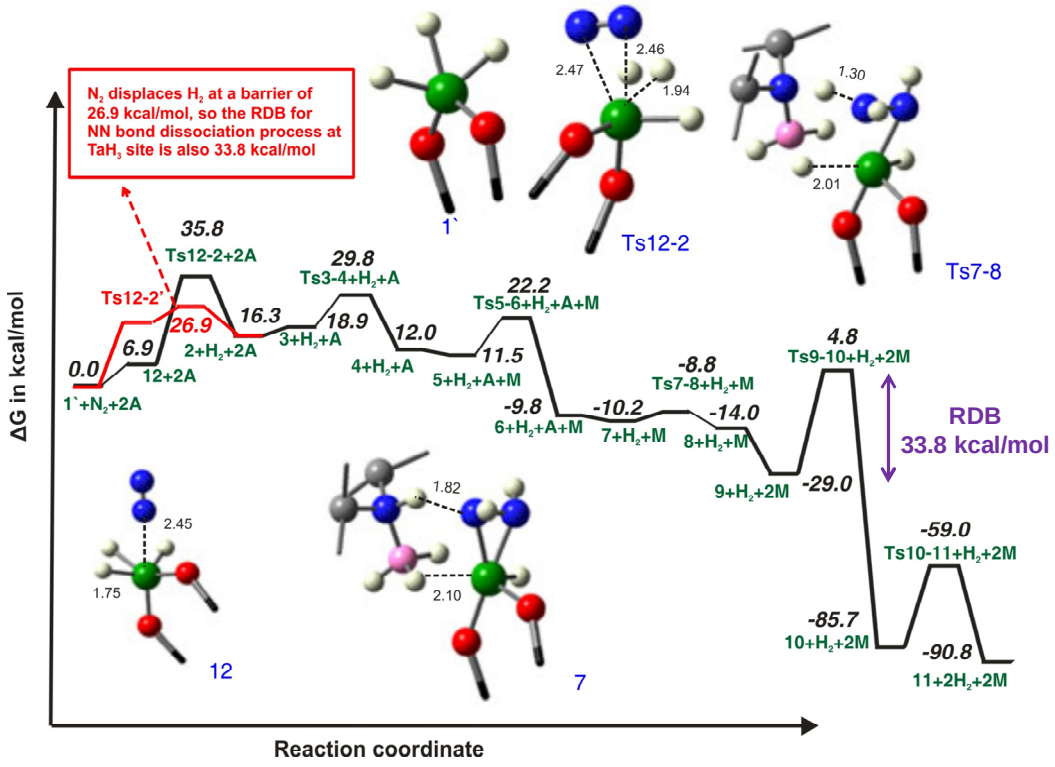


Fig 2: Gibbs free energy profile for N_2 cleavage by the Ta trihydride species linked to silica surface using $^{i}Pr_2NHBH_3$ as hydrogen carrier. All bond lengths in the optimized geometries are in Å. Color code: Ta green, N blue, O red, Si black, H white, C grey, B pink. Isopropyl groups are represented by grey balls and sticks to maintain clarity. The rest of the substituents on Ta centre are omitted for clarity**.** All geometries are optimized at B3LYP/B1.

The free energy profile shown in **Fig. 2**, predicts that **Ts12- 2'**(shown in scheme 2), i. e. binding of N_2 to **1'** leading to formation of **2** along with H_2 removal happens at a free energy barrier of 26.9 kcal/mol. So it turns out that the N_2 bond scission corresponding to **TS9-10** would determine the RDB of the process and as our computations indicate that the RDB would be 33.8 $kcalmol^{-1}$, which is exactly similar to the case of Ta-H case. Though we expect that the surface would be majorly populated by species **2** which can react rapidly with **A** to produce **9** at room temperature, we feel at moderately elevated temperatures of 120^{o}C even the TaH_3 sites would react with amine-boranes at a reasonable rate (2.3×10^{-4} s^{-1} ; Please see S6 for approximate rate determination). The transformation of **1'** to **9** (95 % completion) can happen in less than 7 hours. If the temperature is further raised this would accelerate and 140 ^{o}C the rate is expected to be 1.54×10^{-3} s^{-1}. Note that **A** starts decomposing only at 250 ^{o}C. [13]

S5. Table containing free energies of activation of some important transition state computed by single point calculation on the B3LYP optimized geometries at different DFT functional using extra basis functions on Ta and Si atoms.

Species	B3LYP	M06L	TPSSH	B3PW91
Ts1-2	14.5	7.7	11.1	14.0
Ts3-4	13.5	13.1	5.8	9.0
Ts5-6	10.8	20.6	14.1	12.4
Ts7-8	1.4	2.4	0.7	0.1
Ts9-10	33.8	32.4	28.7	35.6
Ts10-11	26.7	27.0	22.6	24.0

Table 1: Gibbs free energies of activation of some important transition states at different DFT functional. All values are in $kcalmol^{-1}$.

All functional suggest that formation of **9** and other preceding intermediates can happen at room temperature as all the predicted barriers are about 20 $kcalmol^{-1}$ or in general less than that 20 $kcalmol^{-1}$. All of them barring B3PW91 predicts a lower rate determining barrier (corresponding to **Ts9-10**) than B3LYP. We find B3PW91 predicts a barrier which is just 1.8 $kcalmol^{-1}$ higher than the barrier estimated at the B3LYP level of theory. TPSSH tends to predict a barrier 5.1 $kcalmol^{-1}$ lower compared to the barrier predicted by B3LYP. So in general we see that the general chemical findings remain the same and is independent of the functional that we use.

S6. Discussion on the effect of reduction of barrier on N_2 bond cleavage reaction kinetics.

Quadrelli et al. reported that they experimentally observed 95% completion of reaction (i.e. formation of **11** from N_2 splitting by silica supported tantalum hydride (**1**) species in presence of molecular H_2) in 3days at 250°C (523K).[8] If we assume that the reaction follow a first order/pseudo first order reaction kinetics which obeys the rate equation given by,

$kt=\ln(c_0/c)$ …….(1)

where, k=rate constant in s^{-1}, t=time in seconds (s), c=concentration of reactant at any instant time=t, c_0= initial concentration of reactant. From the experimental observation[7] using equation 1, the rate constant of the reaction is estimated to be $k=1.15\times10^{-5}$ s^{-1}.

For simplicity we assume that the rate (k) of a reaction follows Eyring equation:

$$k=(k_BT/h)\exp(-(\Delta G^{\ddagger}/RT)) \quad \text{……(2)}$$

Where, k_B=Boltzmann's constant $=1.38\times10^{-23}$ J/K

h= Planck's constant $=6.63\times10^{-34}$Js

T= Temperature in K

R= Universal molar gas constant = 1.99×10^{-3} $kcalmol^{-1}K^{-1}$

$\Delta G^{\ddagger}$ = Free energy of activation in $kcalmol^{-1}$

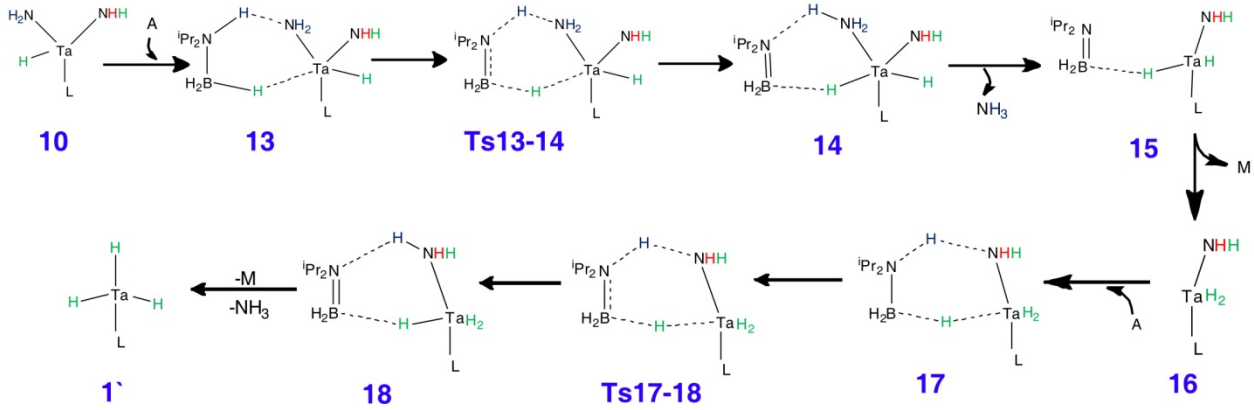
If we now put the value of $k=1.15\times10^{-5}$ s^{-1} in equation 2, we get the $\Delta G^{\ddagger}$ to be equal to 42.9 $kcalmol^{-1}$, which is nearly equal to the $\Delta G^{\ddagger}$ predicted by Li et.al.[3] This finding suggests that the assumptions made by us regarding the reaction kinetics are satisfactory and may be used to check the effect of suppression of barriers on reaction temperatures.

Now according to equation 2, a reaction having $\Delta G^{\ddagger}$ =23.0 $kcalmol^{-1}$ at 298K and 1atm, the rate constant (k_{298K}) is predicted to be 8.9×10^{-5} s^{-1} and the half life of the reaction is estimated to be of 130 min and for 97% completion of the reaction the time required would be 10.8 hours.[10]

For simplicity, we are assuming that Eyring equation (equation 2) is also valid in the amine-borane facilitated NN bond dissociation case. We calculated the rate constant for the RDS i.e for **TS9-10** step using the above equation 2. We found that for N-N bond splitting at an isolated Ta centre on silica surface using amine-borane (A) as a hydrogen carrier, with an associated $\Delta G_{298K,\ Our}^{\ddagger}$ =33.8 $kcalmol^{-1}$ (at 298K, 1atm) the rate constant would be $k_{298K,\ Our}$ = 1.1×10^{-12} s^{-1}. However, if the reaction temperature is raised to 160°C (433K) then a significant rate enhancement can be observed. We calculated the rate constant at 160°C (433K) and 1atm, and it is predicted to be of $k_{433K,\ Our}$= 8.3×10^{-5} s^{-1}. So we can expect that reaction would complete (95 % completion) in a reasonable time frame (less than 12 hours) if the reaction temperature is raised to 160°C (433K). Generally, the default calculations of free energy of activation ($\Delta G^{\ddagger}$) is done at 298K and 1 atm. So, we recalculated the free energy of activation ($\Delta G^{\ddagger}$) at 433K and 1atm. We found that the $\Delta G^{\ddagger}$ remains almost unchanged at 433K and 1atm ($\Delta G^{\ddagger}_{433K,\ our}$ =33.85 $kcalmol^{-1}$). Hence, following our strategy the N-N bond scission can be achieved at a much faster rate ($k_{433K,\ Our}$ $=8.3\times10^{-5}$ sec^{-1}) in less than 12 hours at 433K, which can be a significant development. We also calculated the rate constant for the corresponding RDB for N-N bond cleavage by direct H_2 predicted by Li et.al.[3] by following the above equation 2. They predicted a $\Delta G_{523K,\ Li\ et\ al.}^{\ddagger}$ =43.0 $kcalmol^{-1}$ at 250°C (523K). The rate constant ($k_{523K,\ Li.\ et\ al.}$) is estimated to be $1.24\times10^{-5}s^{-1}$. For comparison, we also calculated the rate constant at 250°C (523K) for the $\Delta G_{523K,\ Our}^{\ddagger}$(33.8 $kcalmol^{-1}$) predicted by us. We found that $k_{523K,\ Our}=8.57\times10^{-2}s^{-1}$. So, $k_{523K,\ Our}/k_{523K,\ Li.\ et\ al.}$ $=6.9\times10^{3}$. These suggest that a

significant amount of rate enhancement would be observed and the NN bon dissociation can be achieved in minutes if we use amine-borane as hydrogen carrier instead of direct dihydrogen for N-N bond splitting at the silica supported tantalum hydride centre.

S7. Possibility of NH_3 formation from intermediate 10.



Scheme 3: Formation of NH_3 from intermediate **10** in presence of excess $^{i}Pr_2NHBH_3$(**A**).

Association of another **A** with **10** can possibly form **13**. From **13**, the proton and hydride of **A** gets transferred to the $(NH_2)(NH_2)$-TaH moiety and produces **14**, a $[(\equiv Si\text{-}O)_2TaH_2(NH_3)(NH_2)]$ species weakly complexed to **M**. The Gibbs free energy barrier for conversion of intermediate **13** into **14** is predicted to be 24.1 kcalmol^{-1}. Dissociation of NH_3 from **14** generates 1**5**, a $[(\equiv Si\text{-}O)_2TaH_2(NH_2)]$ entity feebly linked to **M**. NH_3 removal from **14** is free energetically 7.3 kcalmol^{-1} downhill. Dissociation of **M** from **15** forms $[(\equiv Si\text{-}O)_2TaH_2(NH_2)]$ (**16**). Then again, association of another **A** with **16** can possibly produce **17**. From **17**, the proton and hydride of **A** gets transferred to the (NH_2)-TaH_2 moiety and produces **18**, a $[(\equiv Si\text{-}O)_2TaH_3(NH_3)]$ species weakly complexed to both **M** and NH_3.The Gibbs free energy barrier for conversion of intermediate **17** into **18** is predicted to be 20.3 kcalmol^{-1}. Subsequent dissociation of NH_3 and **M** from **18** produces the trihydride species $[(\equiv Si\text{-}O)_2TaH_3]$ (**1'**). The free energy profile for the overall reaction for formation of NH_3 represented by the equation: **1**+N_2+*4***A** = **1'**+*4***M**+*2*NH_3 is given below.

