<u>Electronic Supplementary Information</u>

Nitrile regio-synthesis by Ni centers on a siliceous surface: implications in prebiotic chemistry

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Computational Details (ORCA)

The ORCA software (version 4.2.1) [1a,1b,1c] was used for all geometry minimizations, potential energy surface (PES) and vibrational frequency analyses using the global hybrid functional PBE0 [2] coupled to the split valence triple-ζ def2-TZVPP basis set with two sets of polarization functions [3] and the atom-pairwise dispersion correction energy with Becke-Johnson damping (D3BJ) [4,5].

The selected level of theory (PBE0-D3BJ/def2-TZVPP) was shown to be one of the most robust, reliable and accurate theoretical tools in the estimation of general main group thermo-chemistry, kinetics and noncovalent interactions after the double hybrid functionals.

To speed up calculations the RI (Resolution of the Identity) [6] and RIJCOSX [7] algorithms were used coupling the Coulomb-fitting basis sets def2/J [8] .

To test if the computed structures represent a minimum or a transition state, frequency calculations within the harmonic approximation were performed on all compound models. The IRC method [9] was used to confirm if the guessed TS were connecting the two considered minima.

Electron correlation effects were considered by running single point calculations on the DFT optimized geometries using the domain-based local pair-natural orbital (DLPNO) approach coupled with the CCSD(T) method [10,11] in conjunction with the cc-pVTZ [12,13] basis set (DLPNO-CCSD(T)/cc-pVTZ). Stability of the HF wavefunction was always analyzed.

The obtained enthalpies and entropies were used to estimate the free energies (G) at T=200 K. The DFT thermal and entropy corrections were added to the single point energies ($E_{El.}$) of the corresponding DLPNO-CCSD(T) levels of theory to obtain the reported H and G values.

Figures were rendered by the program Avogadro [14].

References

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ORCA input: Opt (OptTS)+Freq

```
%MaxCore 1000
! UKS RIJCOSX PBE0 def2-TZVPP def2/J SmallPrint TightSCF Slowconv MORead
! OptTS (or !Opt)
! UNO
! UCO
! GRID5
! GRIDX5
! D3BJ
! DIIS

%moinp "Start.gbw"

%scf Maxiter=350
     end

%base "OPT"
----------------------------- ONLY for TS search--------------------------
%geom
 TS_Mode { B 30 39 }
end
end

%geom
   modify_internal
    { B 30 39 A }
end
end
-------------------------------------------------------------------------------
* xyzfile 0 2 Start.xyz

$new_job
%MaxCore 2000
! UKS RIJCOSX PBE0 def2-TZVPP def2/J SmallPrint TightSCF Slowconv MORead
! UNO
! UCO
! GRID5
! GRIDX5
! D3BJ
! NumFreq
! DIIS

%moinp "OPT.gbw"

%scf Maxiter=350
     end

%base "FREQ"

%freq Temp 100, 200, 298.15
    CentralDiff true
    Increment 0.0030
    end

* xyzfile 0 2 OPT.xyz
```

ORCA input: DLPNO

%MaxCore 12000
! UHF RIJCOSX DLPNO-CCSD(T) cc-pVTZ cc-pVTZ/C NormalPNO TightSCF SCFConvForced
VerySlowConv
! UNO
! GRID6
! GRIDX6
! DIIS
! MORead

%moinp "OPT.gbw"

%base "DLPNO"

%scf sthresh 1e-7
end

%scf Maxiter 1500
    DIISMaxEq 15
    DirectResetFreq 1
end

%method Z_solver Pople
     Z_MaxIter 256
end

%scf GuessMode CMatrix
end

%mdci Maxiter 250
end

%mdci
UseFullLMP2Guess false
end

%mdci LocRandom 0
end

%mdci KCOpt KC_MO
end

%mdci Triples 2
end

* xyzfile 0 2 OPT.xyz

Kinetic calculations

Kinetic constants were derived by using the Eyring equation:

$$k = (k_B T/h) \exp(-\Delta G_a/k_B T)$$

at three different temperatures: 100, 200 and 300 K.
In the following Table the prefactor ($k_B T/h$) as well as the ΔG_a of activation at the corresponding T, are reported.

Reaction (see Figure 4)	$k_B T/h$ (s^{-1})	ΔG_a (kcal/mol)	k
100 K			
2 → (3 TS I L) → 3L	2.0837E+12	9.6	2.18E-09
2 → (3 TS I B) → 3B	" "	5.2	9.00E+00
4L → (5TS II L) → 5L	" "	9.4	5.96E-09
4B → (5 TS II B) → 5B	" "	11.9	2.05E-14
200 K			
2 → (3 TS I L) → 3L	4.1673E+12	9.9	6.33E+01
2 → (3 TS I B) → 3B	" "	5.3	6.73E+06
4L → (5TS II L) → 5L	" "	9.5	1.73E+02
4B → (5 TS II B) → 5B	" "	12.0	3.21E-01
300 K			
2 → (3 TS I L) → 3L	6.2510E+12	10.2	2.32E+05
2 → (3 TS I B) → 3B	" "	5.5	6.16E+08
4L → (5TS II L) → 5L	" "	9.5	7.50E+05
4B → (5 TS II B) → 5B	" "	12.2	8.10E+03

Table S1.

The barrierless reactions, 1 → 2, 3L → 4L, 3B → 4B are considered fast enough to allow the approximations used in the kinetic simulations: 1=2, 3L=4L and 3B=4B.

10^7 particles were used and the initial concentration of the starting compound 2 was set to 1M. In the next Figure S1 (T=100 K), Figure S2 (T=200 K) and Figure S3 (T=300 K) the calculated kinetics are reported.

Kinetic simulations were conducted by the program "Kinetiscope" based on a stochastic algorithm [14,15].

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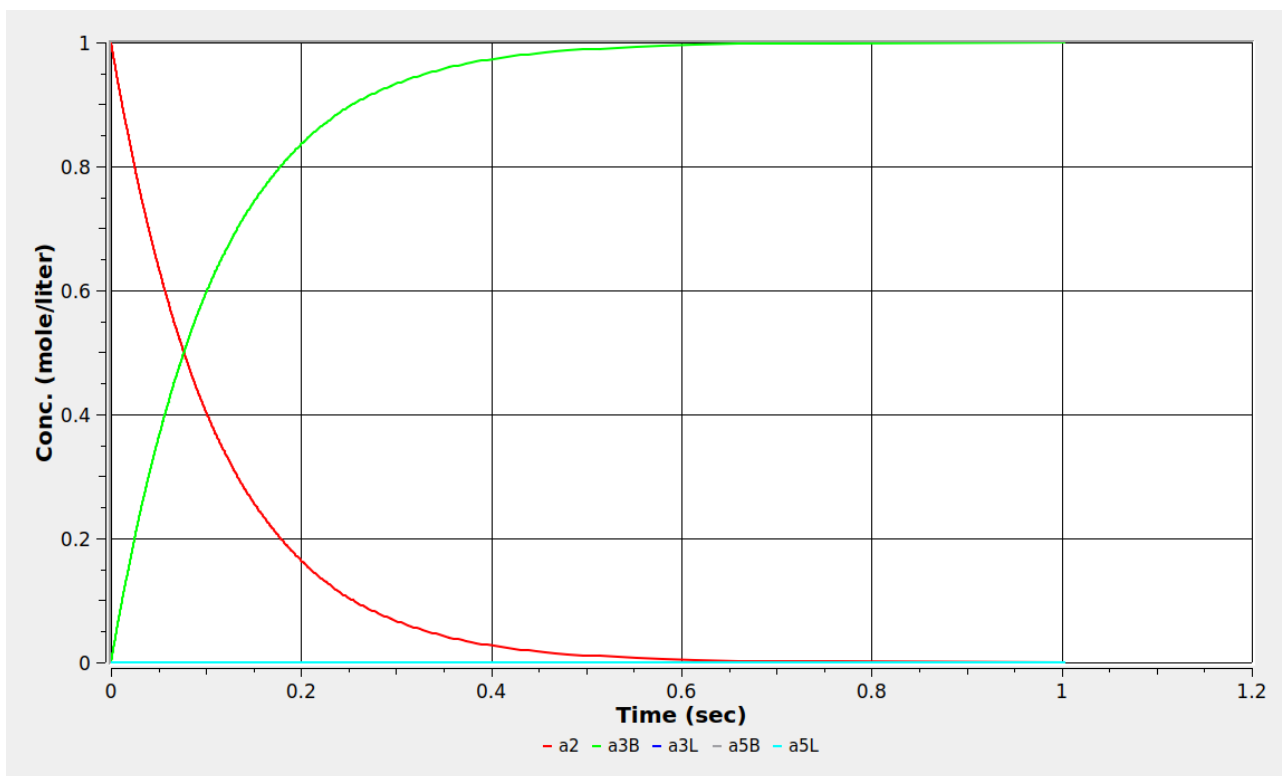
Fig. S1. T=100 K.
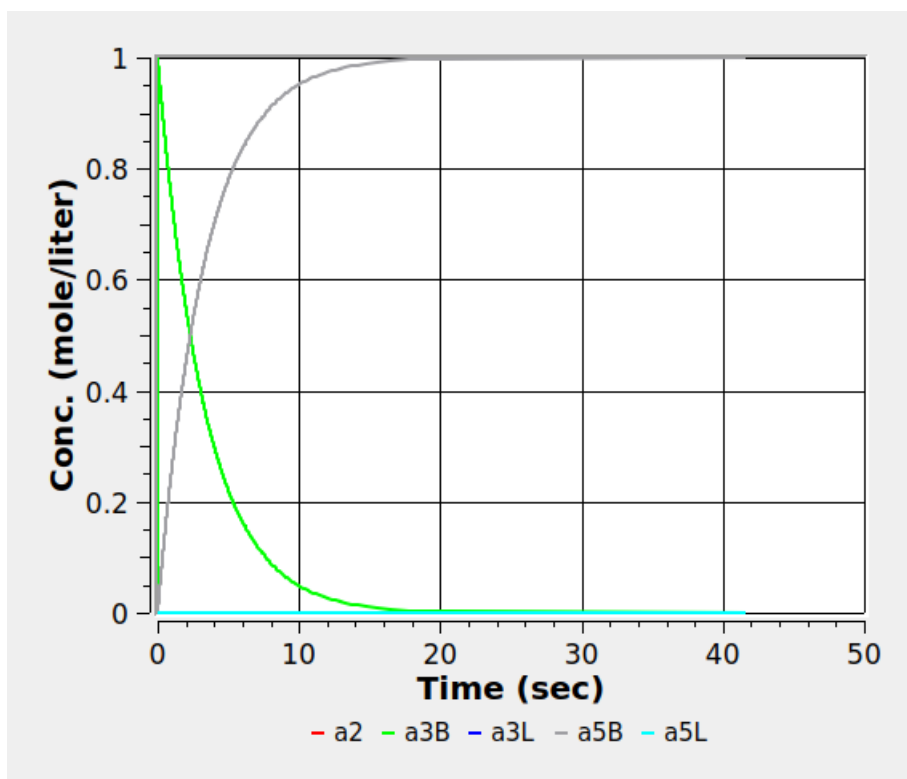
Fig. S2. T=200 K.
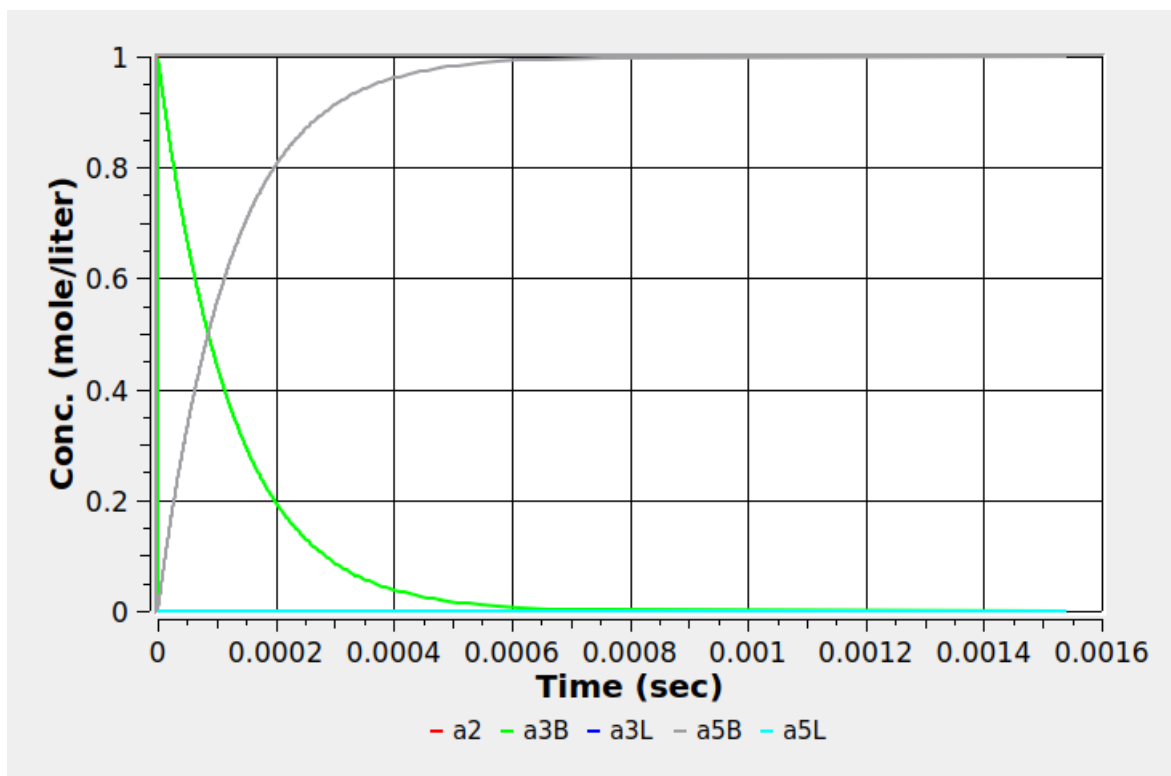
Fig. S3. T=300 K.