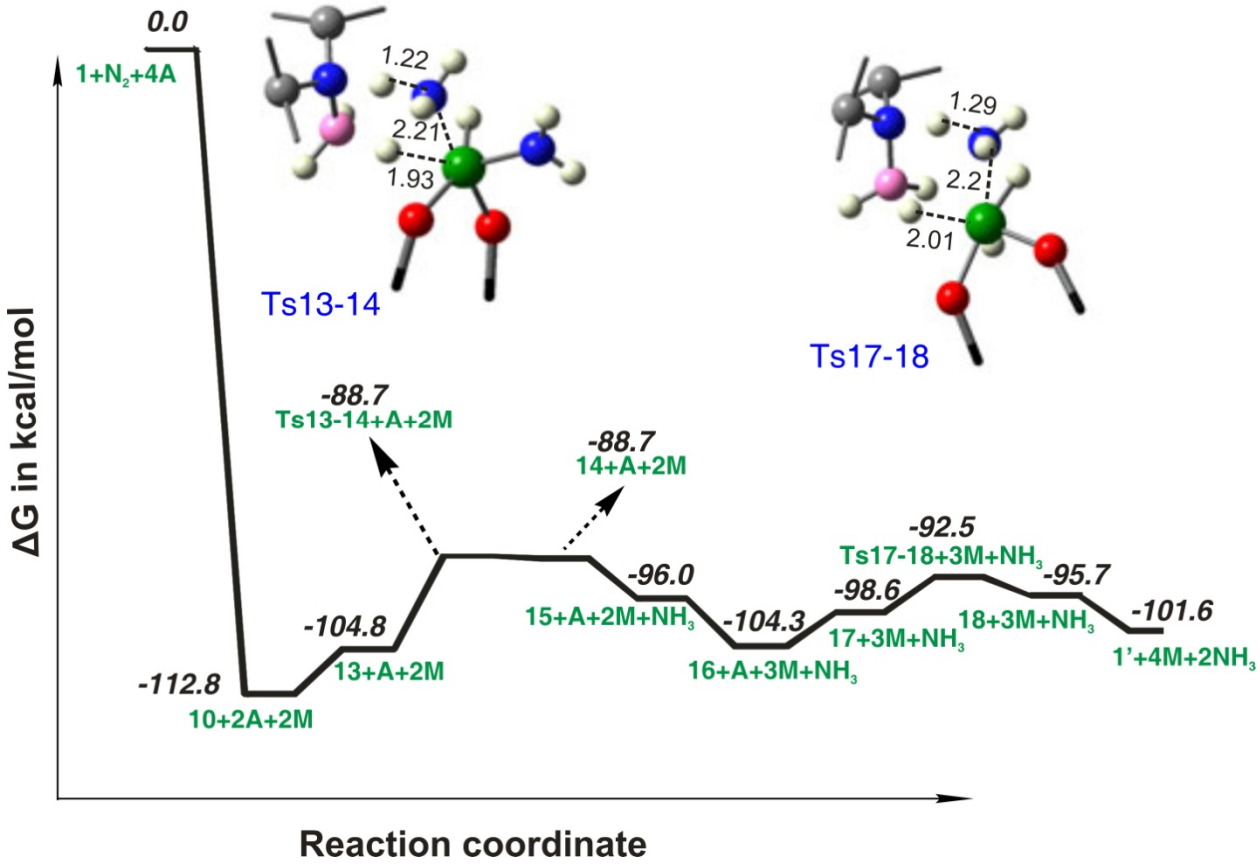


Fig 3. Gibbs free energy profile for possible NH_3formation at the Ta centre linked to silica surface using $^{i}Pr_2NHBH_3$ as hydrogen carrier. All bond lengths in the optimized geometries are in Å. Color code: Ta green, N blue, O red, Si black, H white, C grey, B pink. Isopropyl groups are represented by grey balls and sticks to maintain clarity. The rest of the substituents on Ta centre are omitted for clarity

Intermediate **11** is very similar to **10**, except it has two less number of hydrogen atom. **11** is 5.1 kcalmol^{-1} stable compared to **10**. We believe that in presence of excess **A**, **11** is another possible species from which NH_3 can be formed. In that case the RDS for ammonia formation from **11** and **A** would be associated with a $\Delta G^{\ddagger}$ of 29.2 kcalmol^{-1}.

Although it is known that the surface species **1** consume NH_3,[11] there is still possibility of small amount of NH_3 formation following our strategy if proper reaction monitoring can be achieved. These can be done in the possible following ways:

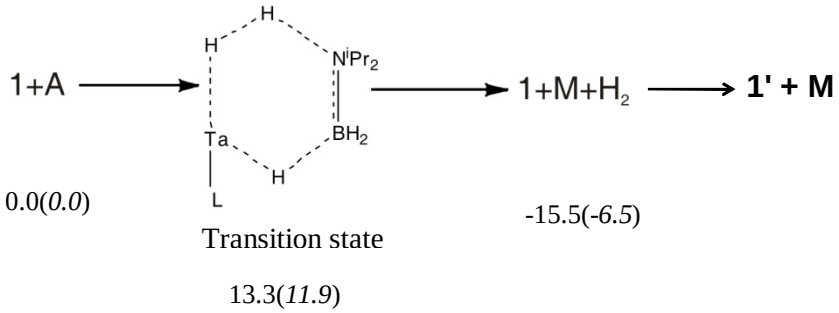
(i) If one can devise a strategy to remove the ammonia (if it is produced) immediately after its generation from the reaction vessel.

(ii) If we can introduce an inert species in to the reaction system, which can trap ammonia and then the trapped ammonia can be released.

(iii) By proper designing of the surface keeping the main active site unchanged, which would not consume ammonia.

S8. Possibility of dehydrogenation of ($^{i}Pr_2NHBH_3$) (A) by species [(≡Si-O)$_2$TaH], 1.

According to the reaction strategy which we mentioned in manuscript and also in S3 the possibility of dehydrogenation of **A** by free **1** species is significantly low. On exposing the surface to N_2 at mildly elevated pressures at room temperature a very large fraction of **1** is likely to get transformed to **2.** Species **2** would react with amine-borane at very low barriers to form **9**, a significantly stable entity. At room temperature conversion of **2** to **9** is practically irreversible as the barrier for **9** reverting to **2** is more than 58 kcal/mol. If our proposed strategy is adopted then bare Ta-H sites (species 1) would be minimized before **A** is introduced in the system. As the number of Ta-H species (**1**) would be minimized largely due to the conversion of those sites to **2**, the small remaining fraction of the sites which are Ta-H sites would either compete in binding N_2 leading to formation of **9** or dehydrogenate amine-borane (as both the rate determining barriers are more or less similar with the former being 14.5 kcal/mol and the later being 13.3 kcal/mol). So we expect only a small amount of loss of amine-borane (**A**) to wasteful would occur due to dehydrogenation of **A** converting Ta-H (**1**) species to TaH_3 (**1'**). Additionally TaH_3 (**1'**) can effectuate N_2 dissociation like the Ta-H (**1**) site on reacting with amine-borane at an overall barrier of 33.8 kcal/mol (which is exactly similar to that in the case of the Ta-H site).



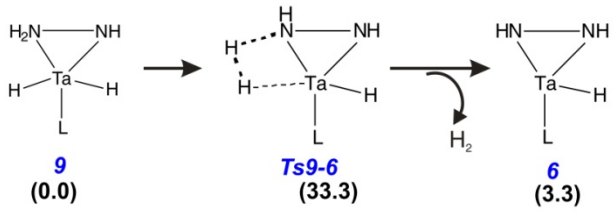
Scheme 4: Dehydrogenation of $^{i}Pr_2NHBH_3$(**A**) by **1**. The relative Gibbs free energy and enthalpy (in parenthesis) of reactants, transition state, and product are given in kcalmol^{-1}.

S9. Possibility of dehydrogenation of 9.

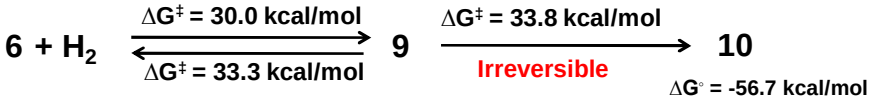
9 can dehydrogenate in three possible ways. These are discussed bellow.

i) **9** can dehydrogenate to intermediate **6**. The free energy activation barrier is estimated to be 33.3 kcal/mol, but the recombination of H_2 to **6** to revert back to **9** is favorable by a barrier of 30 kcal/mol. Hence the reverse reaction is significantly faster. Note that this dehydrogenation leads to a slightly higher energy product. However almost at a similar competitive barrier the NN bond dissociation occurs (with a RDB of 33.8 kcal/mol) producing a hugely thermodynamically favorable product with stabilization gain of 56 kcal/mol (free energy change). Conversion of **9** to **10** would occur irreversibly, as the back reaction from **10** to **9** would happen at an insurmountable barrier over 89 kcal/mol. Note for the original experiment of Basset et al. where only 0.5 Torr H_2 pressure is used to achieve NN bond dissociation, Eisentstein et al. predicts that the RDB for NN bond dissociation in the experiment by Basset et al. is over 47 kcal/mol. This suggests that even at a low dehydrogenation barrier for conversion of **9** to **6** compared to the RDB of 47 kcal/mol, a significant yield of **10** is obtained, suggesting this is thermodynamically controlled reaction and recombination of H_2 to **6** to revert back to **9** is fast. This would hold true in our case also, as it would be carried out in a closed system. Thermodynamic control would inevitably determine the fate of the reaction. **9** would initially loose some H_2 and almost at equal rate **10** would be formed from **9**. As partial pressure of H_2 would

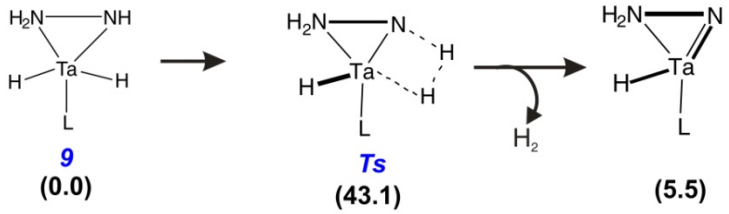
increase in the system recombination of H_2 to **6** to form **9** would become substantial and gradually all of **9** would irreversibly convert to **10**.



Scheme 5 : Dehydrogenation of **9** to form **6**. The relative Gibbs free energy values (in kcalmol^{-1}) are given in parenthesis.

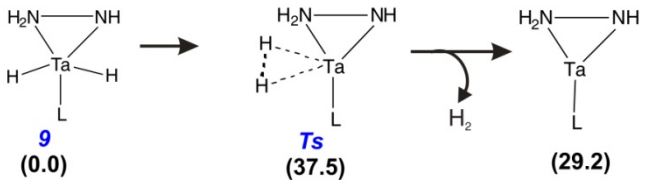


ii) Dehydrogenation of **9** may lead to the formation of an intermediate where the bisprotonated nitrogen, and the other nitrogen making a double bond with the Ta centre. This possibility also has been explored. The Gibbs free energy barrier for this dehydrogenation pathway is estimated to be 43.1 kcal/mol.



Scheme 6 : Possible dehydrogenation pathway of **9**. The relative Gibbs free energy values (in kcalmol^{-1}) are given in parenthesis.

iii) The other way of dehydrogenation of intermediate **9** would lead to the formation of the intermediate [(≡Si-O)$_2$Ta(NH$_2$NH)]. The Gibbs free energy barrier for this dehydrogenation pathway is predicted to be 37.5 kcal/mol.



Scheme 7 : Possible dehydrogenation pathway of **9**. The relative Gibbs free energy values (in kcalmol^{-1}) are given in parenthesis.

All the dehydrogenation reactions of **9** are endoergic and are associated with reasonably high Gibbs free energy barrier of activation or similar to the RDB of NN bond dissociation. On the other hand, the NN bond dissociation step (**Ts9-10**) from **9** is highly exothermic and for all practical purposes is irreversible. So, it is the thermodynamic stability of the product generated from **9**, which turns out to be the deciding factor of the fate of **9** (**THERMODYNAMIC CONTROL OF REACTION**).

S10. Thermodynamics of dehydrogenation of ($^{i}Pr_2NHBH_3$) (A).

The dehydrogenation of **A** can be represented by the equation: $^{i}Pr_2NHBH_3 \rightarrow {}^{i}Pr_2N{=}BH_2 + H_2$

The calculated solvent phase enthalpy change (ΔH_s) for the above reaction in three different solvents at B3LYP, M06L, M062X, M06 and M052X functional is given below.