Observing Fig. S1 it is easy to notice how compound 3B is the only formed intermedia, determining a clear preference for the formation of the branched form.
The reaction does not proceed to the final compound 5B due to TS (5 TS IIB) at +12.0 kcal/mol, a too high barrier to be surpassed at T=100 K.

At 200 K (Fig. S2) and 300 K(Fig. S3) the 5B is strongly favored over the 5L.

The final concentrations are:

200 K: [5L]=10^{-5} and [5B]=0.99999

300 K: [5L]=0.00045 and [5B]=0.99955

PES

H Oxydative Addition

Fig. S4

CN Radical Addition
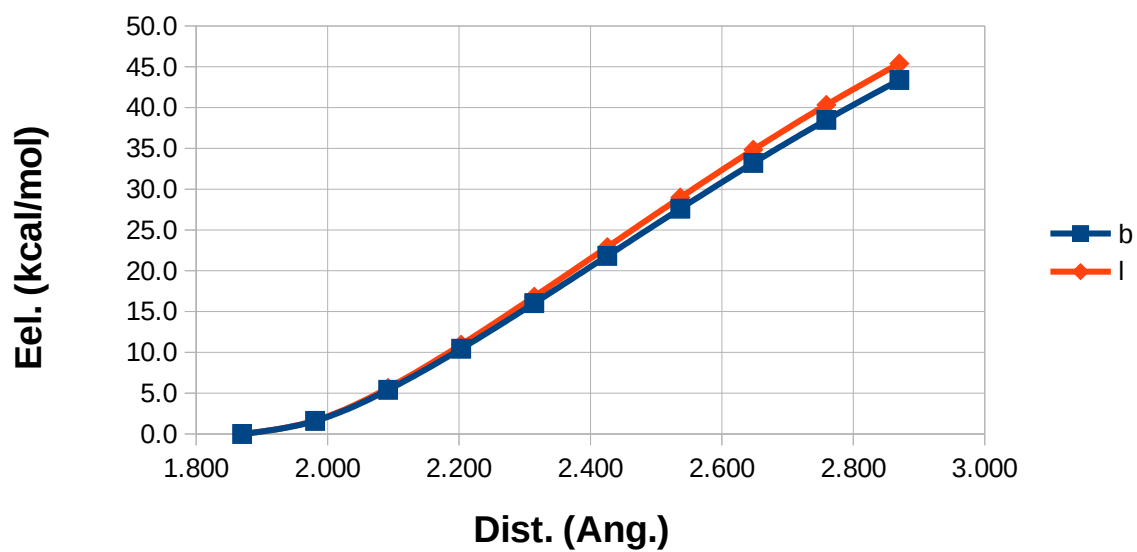
Fig. S5

Spin dependent energies

Free Catalyst

Multiplicity	M2	M4	M6
$\triangle$G (kcal/mol) T=200 K)	0.0	51.4	187.1

Ligand Exchange

Multiplicity	M2	M4	M6
$\triangle$G (kcal/mol) T=200 K)	0.0	49.7	99.5

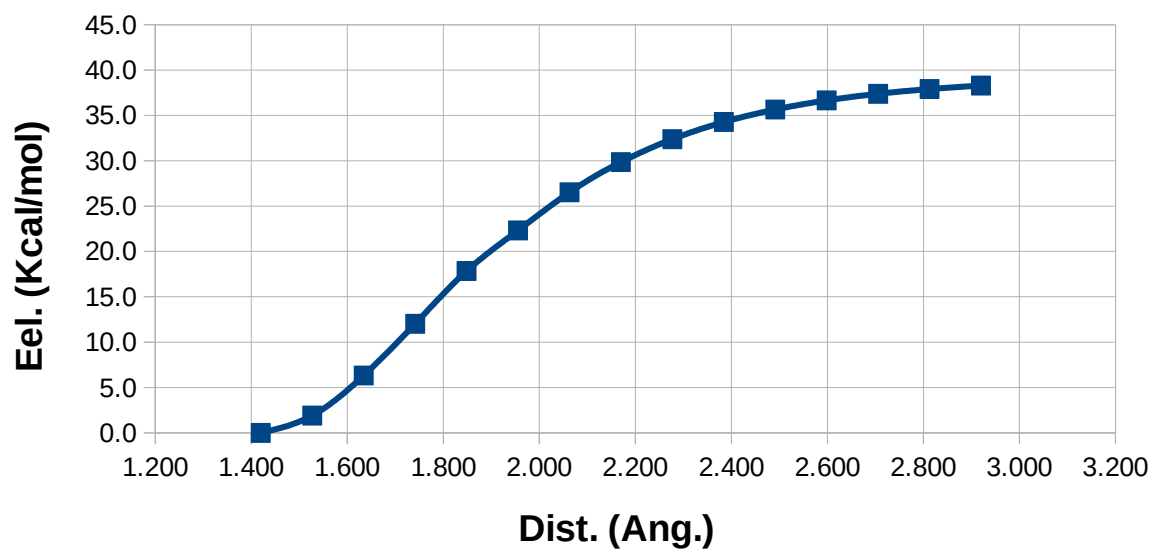**H Oxidative Addition**

Multiplicity	M1	M3	M5
$\triangle$G (kcal/mol) T=200 K)	0.0	26.3	90.7

Configuration dependent energies

The Substrate/Reactant-POSS-Ni system was found to explore mainly three different configurations that can be schematically represented in Figure S6.