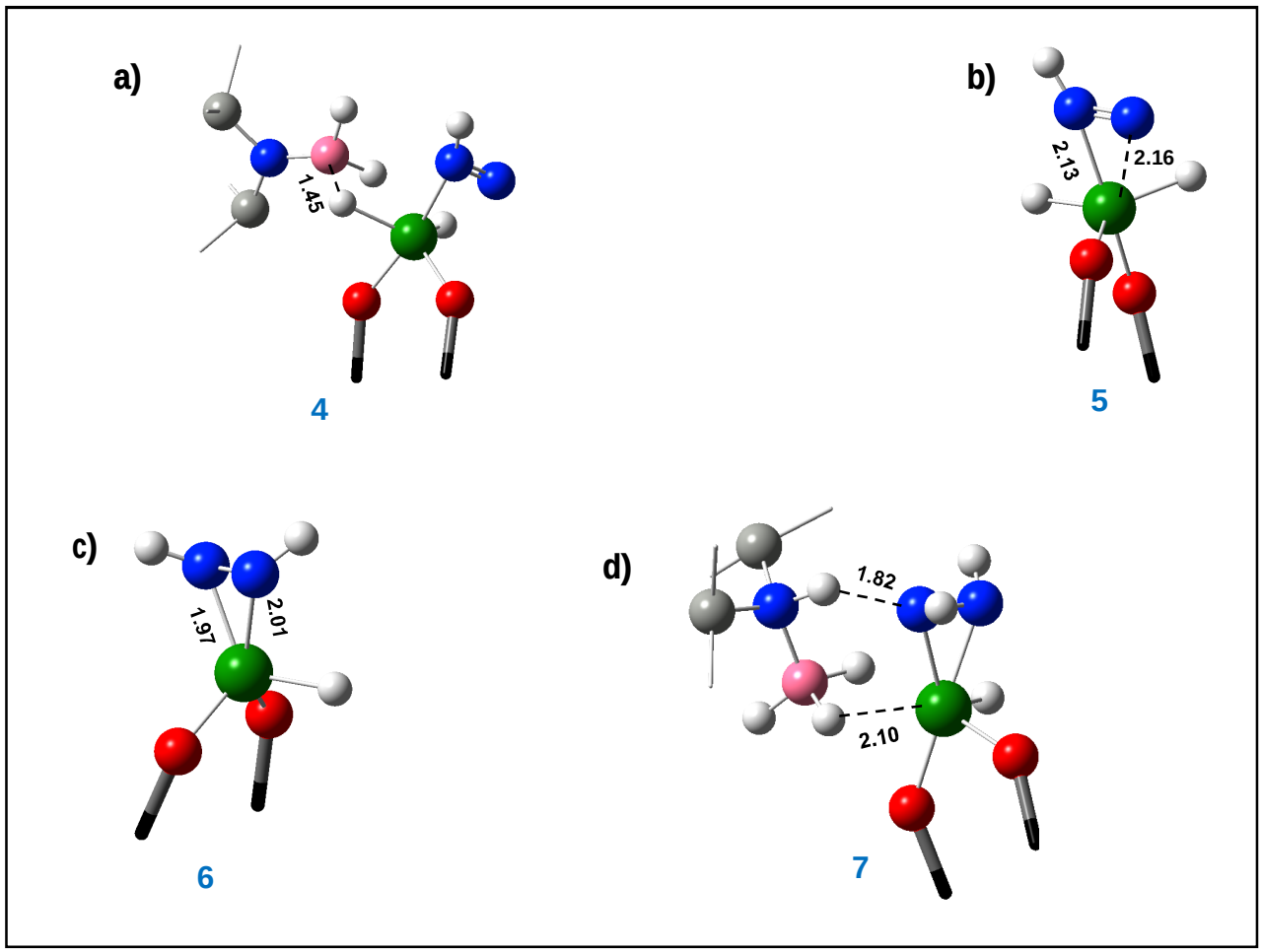
	ΔH_s in kcal/mol
B3LYP/CPCM/THF/6-311++g(d,p)	-2.3
B3LYP/CPCM/Toluene/6-311++g(d,p)	-4.0
B3LYP/CPCM/Acetonitrile/6-311++g(d,p)	-1.6
M06L/CPCM/THF/6-311++g(d,p)	4.9
M06L/CPCM/Toluene /6-311++g(d,p)	3.2
M06L/CPCM/Acetonitrile /6-311++g(d,p)	5.6
M062X/ CPCM/THF/6-311++g(d,p)	1.6
M062X/CPCM/Toluene /6-311++g(d,p)	-0.1
M062X/CPCM/Acetonitrile /6-311++g(d,p)	2.3
M06/CPCM/THF/6-311++g(d,p)	1.3
M06/CPCM/Toluene /6-311++g(d,p)	-0.4
M06/CPCM/Acetonitrile /6-311++g(d,p)	2.0
M052X/ CPCM/THF/6-311++g(d,p)	1.1
M052X/CPCM/Toluene /6-311++g(d,p)	-0.6
M052X/CPCM/Acetonitrile /6-311++g(d,p)	1.8

Solvent phase single point calculation were done using CPCM[12] model on the respective B3LYP and M06L gas phase optimized geometries. For obtaining CPCM enthalpies, (H(s)) thermal corrections for

enthalpies (H_{corr}) were added to the corresponding solution phase total energies (E(s)), which is a fairly standard practice.

The calculated reaction enthalpies (which are consistent in various level of theory) strongly suggest that the reverse reaction i.e. the amino-borane (**M**) can possibly rehydrogenated back into the parent amine-borane (**A**) by proper choice of solvent(preferably acetonitrile) and maintaining other necessary reaction condition. Furthermore, amine-borane (hydrogen carrier) with a general formula $R_2HNBHR'_2$ can be designed by proper choice of R and R' such that the amino-borane ($R_2N{=}BR'_2$) will remain in monomeric and also the rehydrogenation to the parent amine-borane might possibly become more thermodynamically feasible.

S11. Optimized geometries of some important intermediates.



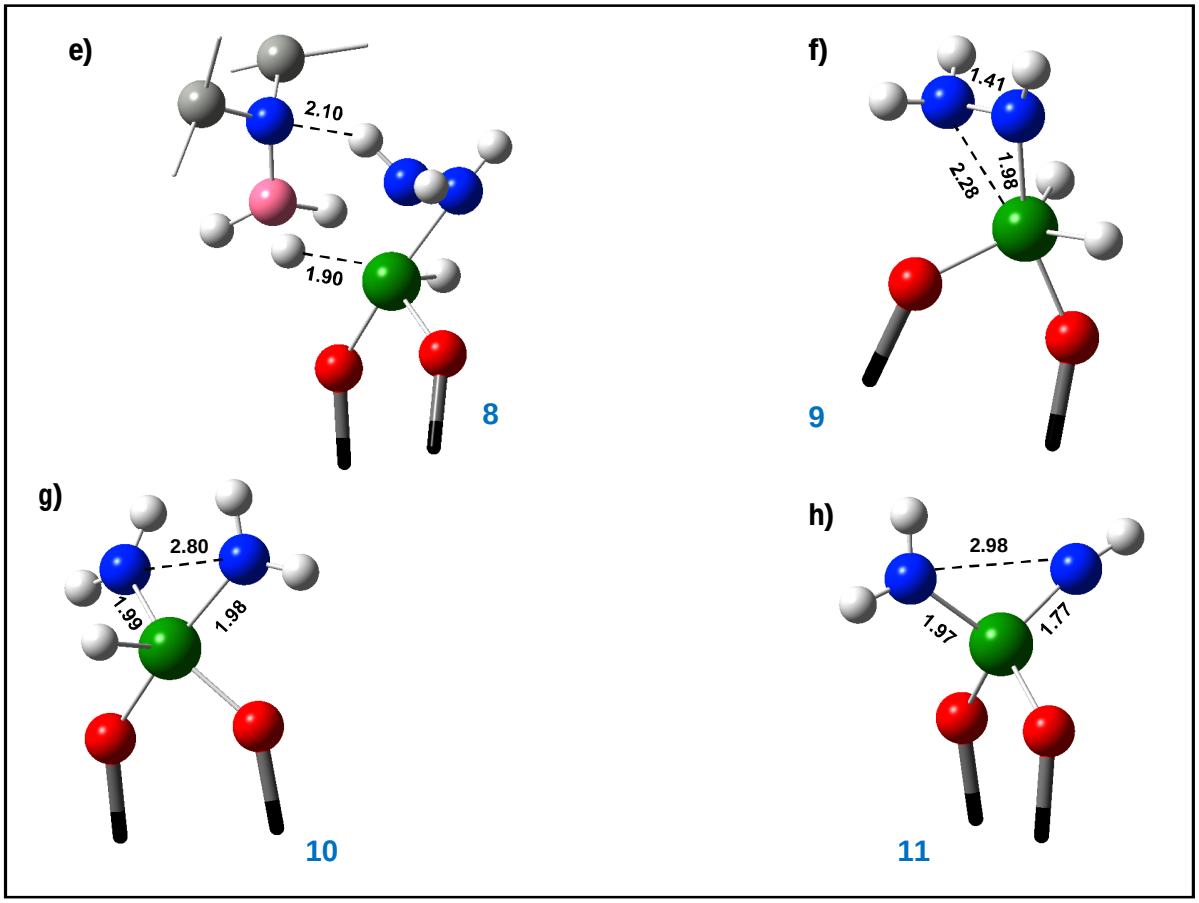


Fig 4: Optimized Geometries of species a) 4, b) 5, c) 6, d) 7, e) 8, f) 9, g) 10, h) 11 optimized at B3LYP/B1 level of theory. All bond lengths in the optimized geometries are in Å. Color code: Ta green, N blue, O red, Si black, H white, C grey, B pink. Isopropyl groups are represented by grey balls and sticks to maintain clarity. The rest of the substituents on Ta centre are omitted for clarity

S12.Table of gas phase total energies, thermal corrections to enthalpy(H_{Corr}) and free energy (G_{Corr}) of all species.

Species	Total Energy in Hartree	H_{corr} in Hartree	G_{corr} in Hartree
1	-1629.926036	0.316279	0.180882
N_2	-109.5596937	0.008875	-0.012863
Ts1-2	-1739.479544	0.325754	0.184345
2	-1739.51884	0.326924	0.185943
A	-319.1797174	0.250981	0.203799
M	-318.0019302	0.228406	0.181684
3	-2058.719894	0.580976	0.414079
Ts3-4	-2058.699184	0.573377	0.412873
4	-2058.727668	0.578408	0.411496
5	-1740.702098	0.346943	0.207362
Ts5-6	-1740.681393	0.344842	0.205894
6	-1740.737766	0.350563	0.21127
7	-2059.945322	0.604619	0.440105
Ts7-8	-2059.938925	0.599267	0.436165
8	-2059.949687	0.603458	0.438413
9	-1741.94641	0.3722	0.232053
Ts9-10	-1741.882462	0.365106	0.225006
10	-1742.03395	0.372902	0.230314
Ts10-11	-1741.983215	0.36744	0.225979
11	-1740.840052	0.352986	0.2118
H_2	-1.179571533	0.01337	-0.001426
1'	-1631.165932	0.332248	0.19664
12	-1740.731149	0.342964	0.200014
Ts12-2	-1740.687043	0.342736	0.202129
13	-2061.226104	0.626113	0.457546
Ts13-14	-2061.196702	0.618028	0.453074
14	-2061.200388	0.624099	0.45606
15	-2004.615634	0.586272	0.426145
16	-1686.594267	0.352216	0.213119
17	-2005.790445	0.607334	0.441862
Ts17-18	-2005.780125	0.601798	0.440117
18	-2005.787545	0.606126	0.441967

Table 2: Gas phase total energies, thermal enthalpy corrections (H_{Corr}) and free energy corrections (G_{Corr}) of all species at their respective optimized geometries at B3LYP/B1.Thermal corrections to enthalpy and free energy are obtained from frequency analysis done at the same level of theory.

S13. B3LYP/B1 optimized geometries of the structures reported in the paper (the atomic symbol followed by the three Cartesian coordinates, in Å).

1

Si	-5.40157700	0.64549300	-1.27384400
Si	-1.87980700	2.53415700	1.65213800
Si	-0.75823800	0.08945400	3.40047500
Si	-4.50007400	-2.09852500	0.09823800
Si	-2.15765100	-3.23522900	-1.75195000
Si	1.57037400	-0.60371500	1.44409000
Si	-2.51843100	2.09817200	-1.43575600
Si	-0.35311000	0.77561400	-3.37538100
Si	0.24064600	4.94357100	1.65221400
Si	2.69620000	4.03263800	-0.22708700
Si	0.52298200	-1.47078600	-1.38599100
Si	3.88761700	1.60933900	1.47928100
Si	2.12716200	2.82575900	-3.17890300
Si	-3.08523800	-2.13670300	3.05673600
O	-4.12863300	1.71377700	-1.46864900
O	-0.95027000	1.53392500	2.60415200
O	-1.94255200	1.90755800	0.11330000
O	-5.03813900	-0.54523200	-0.14184200
O	-0.85377200	-2.33177800	-1.19925200
O	2.58407800	-1.97033700	1.38406500
O	0.83727100	-0.53162100	-0.05123500
O	0.47771200	-0.53432700	-2.73582300
O	3.47761000	3.13866900	0.93861000
O	2.48088100	0.72040200	1.75070200
O	-1.16042000	4.02880300	1.60998900
O	1.23506100	4.56424800	0.35126300
O	1.82075400	-2.57067800	-1.48150800
O	-1.69599300	1.04648900	-2.43654300
O	-3.58918500	-2.55129500	-1.22217400
O	0.43973800	-0.78622000	2.61945800
O	2.47542600	3.06234400	-1.55892900
O	0.61768400	2.11832800	-3.36808100
O	-2.17660400	-0.76290100	3.36674500
O	-3.55640200	-2.20024900	1.45482300
H	-5.64096400	-2.98860300	0.22952600
H	-0.35654800	0.33453900	4.76961100
H	-0.74763000	0.44483200	-4.72812800
H	3.52489600	5.17535000	-0.56847400
H	-6.52956200	1.40589400	-0.74881800
H	-5.69568800	0.01683800	-2.56171700
H	-2.37198100	3.46684000	-1.89268600
H	-0.16670500	6.33679500	1.51356400
H	-3.21274300	2.68507600	2.20321000
H	0.96090600	4.68439000	2.89935800
H	4.56292000	1.77477600	2.75957400
H	-2.17871600	-3.20362200	-3.21162800
H	3.14566000	1.93385800	-3.72643400
H	2.07344100	4.11598600	-3.86304700
H	-2.27369600	-3.32054500	3.32684700
H	-4.27099400	-2.05444500	3.90613500
H	-2.02114100	-4.58557100	-1.21373900
H	4.70567700	0.92365700	0.48046300
Ta	2.95949700	-3.08568500	-0.08007300
H	4.14364100	-4.41963700	-0.12048300

Ts1-2

Si	-5.00708300	-2.51936300	-1.46613300
Si	-3.18907100	0.82544200	1.58069700
Si	-0.81342900	-0.22514500	3.48929400
Si	-2.76778200	-4.08558500	0.19100400
Si	-0.12326900	-3.69738300	-1.65070700
Si	1.48244400	0.59699200	1.54835100
Si	-3.32705200	0.22933400	-1.52614800
Si	-0.74109300	0.37002500	-3.38378100
Si	-3.10063200	4.03001600	1.48229900
Si	-0.53988800	4.82742900	-0.31027600
Si	1.20568600	-0.80882200	-1.23129200
Si	1.90667700	3.77416400	1.44136000
Si	-0.05426600	3.51863900	-3.23713100
Si	-1.34023800	-3.37317800	3.05513300
O	-4.49199800	-0.93843400	-1.67432800
O	-1.85558500	0.67952500	2.56420700
O	-2.80571800	0.28334300	0.05464000
O	-4.15514800	-3.28438600	-0.23476600
O	0.59292800	-2.31355300	-1.01657000
O	3.10774900	0.10687500	1.50840000
O	0.85971500	0.17819400	0.05858800
O	0.67164400	-0.13105100	-2.62980000
O	0.59654200	4.66100200	0.89438000
O	1.40507500	2.20878500	1.81317000
O	-3.60068600	2.43304900	1.49539300
O	-2.01651200	4.29450600	0.22411400
O	2.90068200	-0.94053100	-1.25895400
O	-2.02475800	-0.18447100	-2.48655000
O	-1.66372400	-3.88543500	-1.04084000
O	0.68567600	-0.20401300	2.73774300
O	-0.03791500	3.92537900	-1.61349000
O	-0.78007500	2.02366900	-3.46567200
O	-1.33689000	-1.79085400	3.60416300
O	-2.16622000	-3.46953500	1.60345700
H	-3.05583400	-5.50014800	0.35837800
H	-0.70925100	0.34244700	4.81564800
H	-0.77815100	-0.20143100	-4.71259100
H	-0.63197900	6.23071400	-0.67376800
H	-6.40436000	-2.47580900	-1.05305000
H	-4.81305700	-3.24843600	-2.71949400
H	-3.89578000	1.49489700	-1.94705000
H	-4.28826600	4.83841300	1.23182700
H	-4.31649100	0.09403900	2.12399000
H	-2.45130900	4.35646500	2.75237500
H	2.35934400	4.39728200	2.67758300
H	-0.23496600	-3.55377900	-3.10008000
H	1.33091700	3.45410300	-3.69436800
H	-0.85450000	4.48984500	-3.97981100
H	0.03652500	-3.82009400	2.84901800
H	-2.04563600	-4.16354200	4.05914400
H	0.70637000	-4.83131300	-1.25380700
H	2.94074100	3.71483400	0.40963800

2

Si	-5.17606600	-2.20221000	-1.37947600
Si	-3.07023000	0.96893600	1.69370600
Si	-0.69884800	-0.33200700	3.43801700
Si	-2.96438500	-3.95622000	0.11966300
Si	-0.36531000	-3.66487900	-1.78337700
Si	1.58615100	0.38785000	1.44715500
Si	-3.39402000	0.48191400	-1.41751500
Si	-0.89043600	0.56995800	-3.38362100
Si	-2.79666100	4.16780700	1.69768200
Si	-0.20942100	4.84160200	-0.10460000
Si	1.10507900	-0.83910200	-1.41443900
Si	2.19422400	3.53757100	1.55155000
Si	0.04604800	3.64668600	-3.10189100
Si	-1.51690400	-3.41877800	3.02094600
O	-4.61454700	-0.63079800	-1.53164800
O	-1.70767900	0.69368000	2.60801900
O	-2.78191700	0.46961400	0.13170000
O	-4.31090200	-3.04738100	-0.21082500
O	0.41897600	-2.30728900	-1.16450100
O	3.17455000	-0.21219300	1.35197000
O	0.94413100	0.13154200	-0.07325700
O	0.51778400	-0.08559400	-2.74606100
O	0.92902300	4.51684700	1.06461900
O	1.62037200	1.97610500	1.82876600
O	-3.38172900	2.59985400	1.69251300
O	-1.71460800	4.39388100	0.42990700
O	2.78157800	-1.09058000	-1.57209500
O	-2.16450500	0.04151800	-2.45917700
O	-1.90592900	-3.78051200	-1.15604800
O	0.73807800	-0.44729000	2.57547700
O	0.19710200	3.98196200	-1.46857400
O	-0.81027300	2.22294600	-3.33848200
O	-1.36578800	-1.84051800	3.56239300
O	-2.24801300	-3.43722000	1.51715900
H	-3.34077900	-5.35346800	0.25222700
H	-0.44446200	0.19447700	4.76124400
H	-1.02887700	0.10132300	-4.74530600
H	-0.19615200	6.26662500	-0.38509800
H	-6.55721600	-2.13016400	-0.91950500
H	-5.04408400	-2.88056600	-2.66873600
H	-3.92976300	1.78180100	-1.77184700
H	-3.94130500	5.04327700	1.47482700
H	-4.21850200	0.28552000	2.25571000
H	-2.11557900	4.43682400	2.96451900
H	2.67800600	4.05746400	2.82275500
H	-0.48630400	-3.52285600	-3.23164500
H	1.39120300	3.49218200	-3.64817600
H	-0.71750300	4.70773600	-3.75452200
H	-0.18948300	-4.02015800	2.90673300
H	-2.37021500	-4.11071400	3.98182200
H	0.42245100	-4.82808000	-1.38558200
H	3.22357200	3.48878200	0.51429100
Ta	4.05218100	-0.92133300	-0.17456100
N	5.13359600	-2.66818700	0.23824000
N	5.94958600	-1.90444500	-0.20217800
H	5.05876900	0.41939800	-0.64118900

3

Si	3.78938200	4.67373100	-1.28277600
Si	3.56351800	1.12893800	1.91424600
Si	0.71952500	0.71350800	3.39608000
Si	0.83079600	4.76020900	-0.11945400
Si	-0.76164900	2.95372500	-2.29734900
Si	-0.36963300	-1.34432100	1.32197200
Si	3.89206800	1.45684700	-1.21059600
Si	2.15914200	-0.16053600	-3.32890600
Si	5.30077700	-1.52405000	2.33215300
Si	4.02203100	-3.71187500	0.34147900
Si	-0.50146200	-0.17483800	-1.65174800
Si	1.14534300	-4.14057800	1.62968700
Si	3.31972200	-3.11681400	-2.77572100
Si	-0.42181900	3.62840100	2.67424200
O	4.26085200	3.06755300	-1.34933300
O	2.23462000	0.56365300	2.73281700
O	3.21760900	1.17806900	0.28598500
O	2.48112100	4.88537400	-0.24527300
O	-0.84433200	1.42907200	-1.60409300
O	-1.92699600	-1.98025400	1.13305200
O	0.03375900	-0.73118100	-0.17890300
O	0.60280400	-0.51221300	-2.82243900
O	2.80069100	-4.18067100	1.37024400
O	0.65758300	-2.53486800	1.78424900
O	4.82217100	0.07158400	2.16444600
O	4.84249200	-2.42252400	0.98638800
O	-1.94413700	-1.01123900	-1.94466800
O	2.75591100	1.05836300	-2.36714100
O	0.29247900	3.94002700	-1.46430800
O	-0.35475500	-0.14667100	2.44322100
O	3.33374900	-3.29159700	-1.11178500
O	3.11732000	-1.50485400	-3.19237200
O	0.25227900	2.30140500	3.44013800
O	0.42131500	3.94215400	1.25859700
H	0.24412300	6.09073900	-0.09276100
H	0.72551700	0.19090700	4.74507200
H	2.10995600	0.27942200	-4.70681400
H	4.93747900	-4.82543600	0.16224600
H	4.89979400	5.43588900	-0.72508200
H	3.42196300	5.11761900	-2.62756200
H	5.11295100	0.69872000	-1.40126200
H	6.75781200	-1.51817900	2.39464100
H	3.96477200	2.43340600	2.40270800
H	4.68616000	-2.10252600	3.52749100
H	0.90128900	-4.81207700	2.90005200
H	-0.26175500	2.83500200	-3.66516700
H	2.20328100	-3.89487800	-3.30508200
H	4.60943600	-3.53067200	-3.32486500
H	-1.81890100	3.35591100	2.34857000
H	-0.26862000	4.75949400	3.58641700
H	-2.10597900	3.52192300	-2.23937400
H	0.44374200	-4.75865800	0.50677300
Ta	-2.81700500	-1.98547100	-0.55333600
N	-4.91226600	-2.05540500	-0.60892100
N	-4.55636200	-3.16583600	-0.91359000
H	-2.01399800	-3.46248800	-1.02878200
N	-5.54899300	0.71664200	0.34396600
B	-3.96967100	0.82064200	0.75965500
H	-3.81686600	0.38085000	1.86148700
H	-3.61229800	1.96373800	0.63690000
H	-3.33814700	0.13403100	-0.04656600
H	-5.67383900	-0.22986600	-0.03279200
C	-6.48930400	0.79378900	1.53838200
H	-7.49999100	0.80125700	1.12783500

C	-5.90826600	1.66734000	-0.78674900
H	-5.66038300	2.66356600	-0.41589000
C	-6.37214100	-0.46825200	2.39565100
H	-5.40844900	-0.53227900	2.89928300
H	-7.15960900	-0.45348600	3.15365700
H	-6.50899400	-1.37003400	1.79260900
C	-6.27899500	2.07341000	2.34487000
H	-6.41247100	2.97160500	1.73723500
H	-7.01328400	2.11036200	3.15360400
H	-5.28096000	2.10192900	2.78391000
C	-7.39099800	1.61529300	-1.17470300
H	-8.05512900	2.01155400	-0.40549700
H	-7.54015400	2.22242600	-2.07042700
H	-7.70525200	0.59434700	-1.41437200
C	-5.03507100	1.37100600	-2.00908900
H	-5.27238800	2.08795400	-2.79858400
H	-3.97462900	1.44970600	-1.78114600
H	-5.23510400	0.36870600	-2.40048000

Ts3-4

Si	5.08911600	3.81909600	-1.09123200
Si	4.21944700	-0.04159200	1.86647400
Si	1.47568100	0.59683200	3.39065100
Si	2.22599500	4.72206500	-0.01578000
Si	0.12368500	3.43961600	-2.08463400
Si	-0.38056900	-0.82874800	1.32585700
Si	4.46246000	0.65474900	-1.23728000
Si	2.24216300	-0.33499100	-3.29623700
Si	4.82234700	-3.19050200	1.99680800
Si	2.70378200	-4.63400100	0.04424300
Si	-0.23146100	0.30954500	-1.50119400
Si	-0.05786900	-4.00191200	1.52364300
Si	2.36372800	-3.53866500	-2.98225700
Si	1.19323700	3.77912900	2.94419700
O	5.15327300	2.16010600	-1.29497200
O	2.79937000	-0.15598500	2.72394700
O	3.88148900	0.38461600	0.29586500
O	3.82537600	4.27401500	-0.07591200
O	-0.24194700	1.95290300	-1.39577600
O	-2.00649400	-0.71354000	1.03751800
O	0.35059100	-0.40359300	-0.12349800
O	0.64893800	-0.18693800	-2.80195400
O	1.44651700	-4.62796100	1.13095800
O	0.06679200	-2.34720900	1.77942900
O	4.96229300	-1.52641400	1.88755000
O	4.00145000	-3.80856100	0.66732300
O	-1.83492000	-0.18100100	-1.63775100
O	3.18466700	0.61557900	-2.31059500
O	1.47135100	4.12686300	-1.37543300
O	0.11480900	0.21843500	2.50087200
O	2.18117100	-3.91581200	-1.36239900
O	2.73450700	-1.91487400	-3.18503600
O	1.70807500	2.24104500	3.35672400
O	1.48369100	4.11096500	1.33039700
H	2.13194100	6.17282800	-0.00260400
H	1.31134900	0.15263100	4.75943200
H	2.33272500	0.12495200	-4.66603600
H	3.09260000	-6.00971900	-0.21368200
H	6.32613000	4.23185700	-0.43834900
H	4.90860100	4.44837900	-2.39977800
H	5.47323200	-0.31883100	-1.60379200