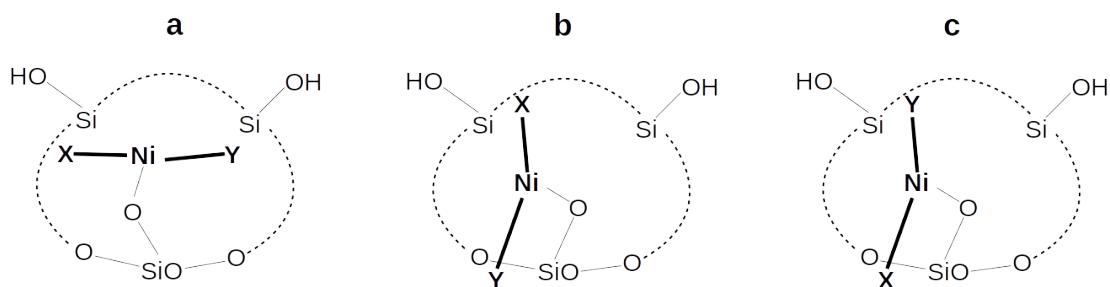
Fig. S6

In configuration **a**, no ligand is in *trans* to the O, while in configurations **b** and **c**, the two ligands are, alternatively, in *trans* to the O atom.

In Figure S7, the three calculated representative conformers (H oxidative addition step) corresponding to the schemes of Figure S6, are reported.
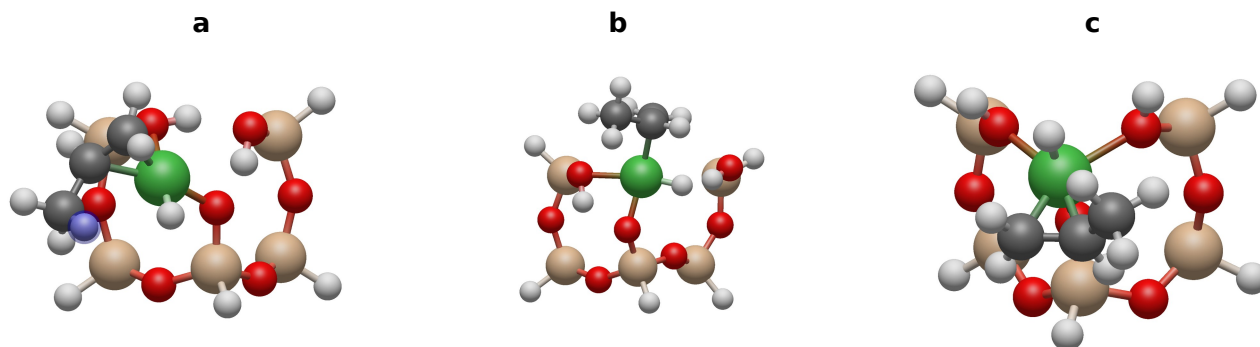
Fig. S7. Background atoms of the POSS have been deleted for clarity

A systematic search was conducted on all the reaction steps and configuration **a** was systematically found to be lower in energy.

Generally, the energy difference compared to the **a** configuration is always $\triangle G<18.0$ kcal/mol with an average of $\triangle G=5\text{-}10$ kcal/mol, depending from the reaction step.

Comparison between DFT and DLPNO-CCSD(T) corrected energies
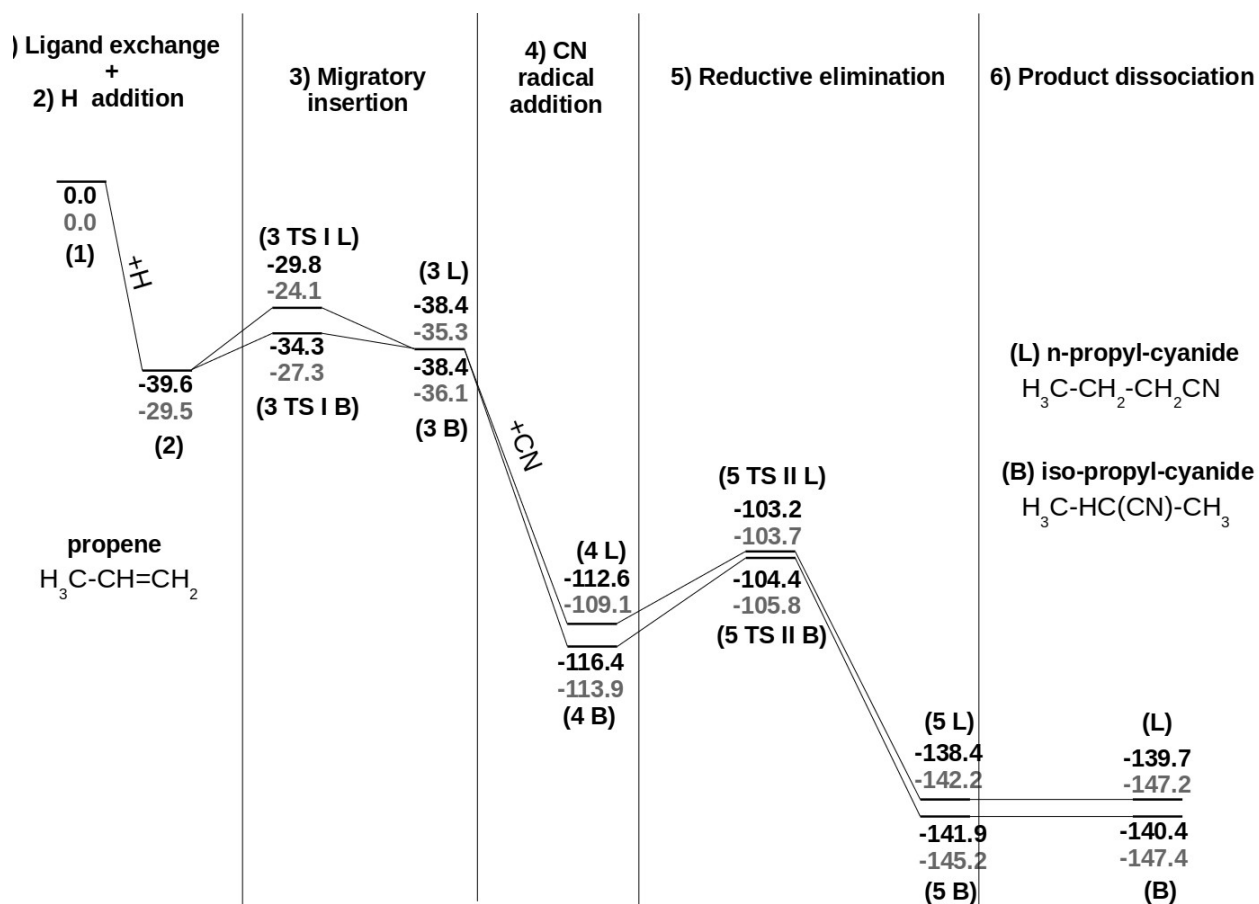
Fig. S8. ΔG energies at the DFT (PBE0/def2-TZVPP – gray color) and DLPNO-CCSDF(T)/cc-pVTZ (black color).