H	6.17919300	-3.72451400	1.96850000
H	5.11618000	0.92369500	2.47343700
H	4.09960400	-3.54666100	3.21844100
H	-0.45666600	-4.62485900	2.77946800
H	0.43326200	3.25361500	-3.50002700
H	1.09627300	-3.82624700	-3.64909100
H	3.48233200	-4.29554100	-3.54104700
H	-0.24850300	3.88381300	3.15736700
H	1.95415500	4.71288800	3.77139400
H	-1.03691200	4.30057400	-1.86805100
H	-0.99942500	-4.26249300	0.43457900
Ta	-3.26221700	-0.66930200	-0.47121700
N	-4.89237300	-0.04208900	-1.56365100
N	-4.63788100	-1.07759000	-2.14939300
H	-3.43228100	-2.40082900	-0.36656800
N	-6.38748500	0.55510100	0.38252200
B	-5.11327100	0.06605200	1.10435900
H	-4.85765800	-1.13032700	0.80177600
H	-5.03484200	0.19966700	2.29234400
H	-4.06479200	0.67496900	0.66620100
H	-5.84074600	0.40527300	-1.17537400
C	-7.57584000	-0.34304400	0.59998700
H	-8.44730900	0.23242600	0.27807600
C	-6.76096900	1.98912700	0.61901500
H	-7.39103400	2.03312500	1.51900500
C	-7.52773300	-1.59623000	-0.28033600
H	-6.68789500	-2.24703000	-0.02657500
H	-8.44353400	-2.17580400	-0.13682600
H	-7.45678800	-1.34488800	-1.34112100
C	-7.80007700	-0.71731700	2.07471400
H	-7.79998900	0.16153700	2.72359300
H	-8.76837300	-1.21415200	2.18416200
H	-7.02946000	-1.40079800	2.43865700
C	-7.56949800	2.54499000	-0.56422100
H	-8.44167800	1.93500200	-0.80686000
H	-7.92863800	3.55211200	-0.33520600
H	-6.94411200	2.61051000	-1.46052900
C	-5.55084900	2.89544700	0.87052200
H	-5.89954500	3.91909800	1.02962500
H	-4.98425500	2.59681600	1.75294700
H	-4.87335100	2.91010000	0.01142900

4

Si	-5.50466600	-3.44692700	-0.69737400
Si	-3.53124200	-0.07719800	2.37894100
Si	-0.52240400	-0.81823200	3.25536300
Si	-2.58207300	-4.58336700	-0.10102400
Si	-0.82090700	-3.23699200	-2.47933800
Si	0.85422800	0.73252400	0.93100500
Si	-4.53382400	-0.37398300	-0.62185500
Si	-2.74361700	0.66103600	-3.04510900
Si	-3.96259600	3.06276000	2.87375700
Si	-2.29538900	4.65112300	0.61631700
Si	0.00277500	-0.22061200	-1.82869900
Si	0.71685500	3.89292200	1.34893500
Si	-2.65361700	3.83526900	-2.49701600
Si	-0.54823800	-3.91536300	2.39251800
O	-5.41604600	-1.77523400	-0.68318700
O	-1.94807200	-0.04913500	2.88709300

O	-3.58877800	-0.38890500	0.74759800
O	-4.17358900	-4.14529100	0.05632000
O	-0.15036800	-1.86406200	-1.78498000
O	2.36991000	0.57815400	0.26655900
O	-0.21349900	0.44687100	-0.32014100
O	-1.09611500	0.42571700	-2.87632700
O	-0.82227100	4.55276800	1.38224900
O	0.63008400	2.22965100	1.57564500
O	-4.19526100	1.41820200	2.67167400
O	-3.42795700	3.76553200	1.44391700
O	1.56683500	0.14352500	-2.27401800
O	-3.53296300	-0.31706000	-1.95673000
O	-2.00091700	-3.89267200	-1.49985000
O	0.63083200	-0.38224000	2.12621000
O	-2.11463700	4.06282800	-0.92846400
O	-3.12905400	2.24655000	-2.74518600
O	-0.72267500	-2.46433500	3.20725400
O	-1.71294100	-4.05937000	1.20339800
H	-2.48637900	-6.03076800	-0.19597900
H	-0.09190500	-0.43388100	4.58290100
H	-3.11955400	0.29998200	-4.39578000
H	-2.70831800	6.04333300	0.57745000
H	-6.67888600	-3.83237200	0.07611300
H	-5.57337000	-3.90486200	-2.08546700
H	-5.45913900	0.74262800	-0.62016500
H	-5.26717300	3.63227200	3.19120400
H	-4.29091900	-1.06786600	3.11654500
H	-2.97185800	3.29768400	3.92495500
H	1.44274200	4.45681400	2.47982500
H	-1.45189700	-2.88275700	-3.74880900
H	-1.54565300	4.15179400	-3.39461500
H	-3.83154500	4.66691600	-2.73604900
H	0.77338400	-3.96863900	1.76718300
H	-0.74381700	-4.97489300	3.37753200
H	0.26349000	-4.20329500	-2.64337300
H	1.35233000	4.17878100	0.06244400
Ta	3.28489900	0.47944900	-1.44584100
N	4.38576900	-0.05466700	-3.18251200
N	3.95308500	1.05669500	-3.44653300
H	3.71504200	2.15677500	-1.24516100
N	5.80507500	-0.53600700	1.01734900
B	5.44818700	-0.30757500	-0.34001700
H	6.18925900	-0.71008600	-1.18654100
H	5.02045300	0.88717000	-0.57914900
H	4.19379700	-0.93033900	-0.73225600
C	6.92412600	-1.44003700	1.36681900
H	6.96472100	-1.47840400	2.45839100
C	5.03942600	0.05258900	2.13509100
H	4.28013300	0.68047500	1.66939500
C	6.68464500	-2.87589300	0.87596900
H	6.64981300	-2.91475900	-0.21610400
H	7.49036200	-3.53672800	1.21075000
H	5.73950400	-3.26683800	1.26005200
C	8.27813200	-0.89969900	0.88378900
H	8.45093200	0.10970000	1.26380000
H	9.09372900	-1.54204500	1.23038100
H	8.31873600	-0.86262100	-0.20757200
C	5.90517500	0.96058800	3.02298200
H	6.38996600	1.73779400	2.42686700
H	5.28149500	1.44910800	3.77720300
H	6.68216200	0.40306000	3.55412100
C	4.29050500	-1.00539300	2.96007900
H	3.68325400	-0.51992200	3.72920700
H	3.61994100	-1.58550600	2.32338700
H	4.97612200	-1.69263500	3.46566200
H	4.99676800	-0.56545300	-3.84056400

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Si	5.20559900	-2.05257100	1.47702900
Si	3.20581700	1.37186200	-1.47891300
Si	1.13836500	-0.15156600	-3.40461300
Si	3.11588800	-3.91779500	-0.05197300
Si	0.44074200	-3.75296100	1.72144900
Si	-1.33060900	0.29469800	-1.56061300
Si	3.36068900	0.59101700	1.60598500
Si	0.70894100	0.46477300	3.36747800
Si	2.50859100	4.50691400	-1.42924000
Si	-0.20562900	4.86739300	0.26943200
Si	-1.05598500	-0.95235700	1.21635000
Si	-2.29216000	3.33857600	-1.61191800
Si	-0.40106900	3.48660900	3.18677900
Si	2.07188000	-3.22391500	-3.08436800
O	4.58892000	-0.51574900	1.71755900
O	1.96958500	0.98553600	-2.52219500
O	2.88956500	0.71892300	0.01659500
O	4.36885900	-2.87457000	0.26999200
O	-0.34744800	-2.42733900	1.06136500
O	-2.82038600	-0.44154400	-1.47951400
O	-0.66820300	0.05469000	-0.04340800
O	-0.62281100	-0.24557400	2.64145600
O	-1.23176300	4.46831000	-0.97581000
O	-1.47512000	1.89750500	-1.90043000
O	3.28251600	3.02561800	-1.35111000
O	1.37118100	4.65160500	-0.20038900
O	-2.71876600	-1.18459100	1.14015600
O	2.06649400	0.04209900	2.50656300
O	2.02886300	-3.82496000	1.20606600
O	-0.36062700	-0.39119400	-2.70159700
O	-0.56180100	3.89450300	1.57125000
O	0.54678500	2.11536800	3.37170600
O	1.97729500	-1.58223000	-3.40217300
O	2.35148400	-3.51402400	-1.46187800
H	3.63116100	-5.27343400	-0.15031900
H	0.97519900	0.31917400	-4.76429100
H	0.80394500	-0.03540900	4.72285100
H	-0.41577600	6.26204000	0.61645600
H	6.58155700	-1.90577600	1.01669300
H	5.11040600	-2.80178200	2.73021700
H	3.84736300	1.85676100	2.12059000
H	3.53122700	5.52310900	-1.20913600
H	4.47860700	0.89467600	-1.98515300
H	1.84022800	4.64730000	-2.72357300
H	-2.74975000	3.86156500	-2.89261600
H	0.46708100	-3.62308400	3.17647700
H	-1.73868800	3.21734300	3.70842300
H	0.27898000	4.56553400	3.90075100
H	0.80362200	-3.85871400	-3.43445400
H	3.19551500	-3.73658400	-3.86487000
H	-0.27568900	-4.94554800	1.27534300
H	-3.38486300	3.10035600	-0.66837400
Ta	-4.06945300	-1.19302400	-0.21414200
N	-5.59032000	-2.18497500	0.90754300
N	-5.55817000	-1.04354900	1.35266000
H	-5.12672700	0.14089100	-0.68350400
H	-4.13685500	-2.65737600	-1.17060800
H	-6.27886900	-2.86915400	1.25635100

Ts5-6

Si	-5.31303000	-1.92719900	-1.51763600
Si	-3.11200700	1.19515300	1.62539800
Si	-0.88539100	-0.24281800	3.45604900
Si	-3.28895100	-3.80067500	0.10026800
Si	-0.60025900	-3.67160300	-1.70277400
Si	1.48354100	0.31284800	1.51292000
Si	-3.37833900	0.64506800	-1.48625200
Si	-0.80423700	0.52715100	-3.36410900
Si	-2.53883600	4.35133900	1.59528800
Si	0.09621200	4.83985000	-0.19178500
Si	0.99733600	-0.92605700	-1.26496800
Si	2.32997700	3.39381200	1.58161900
Si	0.30863900	3.55014000	-3.15298500
Si	-1.82022700	-3.28803000	2.99684100
O	-4.66341100	-0.38836200	-1.64447000
O	-1.80576300	0.83610900	2.58905200
O	-2.84344700	0.61416500	0.08949100
O	-4.55856100	-2.81429500	-0.30534500
O	0.22042100	-2.35627600	-1.05229000
O	2.99793200	-0.37129600	1.36776900
O	0.76332300	0.09850400	0.01646800
O	0.53907200	-0.19431900	-2.66574400
O	1.19419600	4.47924900	1.00416700
O	1.59733100	1.91037800	1.88161800
O	-3.27187400	2.84821000	1.55796200
O	-1.44357300	4.50538300	0.32820100
O	2.65590400	-1.25843800	-1.29154000
O	-2.14008400	0.10763200	-2.47027600
O	-2.16561600	-3.72301900	-1.12855100
O	0.58182900	-0.43149500	2.67136600
O	0.46633800	3.92290300	-1.52879800
O	-0.62730700	2.17485500	-3.36510000
O	-1.64206800	-1.71448400	3.53962600
O	-2.60939500	-3.30452600	1.52310600
H	-3.76283200	-5.16769500	0.23605100
H	-0.67527300	0.26318200	4.79550300
H	-0.93295500	0.03166500	-4.71771700
H	0.20528000	6.25337000	-0.50793000
H	-6.71111500	-1.77963100	-1.13205100
H	-5.15195700	-2.61781300	-2.79746300
H	-3.81266200	1.97153000	-1.87930300
H	-3.59588500	5.33652500	1.39753300
H	-4.33198400	0.64179700	2.17977100
H	-1.83200900	4.52758100	2.86456100
H	2.81552000	3.91958800	2.85050200
H	-0.66758200	-3.52494900	-3.15465500
H	1.64811900	3.30385000	-3.68047800
H	-0.38255200	4.63762200	-3.84243200
H	-0.50214200	-3.89971200	2.83349500
H	-2.64339200	-3.98080900	3.98353800
H	0.11532300	-4.87532400	-1.28761600
H	3.39464000	3.21677900	0.59263400
Ta	4.03787200	-1.26738000	0.00148800
N	5.85519700	-2.01845500	-0.62413400
N	5.76470800	-0.76421000	-0.95432700
H	5.39170500	0.02088400	0.25190300
H	3.95484900	-2.80569500	0.82390100
H	6.76893000	-2.42803800	-0.43309700