The agreement between the two levels of theory is satisfactory with the DFT calculated TS energies showing a clear trend toward lower barriers.

Snapshots of the elementary steps
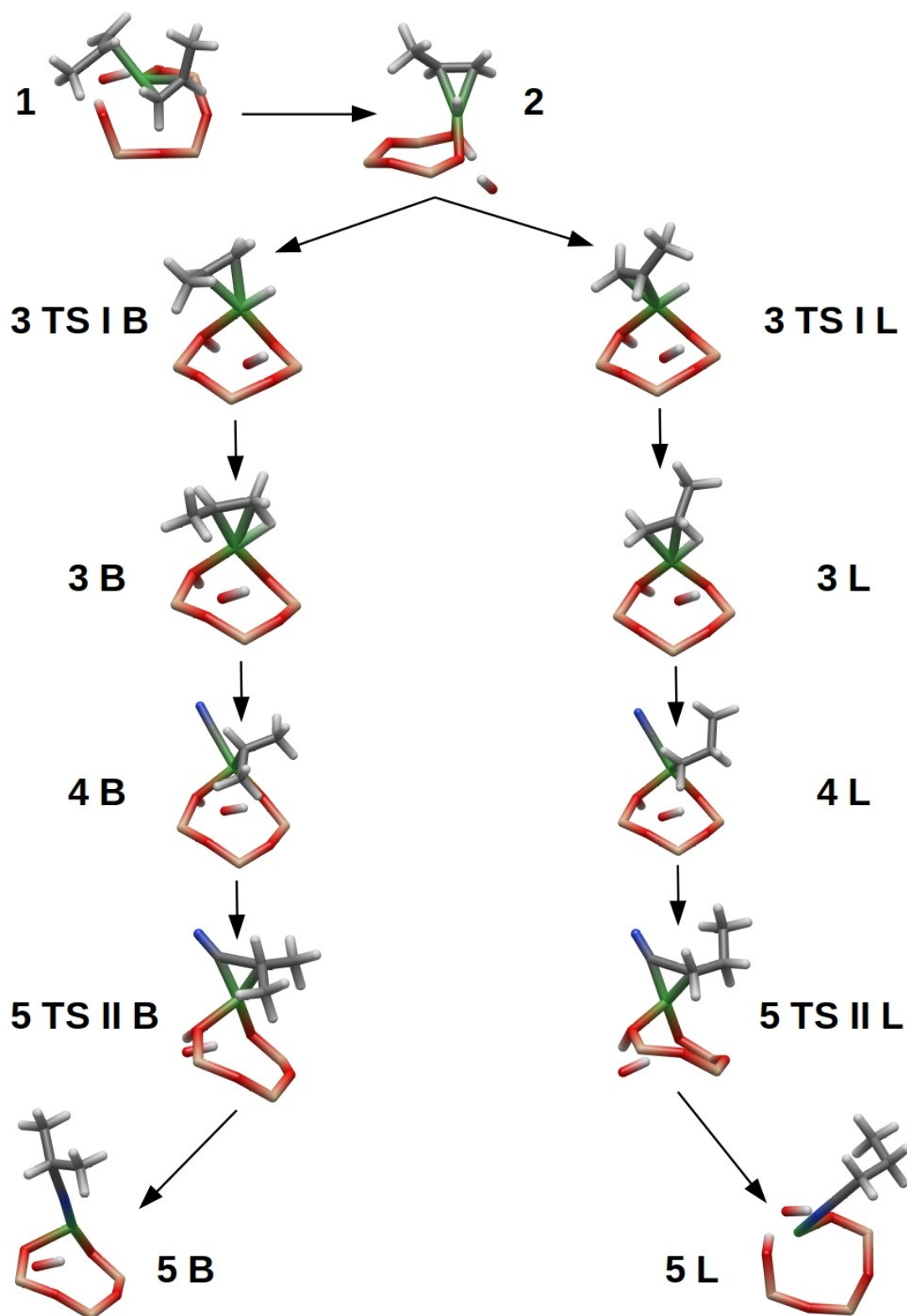
Fig. S9 Snapshots of the minima corresponding to five of the elementary steps as reported in Fig. 4 in the main text.

For clarity, only half of the POSS moiety is depicted and hydrogen atoms on the Si atoms have been deleted. The "free" -OH represents the 2nd silanol (SiOH) of the deleted ring, involved in a hydrogen bond with the SiOH oxygen of the displayed ring.

Propene hydrocyanation no Ni-catalyst

OPT+entropy correction: PBE0/def2-TZVPP   SP: DLPNO-CCSD(T)/cc-pVTZ

H_3C-CH=CH_2
0.0

H

H_3C-CH_2-CH_2*
-28.3

-31.6

H_3C-HC*-CH_3

*CN

H_3C-CH_2-CH_2CN
-139.7 (-111.4)

-140.4 (-108.9)
H_3C-HC(CN)-CH_3
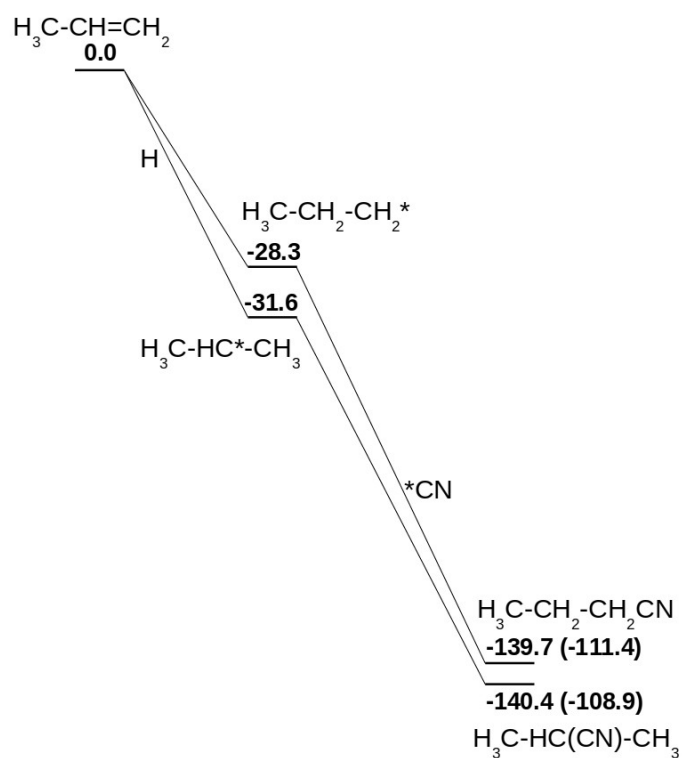
Fig. S10 Radical addition to propene of H and *CN. Energies: ΔG (kcal/mol), T= 200 K.

XYZ

Free Catalyst
M2

O	3.58006541631013	-1.03792606232330	-0.25670872053715
Si	4.75085745146389	-2.26559717318544	-0.30806870590051
O	0.47550734813113	-2.90077695264384	0.40153486559343
Si	0.42744790820548	-4.40319249392168	-0.15979137550861
O	1.74817234603495	-4.74618565115675	-1.08943987665943
Si	3.33831151611109	-4.91857076767130	-1.22165039678587
O	4.07338156417289	-3.44622333073535	-1.14961599127106
Si	1.65063527703423	-3.14465312377305	3.61881939804748
O	1.31679780853864	-4.73220372364855	3.46969173664965
Si	1.10882691279129	-5.96979347895045	2.44194973294554
O	3.07610083660366	-2.87504957875144	2.83146526576428
Si	4.58704582100648	-3.38092413713004	2.57398422138862
O	2.57034721443603	-6.61806070058021	2.10647034688501
O	4.65301940500948	-4.98400080824432	2.36781854410939
Si	4.03477975000464	-6.24317221012651	1.53705484598281
O	0.49707003421184	-2.20390645317630	3.00647888062092
O	0.41039937457829	-5.48675028749812	1.06564394621314
O	5.12632266807494	-2.64449950471320	1.20831186475653
O	3.94980366739582	-5.83388418075721	-0.03393250731520
H	5.92992683126011	-1.71911549031770	-0.98509541057507
H	1.82453430150093	-2.82805894788875	5.04255110399932
H	0.28567740723638	-6.99991706358758	3.07992625894194
H	3.67652072737996	-5.50888125272331	-2.51838998386961
H	5.49058900430649	-2.99914296045209	3.66389873908483
H	-0.75461681235907	-4.66544866133479	-0.99332758161713
H	4.92871469872362	-7.39353034212015	1.68265986996446
H	3.78853946019792	-0.27389084212988	0.28721756073648
H	0.29237657602760	-2.38372138284807	2.06426856225915
Ni	1.81616548561087	-1.77202243761024	-0.06626519390353

Free Catalyst
M4

O	3.15444999513009	-1.25059412252270	-0.09355985011539
Si	4.53453178447716	-2.22765384895351	-0.19686217417354
O	0.30888984330816	-2.96816326446064	-0.06582508519839
Si	0.37324820847059	-4.52474812305728	-0.44967893054151
O	1.77514091298216	-4.86973776597406	-1.26208256565037
Si	3.38752498703385	-4.94885888167922	-1.26763135993794
O	4.11044764840240	-3.47167122270770	-1.12998649713917
Si	1.88268479395494	-3.06355022013439	3.63111974301372
O	1.18418641227317	-4.47533408689684	3.28981619780646
Si	1.04964747789250	-5.80153045666295	2.32024273256283
O	3.49139294542292	-2.97846068966018	3.48635036072832
Si	4.81978402633389	-3.44630152220954	2.64292050592493
O	2.52597982270099	-6.44412872977577	2.11688322905936
O	4.76987949576489	-5.02077225118689	2.28972590278578
Si	4.00865290051177	-6.22532096762875	1.49902021251975
O	1.26956345098283	-1.87633460359265	2.58745243045213
O	0.34820758588816	-5.46853913080200	0.90795959430747
O	5.08647797202806	-2.54605677565880	1.29805433589122
O	3.95338319078641	-5.91455668348042	-0.09074691032584
H	5.57222439775278	-1.44137998309725	-0.87414996131111
H	1.51049426188259	-2.68170656710672	4.99788450406898
H	0.21876372723024	-6.76360537303414	3.04978734582916
H	3.82195369519614	-5.49198047700163	-2.55757974722855
H	5.96213646600365	-3.19934932339353	3.52671895510374
H	-0.74209737739957	-4.96941714429460	-1.29740138351639

H	4.78024077769078	-7.45392632262553	1.70440300049700
H	3.24912037996561	-0.36766287774370	0.27458327144510
H	0.30952521120552	-1.81236739526573	2.53210844395325
Ni	1.93688500612708	-2.67539118939253	0.79793369918887

Free Catalyst
M6

O	3.13434036886476	-1.41000214462631	0.34997878695663
Si	4.45977018215507	-2.28126370297199	-0.16762714576060
O	0.36905650022890	-3.08072035590072	-0.00135424876082
Si	0.48050671454649	-4.74844920090000	-0.29670837783058
O	1.82687749899851	-5.06540838359680	-1.12013614684381
Si	3.45219446593455	-5.00301536164105	-1.24084266057092
O	3.90602950060490	-3.44426127578410	-1.14503155620568
Si	1.70631215702596	-3.08006251071053	3.05924573973441
O	1.55902926242325	-4.75451708400386	3.44851775346657
Si	1.23103930467273	-5.97759119371026	2.46659242030035
O	3.37373622295842	-2.85027593527650	3.05733806750173
Si	4.77310089304766	-3.50468072026918	2.60521319889508
O	2.59666033075500	-6.68950563994270	1.92323761801354
O	4.69366083730603	-5.11714536511691	2.42123299511177
Si	4.11839232675372	-6.32383622148038	1.50563720911792
O	1.35045139847191	-1.36806015849846	2.21286233105504
O	0.39061690183605	-5.47366774071802	1.12615284596799
O	5.19446582113944	-2.85529653115483	1.14960857772465
O	4.14008462887731	-5.85993359414549	-0.05910923594244
H	5.36288904328360	-1.41148750781849	-0.92399850233597
H	1.20365560297453	-2.52989242106478	4.34642930097815
H	0.39975977255692	-7.00128507611291	3.10837429677650
H	3.83993062829814	-5.53976614970997	-2.54586212433415
H	5.83378551812405	-3.19202985845125	3.56649877851509
H	-0.67557424429993	-5.03645336312936	-1.15342883553527
H	4.96768593974237	-7.50683235990137	1.65659038045909
H	3.12464934973846	-1.26372035293109	1.31098314914359
H	0.81101849572087	-0.78858959393291	2.75738477549937
Ni	1.02919457726013	-1.22135019649948	0.24968060890269