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Si	-5.24219000	-1.96563800	-1.32958700
Si	-3.09191600	1.38452700	1.63577000
Si	-0.95424300	-0.24636300	3.37580900
Si	-3.13602600	-3.93742300	0.05137900
Si	-0.49031000	-3.77186900	-1.72585500
Si	1.44395700	0.25133100	1.44433700
Si	-3.43600000	0.70569500	-1.45394900
Si	-0.89079300	0.61129700	-3.37430300
Si	-2.38833400	4.51895600	1.63563700
Si	0.24864900	4.88076300	-0.17849200
Si	0.97713200	-0.92444900	-1.39039400
Si	2.42216500	3.30566500	1.57802000
Si	0.29726300	3.59989800	-3.14578300
Si	-1.98062400	-3.29861400	3.04926400
O	-4.66476100	-0.40385500	-1.49811500
O	-1.80040800	0.94993300	2.59269000
O	-2.84396200	0.80319600	0.09809700
O	-4.34978300	-2.82949400	-0.19458000
O	0.18508000	-2.34118500	-1.16104600
O	2.95183800	-0.51519400	1.36201500
O	0.77842900	0.07779800	-0.07219600
O	0.46435800	-0.14817400	-2.74662900
O	1.32526800	4.42822200	1.00698300
O	1.65840900	1.82913000	1.83269000
O	-3.17198200	3.04183700	1.59208500
O	-1.30507900	4.65499300	0.35638700
O	2.62970800	-1.24571800	-1.46722900
O	-2.20823500	0.18585400	-2.45690100
O	-2.08969600	-3.87686500	-1.24355000
O	0.50304400	-0.47205700	2.57775800
O	0.54313200	3.95426900	-1.52681200
O	-0.69057200	2.25717000	-3.32461600
O	-1.82024400	-1.65635100	3.34591100
O	-2.29137700	-3.59442300	1.43434600
H	-3.71137900	-5.26814900	0.14860400
H	-0.69811200	0.15537200	4.74313500
H	-1.06745400	0.16374100	-4.73943200
H	0.45814000	6.28598000	-0.47961400
H	-6.60611400	-1.86926400	-0.82295300
H	-5.16833000	-2.64401400	-2.62379700
H	-3.96399000	1.98079900	-1.89996600
H	-3.41290500	5.54196900	1.46305900
H	-4.33763500	0.88404100	2.18431500
H	-1.65853800	4.65365500	2.89696500
H	2.90096400	3.78504800	2.86720000
H	-0.48312300	-3.76680700	-3.18621800
H	1.60378100	3.31749900	-3.73448000
H	-0.38856900	4.71664700	-3.79236100
H	-0.72971100	-3.97165300	3.38880500
H	-3.11040800	-3.75917400	3.85282000
H	0.27339100	-4.87890300	-1.15722600
H	3.49989100	3.12022300	0.60368000
Ta	3.92035800	-1.34659800	-0.04912900
N	5.86184000	-1.81210000	0.24131600
N	5.68657700	-0.63361800	-0.57386900
H	6.12526000	0.19697400	-0.18256700
H	3.76053500	-3.07130900	0.18634900
H	6.36168300	-2.53653400	-0.26623300

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Si	5.15761800	3.79486400	-1.03038300
Si	4.15139500	-0.01689500	1.98532900
Si	1.34489900	0.63763500	3.37933700
Si	2.25285200	4.68244700	-0.06574600
Si	0.27345500	3.35892400	-2.24539100
Si	-0.46751300	-0.76548400	1.25503700
Si	4.53066300	0.63147900	-1.11538500
Si	2.39910300	-0.41194800	-3.23889300
Si	4.73449900	-3.16565600	2.19265900
Si	2.67540900	-4.64299600	0.20570800
Si	-0.17156800	0.26119300	-1.58991400
Si	-0.15619400	-3.93039300	1.50838200
Si	2.51474400	-3.60886000	-2.86014800
Si	1.11895700	3.80483300	2.87695200
O	5.23260900	2.13208200	-1.19253000
O	2.69616000	-0.12484300	2.78047700
O	3.89032500	0.41567700	0.40234600
O	3.86411200	4.27348900	-0.06476900
O	-0.19459900	1.91221800	-1.54032800
O	-2.06263600	-0.61229400	0.90196300
O	0.35540500	-0.40333300	-0.16784200
O	0.78605000	-0.25257200	-2.83128900
O	1.37591900	-4.56070800	1.23570200
O	-0.05351100	-2.27850600	1.77240000
O	4.88514200	-1.50628900	2.03530500
O	3.97042200	-3.82965000	0.85240700
O	-1.75939300	-0.23538700	-1.80627500
O	3.29804900	0.56596600	-2.23795500
O	1.56448600	4.05102900	-1.44168400
O	0.02294000	0.29626700	2.42625700
O	2.23739100	-3.97044500	-1.25110900
O	2.89162400	-1.98646700	-3.06134000
O	1.60310900	2.28188100	3.37096200
O	1.48195000	4.07755000	1.26648800
H	2.12600500	6.13126000	-0.07796100
H	1.11541900	0.19170200	4.73868900
H	2.55885500	0.01070700	-4.61488900
H	3.04025000	-6.03674200	0.01644500
H	6.37341800	4.22848200	-0.35125700
H	5.01695000	4.39251400	-2.35875100
H	5.55148400	-0.35602100	-1.41027800
H	6.09009300	-3.70227100	2.23778300
H	5.02630700	0.94243500	2.63287300
H	3.96229900	-3.48015200	3.39541400
H	-0.64553700	-4.55394600	2.73251600
H	0.70710200	3.11624900	-3.61932900
H	1.29160500	-3.91159100	-3.59915600
H	3.66790700	-4.36724800	-3.34217800
H	-0.33000300	3.93004700	3.02410000
H	1.84912900	4.76492400	3.70230600
H	-0.87901900	4.25539000	-2.17146200
H	-1.00808200	-4.20474600	0.35168100
Ta	-3.25803000	-0.64800600	-0.70237500
N	-4.89381000	0.13291600	-1.78871100
N	-4.56583800	-1.23003700	-2.10341400
H	-3.21195300	-2.37814800	-0.52746200
N	-6.31474200	0.58390600	0.56474600
B	-4.93851900	0.05174400	1.16058100
H	-4.78191700	-1.10990800	0.76085900
H	-4.84724300	0.10816000	2.34698100
H	-4.04536400	0.74309400	0.66327700
H	-6.09439500	0.53179000	-0.46652000
C	-7.50721600	-0.32501500	0.83596000
H	-8.39003100	0.27830400	0.61394900

C	-6.66534500	2.03236000	0.88484900
H	-7.23887000	1.99728300	1.81482900
C	-7.51845800	-1.52069400	-0.11672300
H	-6.68033400	-2.19423300	0.06944900
H	-8.44119300	-2.08672500	0.03214200
H	-7.48520000	-1.19760900	-1.15982500
C	-7.58648200	-0.75925800	2.30016400
H	-7.53064700	0.08786300	2.98711100
H	-8.54248100	-1.26188300	2.46796500
H	-6.78607500	-1.45415600	2.55811000
C	-7.53687800	2.61809400	-0.23282500
H	-8.43369300	2.02787400	-0.43036800
H	-7.86159300	3.62372700	0.04349400
H	-6.96771800	2.69139400	-1.16367000
C	-5.44024200	2.91694200	1.11838100
H	-5.78583200	3.92518500	1.36112500
H	-4.82528500	2.56340000	1.94482300
H	-4.81593100	2.98614100	0.22435200
H	-5.35122700	-1.86500600	-2.02767900
H	-4.62086400	0.72280000	-2.57531700

Ts7-8

Si	5.16010600	3.77348900	-1.04069900
Si	4.20717900	-0.07231200	1.91446200
Si	1.44252800	0.59586400	3.38574500
Si	2.28408100	4.69778000	-0.01829900
Si	0.21973400	3.43417300	-2.14380100
Si	-0.40312600	-0.79731400	1.28519200
Si	4.49570200	0.61836600	-1.18772500
Si	2.29513900	-0.34995400	-3.27779700
Si	4.76393200	-3.22854600	2.05716100
Si	2.65952400	-4.65483400	0.07926100
Si	-0.21081600	0.32228700	-1.53925400
Si	-0.11130900	-3.96957100	1.51015700
Si	2.36617400	-3.55355900	-2.95305600
Si	1.19600600	3.77325500	2.92764700
O	5.20771500	2.11459000	-1.24771400
O	2.77552800	-0.17054300	2.75304900
O	3.89822300	0.36734300	0.34181500
O	3.88302800	4.24460200	-0.05002600
O	-0.21566400	1.96982400	-1.45185400
O	-2.01588600	-0.66989100	0.98139100
O	0.36046600	-0.38132300	-0.15333400
O	0.69400800	-0.17652400	-2.82566800
O	1.38909900	-4.62909400	1.14912900
O	0.04256900	-2.31653500	1.74777600
O	4.92985500	-1.56753500	1.93790500
O	3.96236100	-3.84779500	0.71691900
O	-1.81011200	-0.16012400	-1.70727800
O	3.23016900	0.59067700	-2.27495200
O	1.55202900	4.10332700	-1.38966900
O	0.09727600	0.24542600	2.46606300
O	2.16758700	-3.93342300	-1.33658000
O	2.76529900	-1.93619400	-3.15110200
O	1.70026200	2.23851800	3.36315100
O	1.51790700	4.09481500	1.31750800
H	2.19608100	6.14924700	-0.01046700
H	1.24383000	0.15174200	4.75029800

H	2.42698500	0.10251100	-4.64708900
H	3.03336100	-6.03624900	-0.17147700
H	6.38902900	4.17052700	-0.36286000
H	5.01487800	4.40760900	-2.35148500
H	5.49799100	-0.37004800	-1.53787400
H	6.11385400	-3.78101100	2.06014800
H	5.10995900	0.87707600	2.53762400
H	4.01344500	-3.56505700	3.26762200
H	-0.53731800	-4.57363900	2.76698900
H	0.58399600	3.22160400	-3.54263400
H	1.09892500	-3.81957600	-3.62951600
H	3.47541000	-4.32781400	-3.50736100
H	-0.24942200	3.88409400	3.11208400
H	1.94208100	4.71276800	3.76217600
H	-0.92617800	4.32864700	-1.99125400
H	-1.03880000	-4.23398800	0.41073300
Ta	-3.26066200	-0.63946900	-0.56212000
N	-4.95666700	0.16846800	-1.65502500
N	-4.60430000	-1.18710100	-1.91709800
H	-3.20140600	-2.37228200	-0.43384600
N	-6.28603200	0.56796800	0.49505000
B	-4.98157600	0.08211500	1.19942000
H	-4.76652100	-1.10436800	0.88216400
H	-4.88601200	0.21749500	2.38174100
H	-4.02069000	0.72688800	0.70733800
H	-5.82698700	0.42751400	-0.71144000
C	-7.48715800	-0.31227100	0.74681800
H	-8.35762300	0.28114000	0.45650700
C	-6.65451300	2.01546200	0.71784400
H	-7.29236100	2.05359400	1.60915700
C	-7.48602000	-1.56018200	-0.14048500
H	-6.63807200	-2.21185700	0.07844700
H	-8.40019700	-2.13241900	0.03759500
H	-7.46167000	-1.29198100	-1.19949700
C	-7.65920000	-0.68550400	2.22530100
H	-7.62035300	0.19160800	2.87513000
H	-8.63057000	-1.16676900	2.36983300
H	-6.88463500	-1.38022100	2.55661400
C	-7.45167600	2.55686700	-0.47916200
H	-8.31697000	1.93965400	-0.72884900
H	-7.81914800	3.56231900	-0.25831800
H	-6.81747900	2.62098600	-1.36820100
C	-5.44980800	2.92358300	0.98104800
H	-5.80820700	3.94408400	1.13991300
H	-4.88936400	2.62409200	1.86632800
H	-4.76543500	2.94447100	0.12846700
H	-5.36941400	-1.83263200	-2.05466900
H	-4.78117400	0.76895600	-2.45920300

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Si	5.15613400	3.79946600	-1.04027500
Si	4.18008500	-0.02011400	1.94894800
Si	1.39449700	0.62155800	3.39814200
Si	2.26740200	4.68458500	-0.03122900
Si	0.25886000	3.38818800	-2.19786100
Si	-0.39931100	-0.79058400	1.27177200
Si	4.49830800	0.64193700	-1.15527800
Si	2.33872500	-0.38355400	-3.26066700
Si	4.76266700	-3.17340400	2.11039100
Si	2.69299800	-4.64919300	0.13134500
Si	-0.19474500	0.28386600	-1.56547000

Si	-0.10855900	-3.96203900	1.50556900
Si	2.47258600	-3.58670100	-2.91828600
Si	1.13994100	3.79147900	2.91086000
O	5.20350600	2.13942500	-1.24253900
O	2.73997200	-0.12880200	2.77215800
O	3.88720100	0.42384800	0.37452500
O	3.87789700	4.27337700	-0.05244400
O	-0.20964100	1.93292600	-1.50797300
O	-2.01389000	-0.67228500	0.93564400
O	0.37479500	-0.38972200	-0.16103900
O	0.72793600	-0.23255600	-2.83308300
O	1.40454900	-4.60772300	1.17901000
O	0.02573900	-2.30753000	1.75381600
O	4.90881500	-1.51223800	1.97242300
O	3.97911600	-3.81764100	0.77076300
O	-1.78665500	-0.21131800	-1.72934400
O	3.24254400	0.58199300	-2.25344200
O	1.56534200	4.06052600	-1.40486400
O	0.06707100	0.26426300	2.45119100
O	2.21833500	-3.96313100	-1.30846600
O	2.83267800	-1.96011200	-3.11170000
O	1.63054900	2.26596500	3.39533900
O	1.50983800	4.06824700	1.30264100
H	2.14077200	6.13319100	-0.03270300
H	1.18075800	0.16050800	4.75429400
H	2.48214000	0.05707500	-4.63278500
H	3.07901200	-6.03338800	-0.08179300
H	6.38365800	4.19975800	-0.36201500
H	5.01283200	4.42769100	-2.35396100
H	5.50724500	-0.35023800	-1.47445500
H	6.11877700	-3.70981700	2.12969300
H	5.06990400	0.93188700	2.58627500
H	4.00539400	-3.50508200	3.31790300
H	-0.56367200	-4.57242400	2.74840500
H	0.67072200	3.15751200	-3.58078400
H	1.24096200	-3.89230400	-3.64247800
H	3.62390700	-4.33290400	-3.42255800
H	-0.30946600	3.90676800	3.05429200
H	1.86621300	4.74817000	3.74296500
H	-0.88879900	4.28761300	-2.09754300
H	-1.00541400	-4.22412600	0.38001100
Ta	-3.26467800	-0.62955800	-0.57121000
N	-4.79231500	0.23281700	-1.97357600
N	-4.57379100	-1.16041800	-1.95891500
H	-3.32051600	-2.35455600	-0.36138600
N	-6.35161600	0.57341400	0.51124600
B	-5.00900100	0.15790400	1.07884200
H	-4.74234800	-1.04441600	0.81952700
H	-4.73030800	0.38517500	2.22544700
H	-4.05599300	0.77836100	0.44598400
H	-5.63903000	0.54507400	-1.47061500
C	-7.45498500	-0.39574600	0.79536400
H	-8.38852000	0.14240200	0.61324000
C	-6.77707800	1.96728500	0.82661000
H	-7.28525500	1.97928400	1.80537900
C	-7.45149600	-1.58870900	-0.16648500
H	-6.54542000	-2.18935400	-0.06655800
H	-8.30718500	-2.23851800	0.04053200
H	-7.53019400	-1.25146000	-1.20393900
C	-7.49983600	-0.87520300	2.25908200
H	-7.47543200	-0.03424300	2.95643200
H	-8.41955100	-1.43836700	2.44488100
H	-6.65446000	-1.52741200	2.49394900
C	-7.76498500	2.49812200	-0.22664900
H	-8.62631500	1.84343100	-0.37127700
H	-8.14657400	3.47960400	0.07054400
H	-7.26404200	2.61175800	-1.19411600