Ligand Exchange
M2

O	-1.56503605214373	-0.34911891916903	-2.63764704019399
Si	-2.17249372381460	-0.69257097027490	-4.13545137752031
O	-0.32368146032097	-2.52704037937914	-1.06111725600991
Si	-0.45869851399978	-4.03575093130353	-1.58733065948560
O	-1.76816221359287	-4.20016785024110	-2.59095608816991
Si	-2.28301409474131	-3.85458480566575	-4.09138997889986
O	-2.61903054665774	-2.25868080344109	-4.23692273466454
Si	2.16538086225386	-1.05129133427284	-3.30841046510741
O	2.59606100394519	-2.62407452707503	-3.21600085596384
Si	2.05078019167538	-4.14179460249729	-3.47778554949491
O	1.56915316477773	-0.71249880204719	-4.79794043845837
Si	0.37687609507241	-0.83867548670807	-5.90083576898722
O	1.50094975391253	-4.25848550193759	-5.01620668100847
O	0.22319075890533	-2.37553908557055	-6.42811748565889
Si	0.22035546308719	-3.94602670808487	-5.97531391528502
O	1.03708861011972	-0.71780251825763	-2.17478146398538
O	0.87296153045690	-4.52379432903570	-2.42294281506622
O	-1.04331752721435	-0.33658032059747	-5.25984136640039
O	-1.16910720286559	-4.29927550664330	-5.19889690962216
H	-3.37411133645495	0.11805942453549	-4.36161675581157
H	3.35338157978656	-0.21071488795930	-3.11534476758109
H	3.16672469596317	-5.07890607832974	-3.32059599610091

H	-3.52084342828034	-4.60025130195266	-4.34224729980360
H	0.70126447939640	0.02312332126227	-7.04071760212148
H	-0.67503500992430	-5.00210060566884	-0.49437693873513
H	0.31641559997780	-4.76718476927081	-7.18539484886453
Ni	-1.91587715383926	-1.45399025471796	-0.65827261287933
C	-0.93249289039415	-0.35225660168078	0.81563438127796
C	-2.11825582707667	0.29750275819414	0.59060434360765
C	-2.25248123955341	1.52362955067656	-0.26072266647615
H	-1.37513612445707	1.67193965324540	-0.89376762317090
H	-2.36479004687000	2.40389935336355	0.38616931221625
H	-3.13680266135003	1.47702526837274	-0.90463357973776
C	-3.45531925651653	-2.70749759805096	-0.03148105165328
C	-3.60094156628270	-2.83881573653216	1.45562263338485
C	-3.96637515309105	-1.65608891767043	-0.77824289827553
H	-2.69294659902266	-3.23687169768952	1.92060320360765
H	-4.41292295658933	-3.54101132414265	1.68734589594989
H	-3.84908324565194	-1.88295734657332	1.92629040167060
H	-4.51346292747358	-0.84153080697864	-0.30997639445808
H	-4.13390548673813	-1.78430559723796	-1.84762821059542
H	-3.21501392157164	-3.62924600265177	-0.56357240174552
H	-2.95703155766599	0.07756277210347	1.24918544566159
H	-0.01630594296530	-0.02143801982485	0.32812361948636
H	-0.82136697328834	-1.06605516873657	1.62769522407832
H	-0.57737515200503	-0.29876734016013	-2.58733011706374
H	0.61176400308330	-1.51420866372221	-1.67812384588435

Ligand Exchange
M4

O	2.84422900267682	-2.64422585235319	-3.56901329332850
Si	3.99490141816942	-3.55138760117672	-2.89464445105394
O	0.45896806406227	-3.19862953162757	-2.49467535553796
Si	-0.10804590402397	-4.68915758653855	-2.61951968600211
O	1.06588694450908	-5.71588874636217	-3.09737281893618
Si	2.55658659367814	-6.28913218437898	-2.81910990236495
O	3.67839501367997	-5.14562957162031	-3.05850703760461
Si	0.88309026075437	-2.36526353696987	0.99348826445034
O	-0.06451078369044	-3.65560104547868	0.88182216971427
Si	-0.30246068704647	-5.20111796501738	0.39520410680592
O	2.42083474982544	-2.63988229909119	0.63094671683245
Si	3.76085837413603	-3.49317468616739	0.24918717213605
O	1.03789540769961	-6.06277881334605	0.69486980263658
O	3.48099132118546	-5.06083819279589	0.55258995863950
Si	2.57810970285247	-6.38465678018985	0.27908795146808
O	0.25504568779668	-1.25758707717251	-0.08762715099491
O	-0.68678602681637	-5.21660182006260	-1.17157829155108
O	4.13516162978420	-3.24018363774403	-1.29179920951898
O	2.66055520436398	-6.81401730196219	-1.27758633721644
H	5.28137618527404	-3.24977718218204	-3.53158570438006
H	0.78954511190183	-1.76422609392582	2.33167696172738
H	-1.41234864647584	-5.75189293133791	1.17754428906935
H	2.81471351669733	-7.42051030668362	-3.71390532435365
H	4.85481679985081	-3.02969938846815	1.10790888881683
H	-1.22079379863099	-4.81845560231403	-3.57867135661981
H	3.07151565506431	-7.48195102010427	1.11423114862846
H	1.93211226213970	-2.84735174631835	-3.26508917539672
H	0.56155723388838	-0.35105417717659	-0.00385899497447
Ni	-0.08902901647887	-1.40371485533229	-2.15866899596207
C	-2.31375994928847	-2.00826954040306	-2.04611378586653
C	-2.37090981868997	-0.66345416330929	-2.05809549038298
C	-2.54452949184907	0.19304918060031	-0.85466407312620
H	-2.40351844964875	-0.36799594748711	0.06834093353372