C	-5.59875000	2.94427200	0.92546400
H	-5.97786100	3.94767800	1.13687100
H	-4.90294000	2.67699000	1.72084900
H	-5.04406300	2.99448900	-0.01736100
H	-5.23371900	-1.75518600	-2.43786500
H	-4.57166500	0.70978500	-2.84313900

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Si	5.07463100	-2.41951700	1.47192600
Si	3.34567200	1.18222400	-1.46067000
Si	1.17129900	-0.16009900	-3.39632400
Si	2.84987500	-4.08370400	-0.09000900
Si	0.20005000	-3.73608000	1.70881200
Si	-1.28157200	0.39690300	-1.54753300
Si	3.40840400	0.34124300	1.61498500
Si	0.74699700	0.39540400	3.36379900
Si	2.87170700	4.35600800	-1.36215400
Si	0.16484800	4.88460100	0.30193200
Si	-1.14837700	-0.86393600	1.22619900
Si	-2.01790000	3.50522800	-1.58657500
Si	-0.13426100	3.49578900	3.20951800
Si	1.91241800	-3.28281500	-3.13012500
O	4.55081100	-0.85324400	1.73871600
O	2.08846200	0.90977400	-2.51378800
O	2.98266000	0.51655200	0.01809300
O	4.19801300	-3.17174700	0.24773000
O	-0.55785500	-2.39445100	1.05099400
O	-2.80503400	-0.25940900	-1.50922500
O	-0.65801000	0.12200400	-0.01767100
O	-0.64009600	-0.22164500	2.66149400
O	-0.87001700	4.55112200	-0.95392400
O	-1.31706600	2.00860200	-1.88517800
O	3.53875300	2.82320400	-1.29246500
O	1.73120000	4.56708600	-0.14604400
O	-2.81728000	-0.95318800	1.16717500
O	2.06157200	-0.11967800	2.48627300
O	1.77184500	-3.88603500	1.16255900
O	-0.32283400	-0.33541300	-2.67145400
O	-0.26723300	3.94119200	1.60248600
O	0.70564200	2.05427700	3.37461600
O	1.92975600	-1.63648600	-3.43477600
O	2.14311300	-3.60373500	-1.50512100
H	3.23004900	-5.48350200	-0.19057200
H	1.01593500	0.34570500	-4.74450500
H	0.82483800	-0.10888000	4.71934000
H	0.04242800	6.29067100	0.64613700
H	6.45934500	-2.35071900	1.01925000
H	4.92901500	-3.18211400	2.71226300
H	3.97599500	1.56311500	2.15280200
H	3.96041600	5.29484800	-1.11607800
H	4.58335400	0.62918400	-1.97683900
H	2.23250900	4.55929900	-2.66283700
H	-2.43900900	4.06864900	-2.86305300
H	0.26531600	-3.59174000	3.16180400
H	-1.48820700	3.32232400	3.73085600
H	0.62524900	4.50963100	3.93898700
H	0.61399100	-3.83508100	-3.50901000
H	3.01547400	-3.86047900	-3.89467600
H	-0.57247400	-4.90699800	1.29796800
H	-3.12018800	3.35517000	-0.63683100
Ta	-4.14242800	-0.88112700	-0.24295300

N	-5.35099700	-2.29086900	1.09368400
N	-5.86846800	-1.02568500	0.72633300
H	-4.83850500	0.70340800	-0.48878500
H	-4.54406400	-2.17988000	-1.37371900
H	-5.83999100	-3.09435500	0.71432300
H	-6.76046500	-0.74523300	1.10799900
H	-5.10177700	-2.39261800	2.07374500

Ts9-10

Si	-5.21788400	-2.22461000	-1.54641300
Si	-3.21969400	1.04004300	1.58267200
Si	-0.91554000	-0.21091500	3.45503100
Si	-3.11241700	-3.93862000	0.14708500
Si	-0.39023000	-3.66462000	-1.59944000
Si	1.43278600	0.46752000	1.52248500
Si	-3.40970200	0.43703100	-1.52306200
Si	-0.80655200	0.44232000	-3.36177400
Si	-2.83804300	4.22266700	1.49381500
Si	-0.20586500	4.85642100	-0.25587400
Si	1.05915000	-0.83962500	-1.20945400
Si	2.08968700	3.58920100	1.57374600
Si	0.12042400	3.52996100	-3.19123800
Si	-1.67231300	-3.30832200	3.02490800
O	-4.63911100	-0.66003500	-1.69894600
O	-1.90534600	0.78785800	2.56714100
O	-2.90547100	0.44058500	0.06273000
O	-4.43760200	-3.05370600	-0.31062300
O	0.34749700	-2.30183100	-0.95263400
O	2.97327000	-0.12964600	1.37848800
O	0.72399200	0.21748900	0.02438200
O	0.56858100	-0.18902200	-2.64427100
O	0.90294500	4.59721200	0.95527100
O	1.44319900	2.07260300	1.89143000
O	-3.48044200	2.67887800	1.47128100
O	-1.72408500	4.41687400	0.24879600
O	2.72119600	-1.08006200	-1.20788300
O	-2.13007000	-0.04266700	-2.48308400
O	-1.95943600	-3.79753300	-1.04706600
O	0.56228500	-0.31874900	2.68066500
O	0.24486700	3.95236300	-1.57721500
O	-0.73176000	2.09963800	-3.38323800
O	-1.57613400	-1.72760200	3.56506000
O	-2.52401200	-3.37629200	1.58667000
H	-3.49199400	-5.33450100	0.28810100
H	-0.75030400	0.33166200	4.78655100
H	-0.88959400	-0.07252100	-4.71218500
H	-0.19667000	6.26990600	-0.59162900
H	-6.62569100	-2.13565100	-1.17791500
H	-5.01307000	-2.93114000	-2.81140400
H	-3.90250000	1.73816800	-1.93188700
H	-3.94645900	5.13967600	1.25205700
H	-4.40940500	0.42735700	2.14038600
H	-2.17377900	4.46747500	2.77475600
H	2.52167000	4.17093400	2.83783000
H	-0.44563600	-3.54071000	-3.05445100
H	1.47759500	3.35080500	-3.70218500
H	-0.62295200	4.56120900	-3.91250700
H	-0.32551600	-3.83478800	2.80450400
H	-2.40650800	-4.05507400	4.04193400
H	0.37909200	-4.82691400	-1.16180400
H	3.18015700	3.46352800	0.60470100

Ta	4.13729100	-1.02405800	0.08462900
N	5.21103800	-2.50871800	-1.25250600
N	5.86690100	-0.74878100	-0.53544400
H	5.34898500	0.42658300	0.34898800
H	4.30324000	-2.38815000	1.17193300
H	5.97051500	-3.10092600	-0.94603800
H	6.67795500	-0.41287500	-1.03998600
H	5.18484900	-2.42450000	-2.26247900

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Si	-5.36394900	-1.96235400	-1.45091700
Si	-3.12479300	1.08741700	1.68064000
Si	-0.81399900	-0.26248200	3.46202300
Si	-3.29985500	-3.80409300	0.15022700
Si	-0.63677700	-3.60925200	-1.70312900
Si	1.51203700	0.33823600	1.47521500
Si	-3.40796600	0.58979100	-1.43772100
Si	-0.86362800	0.48943100	-3.35679600
Si	-2.70845900	4.26713200	1.59193000
Si	-0.09314600	4.80629100	-0.20586200
Si	1.00193500	-0.89392600	-1.26432800
Si	2.24542900	3.45927300	1.51888600
Si	0.16316700	3.54152600	-3.18110500
Si	-1.71920200	-3.31177200	2.97730500
O	-4.70351000	-0.43042900	-1.60600000
O	-1.77873500	0.79254300	2.61098600
O	-2.86872100	0.52762200	0.13545000
O	-4.59418600	-2.84616000	-0.24655900
O	0.19960500	-2.31645500	-1.03796900
O	3.00861200	-0.35980100	1.27260300
O	0.74048300	0.14962000	0.00394200
O	0.50945700	-0.17591300	-2.66955200
O	1.02332400	4.46711100	0.97936100
O	1.64316600	1.93294000	1.86486500
O	-3.36854100	2.73180600	1.62312700
O	-1.61732500	4.41465700	0.31914300
O	2.63745500	-1.21900600	-1.27744000
O	-2.17923100	0.06057800	-2.43627500
O	-2.18168800	-3.69373500	-1.07849800
O	0.64412700	-0.41307300	2.65804100
O	0.29987000	3.92298700	-1.55710300
O	-0.73289000	2.14349800	-3.40297000
O	-1.53402700	-1.75285800	3.55726200
O	-2.64100300	-3.30024200	1.58127900
H	-3.74211500	-5.18275200	0.27690300
H	-0.60011400	0.24633600	4.79990100
H	-1.00754800	-0.03377300	-4.69889900
H	-0.03216900	6.22711800	-0.50417600
H	-6.75333500	-1.80057100	-1.03966900
H	-5.23567700	-2.66492200	-2.72806400
H	-3.83420300	1.92587200	-1.80666700
H	-3.80924200	5.19277300	1.34851400
H	-4.30299000	0.47629100	2.26340600
H	-2.01425400	4.53741800	2.85169400
H	2.74627300	4.02903700	2.76322500
H	-0.75707100	-3.41941500	-3.14745400
H	1.51437900	3.33466600	-3.69673400
H	-0.54944500	4.61112900	-3.87692900
H	-0.40642100	-3.88303500	2.67756400
H	-2.43424000	-4.05987600	4.00685300
H	0.09070800	-4.82870100	-1.35826200

H	3.28347100	3.35012100	0.49114600
Ta	4.15041100	-1.23755200	-0.05610800
N	5.26472100	-1.88025700	-1.58552000
N	5.70625800	-0.20412800	0.61986800
H	5.61897100	0.38426800	1.44097600
H	6.57069400	-0.00469400	0.13309400
H	6.26363200	-2.05234900	-1.60686800
H	4.86384100	-2.09012500	-2.49291100
H	4.22895100	-2.74144000	0.82007800

Ts10-11

Si	-5.34643300	-1.86552000	-1.35145900
Si	-3.11238200	1.41945800	1.63983900
Si	-1.00435700	-0.24373400	3.39869000
Si	-3.25435400	-3.85302600	0.01072100
Si	-0.64419800	-3.67444800	-1.84108300
Si	1.39119600	0.23020100	1.46600100
Si	-3.44203300	0.73609600	-1.45836300
Si	-0.86775200	0.60988000	-3.33563500
Si	-2.28164900	4.52289300	1.65170700
Si	0.35031800	4.88432000	-0.16893700
Si	0.93723000	-0.92589700	-1.31063200
Si	2.44263600	3.23946100	1.61471100
Si	0.33474500	3.59419200	-3.13058800
Si	-2.02908100	-3.28251400	3.00387500
O	-4.69982300	-0.33733900	-1.56544000
O	-1.84339300	0.95387700	2.60813100
O	-2.91130300	0.78991200	0.11597200
O	-4.48040900	-2.75336900	-0.21402300
O	0.14847300	-2.36259600	-1.16388000
O	2.86587300	-0.51488600	1.30541100
O	0.63027000	0.06815800	-0.01397300
O	0.47703400	-0.15647500	-2.69973900
O	1.42996200	4.42732600	1.00884900
O	1.57930400	1.82072600	1.85611800
O	-3.11786500	3.07821800	1.55228900
O	-1.20617800	4.68024300	0.36928400
O	2.57755900	-1.23011100	-1.28758200
O	-2.19732700	0.19500900	-2.42932800
O	-2.22279200	-3.75956100	-1.29281100
O	0.46349400	-0.47681700	2.63367100
O	0.62293800	3.95337800	-1.52095100
O	-0.66222200	2.25705800	-3.29005800
O	-1.87866600	-1.65298800	3.35750900
O	-2.40987700	-3.52996700	1.39617100
H	-3.81783300	-5.19061100	0.08928500
H	-0.78206900	0.15366700	4.77371300
H	-1.03985200	0.16572800	-4.70321500
H	0.57324600	6.28626800	-0.47628600
H	-6.69646200	-1.70052500	-0.82471900
H	-5.32775600	-2.56988200	-2.63378800
H	-3.91732900	2.03200800	-1.90435100
H	-3.27186400	5.58714500	1.53325400
H	-4.37706700	0.98946800	2.20534900
H	-1.53783300	4.58001800	2.91092300
H	2.92131600	3.71038700	2.90804900
H	-0.70428000	-3.51413900	-3.29213800
H	1.62703500	3.30444900	-3.74888700
H	-0.35611200	4.71405800	-3.76697400
H	-0.75624400	-3.95207500	3.26278200
H	-3.11457500	-3.79347700	3.83790500

H	0.07703300	-4.88013900	-1.43893500
H	3.53061400	2.99418200	0.66531300
Ta	4.04925400	-1.32701100	-0.02795000
N	4.73847500	-2.97908900	0.42492100
N	5.32125200	-0.43977100	-1.26145000
H	4.99980300	0.23755500	-1.94332900
H	6.33051400	-0.49666500	-1.26284200
H	5.33449500	-2.05826800	1.17022700
H	4.97055200	-3.90439200	0.75134900
H	5.36616400	-0.96837200	1.33457800

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Si	5.26404900	-1.61761000	1.20665400
Si	3.00939000	1.57129200	-1.55544100
Si	1.16104600	-0.51838700	-3.24486500
Si	3.22216700	-3.78654000	0.07589900
Si	0.68677400	-3.64221200	2.04605300
Si	-1.32059000	0.07622400	-1.44297500
Si	3.44100400	1.06374000	1.58188100
Si	0.83310300	0.77699200	3.36578100
Si	2.10651900	4.62724400	-1.75875800
Si	-0.57122900	4.88022100	-0.00633400
Si	-0.96507400	-0.94405100	1.45111400
Si	-2.44873400	3.03111500	-1.82734800
Si	-0.57192000	3.64780000	2.97889000
Si	2.04775700	-3.59216100	-2.95482500
O	4.60955800	-0.08859600	1.36453400
O	2.14816500	0.32444100	-2.21386800
O	2.88062800	1.56202600	0.10186200
O	4.35837100	-2.57453300	0.16251800
O	-0.22015400	-2.41078200	1.35998500
O	-2.81160600	-0.67455100	-1.34697400
O	-0.65786000	-0.04112900	0.08612300
O	-0.45396900	-0.11301900	2.77917500
O	-1.55638300	4.30819400	-1.21624000
O	-1.48878500	1.65028700	-1.89244000
O	2.37726600	3.00821900	-2.10200500
O	1.01276300	4.83902500	-0.50299600
O	-2.61311200	-1.21574400	1.47927800
O	2.19195300	0.40812500	2.47667500
O	2.23217400	-3.67287200	1.40774400
O	-0.34259600	-0.68064400	-2.52793000
O	-0.78952900	3.93258200	1.34351100
O	0.52102000	2.40256200	3.24370400
O	1.78638500	-2.03033000	-3.49211100
O	2.30807500	-3.64438300	-1.29831500
H	3.89360600	-5.07634200	0.08527700
H	1.05182800	0.14305200	-4.52905000
H	1.03247400	0.40787500	4.75216700
H	-0.93850700	6.25449500	0.28698800
H	6.58217700	-1.45654500	0.60411100
H	5.31960700	-2.25285300	2.52415000
H	4.02094900	2.19227700	2.28417600
H	3.35547200	5.24785100	-1.32205300
H	4.40113100	1.44632100	-1.95372400
H	1.57278400	5.22812300	-2.97818800
H	-2.82508600	3.38963200	-3.18888800
H	0.82259200	-3.40791400	3.48146800
H	-1.86836900	3.27016800	3.53625000
H	-0.00801100	4.83858900	3.61207400
H	0.86005900	-4.39667000	-3.22849700

H	3.23309200	-4.09024500	-3.65019800
H	0.00650400	-4.89896700	1.74128200
H	-3.60321700	2.77927700	-0.96480200
Ta	-3.94077500	-1.34425800	0.07573600
H	-4.01827100	-3.96389900	-0.47133000
N	-4.61644700	-3.17586200	-0.24903800
N	-5.38608700	-0.36023500	0.38757400
H	-6.07007100	0.35224500	0.59284400
H	-5.58496900	-3.46536100	-0.23048300

1'

Si	-5.41662700	0.33706500	-1.33268400
Si	-2.04104700	2.44006800	1.61516800
Si	-0.79690200	0.06715600	3.37590800
Si	-4.39450400	-2.33647600	0.09389800
Si	-1.95168200	-3.37100900	-1.67357400
Si	1.59429500	-0.50596400	1.45720600
Si	-2.63496200	1.97294900	-1.47247700
Si	-0.38769300	0.76727300	-3.39424000
Si	-0.09558800	4.99806900	1.60772200
Si	2.44263700	4.18572500	-0.20445600
Si	0.60497200	-1.43146100	-1.39665300
Si	3.75209600	1.86534900	1.56263300
Si	1.99410500	2.92913100	-3.15011300
Si	-3.04959900	-2.24690200	3.07976900
O	-4.22012200	1.49525900	-1.49794400
O	-1.06007700	1.49708600	2.57429800
O	-2.03897200	1.81450400	0.07329200
O	-4.99777200	-0.81281300	-0.17741400
O	-0.72830100	-2.34414200	-1.14123300
O	2.68550800	-1.81244800	1.42393900
O	0.93282300	-0.47368300	-0.07541200
O	0.49144800	-0.50851800	-2.74761300
O	3.24188500	3.35261200	0.99382200
O	2.41263000	0.86757300	1.79705200
O	-1.42269700	3.97863900	1.58588700
O	0.94214300	4.64541900	0.33298500
O	1.93466300	-2.49196300	-1.51047800
O	-1.75612700	0.97068100	-2.47662300
O	-3.43792900	-2.76618300	-1.20240900
O	0.42544700	-0.76269500	2.57864200
O	2.30498200	3.18354200	-1.52448800
O	0.52244000	2.15083300	-3.36047700
O	-2.17621600	-0.84534100	3.36473100
O	-3.46847200	-2.37630100	1.46670400
H	-5.49502900	-3.27668100	0.21763900
H	-0.38625700	0.33765900	4.73751700
H	-0.74263700	0.42395000	-4.75440000
H	3.21652300	5.36596800	-0.54661000
H	-6.61194100	1.01800800	-0.84981600
H	-5.62374200	-0.32359200	-2.62144800
H	-2.57037200	3.34782600	-1.92937200
H	-0.60357000	6.35047500	1.41054700
H	-3.38806000	2.50086500	2.14883300
H	0.62484500	4.84088700	2.87165000
H	4.37022400	2.08950200	2.86214300
H	-1.94310400	-3.41056700	-3.13283900
H	3.06162200	2.08437100	-3.67849700
H	1.89074900	4.21431900	-3.83784700
H	-2.22392400	-3.40354800	3.41625200
H	-4.26157800	-2.15746600	3.89035600
H	-1.72593600	-4.67811600	-1.06384600
H	4.65083200	1.23707800	0.59538400

Ta	3.10519800	-2.89312200	-0.07630800
H	4.39546800	-4.06943100	-0.14155100
H	4.65206300	-2.26980600	-0.60420800
H	2.66306500	-4.51395200	0.40901300

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Si	4.85775000	-2.57439300	1.57088400
Si	3.34104200	1.07945500	-1.37023800
Si	1.17429400	-0.17978100	-3.36428200
Si	2.68465600	-4.23758100	-0.08651500
Si	-0.07492100	-3.85757500	1.46287900
Si	-1.28075400	0.54676900	-1.59080500
Si	3.32567600	0.26483500	1.70152300
Si	0.62937400	0.36513600	3.40600600
Si	3.08270200	4.28131200	-1.24435300
Si	0.34784300	4.88856000	0.35275400
Si	-1.20534000	-0.85975100	1.18740700
Si	-1.85257300	3.70487200	-1.63883500
Si	-0.20669100	3.47315300	3.20994200
Si	1.83050100	-3.34772000	-3.12581200
O	4.42306500	-0.97287900	1.78606800
O	2.09153500	0.85957900	-2.44904800
O	2.87843700	0.48859100	0.11391500
O	3.98252800	-3.28428800	0.32100100
O	-0.52798600	-2.33088200	0.92676700
O	-2.88836200	-0.00699000	-1.66518300
O	-0.79656900	0.19429300	-0.03898300
O	-0.73631100	-0.21371600	2.62570200
O	-0.66472400	4.65790900	-0.94828700
O	-1.25096800	2.15202600	-1.89876400
O	3.64500900	2.70538500	-1.24514600
O	1.90215800	4.48901100	-0.06553600
O	-2.87895800	-1.04723400	1.12341700
O	1.97134400	-0.15778400	2.57870000
O	1.54139200	-4.12333200	1.12079000
O	-0.35975100	-0.25438600	-2.68696800
O	-0.18660900	3.92458500	1.59728900
O	0.60448000	2.02301700	3.43607000
O	1.85376900	-1.68771200	-3.35517600
O	2.00204500	-3.73661700	-1.51012400
H	3.12121700	-5.61750400	-0.21384100
H	1.07919500	0.31710700	-4.72071300
H	0.63756900	-0.16391000	4.75311900
H	0.29584100	6.28723700	0.74049800
H	6.26155100	-2.59291600	1.17694700
H	4.61128400	-3.30668800	2.81325600
H	3.94616800	1.45539300	2.25019300
H	4.21596600	5.13023100	-0.89599700
H	4.54922300	0.42590400	-1.83526800
H	2.51620500	4.60212200	-2.55489500
H	-2.16395600	4.27993300	-2.94005900
H	-0.22463000	-3.92582100	2.91396100
H	-1.60329500	3.30837600	3.60430800
H	0.49482000	4.47667000	4.00775100
H	0.54413500	-3.87444900	-3.57434900
H	2.95982500	-3.88957200	-3.87747200
H	-0.89921000	-4.83773100	0.76073600
H	-3.01233200	3.62260200	-0.75144600
Ta	-4.05023200	-0.75701300	-0.38753100
H	-5.72914600	-0.91736500	-0.93371100
H	-5.07850400	0.54873000	0.17541700

H	-4.44129200	-2.38837200	-0.90328800
N	-5.53744700	-1.70166300	1.31780400
N	-6.23507900	-2.12243800	2.05002700

Ts12-2

Si	4.81896200	-2.75204200	1.38566000
Si	3.30369300	0.93702500	-1.54635900
Si	0.98554000	-0.27706900	-3.39736700
Si	2.46580600	-4.33435900	-0.09079500
Si	-0.15959700	-3.79434900	1.64461900
Si	-1.34009200	0.57745500	-1.50587100
Si	3.43035700	0.15955300	1.53474000
Si	0.84417400	0.41682800	3.38563900
Si	3.13113800	4.14440300	-1.48849200
Si	0.54440100	4.89743900	0.28580000
Si	-1.16877700	-0.75342900	1.29571900
Si	-1.83750400	3.73979400	-1.49890500
Si	0.16603000	3.56425600	3.21141500
Si	1.49078200	-3.46696800	-3.09623800
O	4.47211600	-1.12715800	1.58341200
O	1.99264400	0.73898400	-2.55386100
O	2.90937200	0.37888100	-0.03055900
O	3.83997300	-3.45000400	0.20797100
O	-0.61855200	-2.28217500	1.07458100
O	-2.96419200	0.07825900	-1.47298500
O	-0.74810700	0.21466900	0.00630600
O	-0.59131100	-0.09292600	2.68602000
O	-0.57252300	4.67341200	-0.92762900
O	-1.28321000	2.18100000	-1.82439600
O	3.65698000	2.55589000	-1.46366900
O	2.04744800	4.42874000	-0.23562800
O	-2.85353500	-0.80108300	1.29522100
O	2.10771400	-0.18581400	2.49104000
O	1.41485200	-4.12620800	1.18502800
O	-0.52062300	-0.25462600	-2.65898600
O	0.07196500	3.98593200	1.59353000
O	0.91121600	2.07331800	3.39852200
O	1.59037100	-1.81695600	-3.37083300
O	1.72142700	-3.82675000	-1.48099800
H	2.81441800	-5.73985600	-0.21092100
H	0.85663500	0.18451500	-4.76349200
H	0.89871400	-0.10210700	4.73567200
H	0.57282900	6.30617900	0.63772600
H	6.19445900	-2.84693400	0.91118900
H	4.61293600	-3.44217400	2.65913000
H	4.13354000	1.32845300	2.02741700
H	4.30648000	4.97709800	-1.26141600
H	4.46600300	0.24335300	-2.06711900
H	2.47475100	4.42642100	-2.76561200
H	-2.26772900	4.32625800	-2.76082900
H	-0.18983500	-3.79103800	3.10459000
H	-1.19787100	3.48721400	3.72770000
H	0.99031000	4.53775100	3.92448100
H	0.15732000	-3.93407500	-3.46695600
H	2.55002800	-4.08798600	-3.88782900
H	-1.06556400	-4.77865800	1.05894200
H	-2.90333900	3.66910400	-0.50047800
Ta	-4.10698800	-0.57856000	-0.13096600
H	-5.80070800	-0.77673900	-1.06288800
H	-5.14285100	0.79426100	0.14343800
H	-5.31108000	-1.42238600	-1.37242800
N	-5.20021800	-2.60827100	0.73852700
N	-5.86553500	-1.77835100	1.12713200

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