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H  -3.55784631249698    0.60511218700525   -0.85741715720772
H  -1.85769039943761    1.03983705128209   -0.87496191456867
H  -2.34201466552936   -2.57893867613084   -2.96657108194179
H  -2.35441270015433   -2.56931146198582   -1.11847312705787
H  -2.39428034285326   -0.14405525999417   -3.01292063337196
H  -0.40108795352069    0.80785971614665   -4.52272375289078
C  -0.30106295597927    1.24738225345627   -3.53423058741514
C  -0.60161713850721    2.69332189296236   -3.38626791396579
C   0.45811811652425    0.50202174468170   -2.50955870819453
H   1.51640667046624    0.38308813503954   -2.80280750548963
H   0.47509001330488    1.08486567696626   -1.57578011093267
H  -1.31310129274024    3.05205515193030   -4.13256355344895
H   0.30589503089482    3.31140488411973   -3.48057304417283
H  -1.00895763732246    2.91914670901827   -2.39335183862822
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Ligand Exchange
M6
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O   2.56702409455784   -2.09783265117795   -3.72270253531119
Si  3.71823676332421   -3.12953306910574   -3.25055932863859
O   0.25385461298918   -2.59391241732454   -2.41811647564254
Si -0.40228766081324   -4.05841139684570   -2.46616774052493
O   0.66219881469920   -5.12105325202155   -3.09602092556292
Si  2.13977947556342   -5.78421285011888   -3.06736770278006
O   3.26741670259773   -4.68525661001099   -3.45109369926172
Si  1.03751113589814   -2.00859099660342    1.05649597251467
O   0.20066261782876   -3.37787293437650    1.20033997587390
Si -0.27086237801210   -4.80054104398508    0.54642182782723
O   2.40241021940569   -2.16687836224379    0.22124818439772
Si  3.70162549131940   -3.10101922755875   -0.11825503474030
O   0.98834792907893   -5.82283408840112    0.56878782827157
O   3.34156546970211   -4.64135134846473    0.23928289204044
Si  2.50083648939831   -6.01326835497355   -0.00155594675933
O   0.13204394261941   -0.90570781404533    0.20089060798591
O  -0.80867206926509   -4.56853424461240   -0.95886757091494
O   4.08766328128276   -2.92073153714848   -1.66813713371942
O   2.44950991283066   -6.37203835135323   -1.57845077617278
H   4.92997596432465   -2.87661897905353   -4.03728688623209
H   1.27972254449865   -1.46116233453283    2.39779983790024
H  -1.34886958102002   -5.34593102416526    1.37502354981870
H   2.19692796400156   -6.89244518264631   -4.02412709461161
H   4.82815302935911   -2.67326358039262    0.71790022739208
H  -1.63321727393847   -4.12287702186397   -3.27115928633512
H   3.14684768948004   -7.10604871382553    0.72903439852971
H   1.68024142736908   -2.25342467574925   -3.32984770909445
H  -0.80810113241471   -0.77502001429367    0.50578517538732
Ni -0.34038788131603   -0.94602406995229   -1.76914501936145
C  -2.29347914544753   -0.52497136285996   -1.45535424602002
C  -2.62220004669278   -0.69561311198678   -0.01791722626037
C  -3.13505570569320   -1.99931914875249    0.47294019713072
H  -2.60730477384426   -2.83578513597654    0.00736396703483
H  -4.19591113268753   -2.12358247839421    0.20692149625819
H  -3.06420665237864   -2.10077732712913    1.55775344939736
H  -2.43092175075916    0.50470944142134   -1.79711590583617
H  -2.88737648429789   -1.18952991838024   -2.09221019610740
H  -2.84983261943712    0.18781478639523    0.57494051020348
H  -0.37732549439261   -0.17906779095860   -4.41632614564555
C   0.37548295869047    0.53577693190312   -4.09615972109733
C   1.10270617303992    1.30104651639058   -5.14359493573931
C   0.86451844114423    0.52614997227843   -2.72148260119765
H   1.84461234208239    0.07179390102965   -2.54153249801358
H   0.68047157083038    1.40673390721289   -2.10052451318184
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H   0.54939894840653      1.31506931912007     -6.08281467821392
H   2.08555631190328      0.85089812172532     -5.33759235272842
H   1.28460146418424      2.33378152380850     -4.83083321225888
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H Oxydative Addition
M1
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O    2.39656774509667     -1.36892736443263    -1.03300515917186
Si   3.58727174494926     -2.32595878802069    -1.67310051761751
O   -0.08628061398275     -2.56153890557366    -1.37891071152094
Si  -0.56975807474252     -3.83762194720956    -2.22710589952784
O    0.57984090421026     -4.26159317255030    -3.32961410506473
Si   2.17189382232351     -4.48478869486738    -3.46426102448186
O    2.97640519915240     -3.17046099334196    -2.91223617243505
Si   1.27049062397523     -3.76144596826367     1.76298700116332
O    0.33197310856843     -4.95712522030419     1.19388672137524
Si  -0.09216418449702     -5.94779804985488    -0.02240182945092
O    2.84519348331234     -4.15626006969279     1.60703710523214
Si   4.03945260509862     -4.49283874931226     0.56680554029760
O    1.23636561362217     -6.71302584388223    -0.56878851289043
O    3.73381452292672     -5.87808420205555    -0.21769227998160
Si   2.70847056512741     -6.62436561514107    -1.23542569609038
O    0.97889421742342     -2.40340876684912     0.90785613272541
O   -0.78626877099433     -5.11315605168994    -1.22313861378403
O    4.18094633341792     -3.27390293601882    -0.50845475398140
O    2.65129687879626     -5.78776980271870    -2.62530519129438
H    4.64114084386414     -1.44944475667657    -2.19749637611594
H    1.00508615628783     -3.55604617976425     3.19104099069094
H   -1.03454591337932     -6.94722333786781     0.48794584643540
H    2.52204038813052     -4.66973726430888    -4.87596611992155
H    5.30232936379279     -4.61995788755636     1.29666675789324
H   -1.82292964055943     -3.63205270717312    -2.96862977453946
H    3.20781866118892     -7.97576823860901    -1.49874568021536
H    2.02462767163918     -1.68304673095027    -0.16798030484273
H    0.39433333521995     -2.51644885972016     0.09317580147967
Ni   0.67993221775417     -1.08928974688836    -2.20523726816977
H    2.74036959531867     -0.13859937582035    -3.29374359998054
C    1.70010088779745      0.08392762091414    -3.51811696612041
C    1.28881199343667     -0.15887048918412    -4.93152156710445
C    0.99997803883614      0.83970850290442    -2.60790534864284
H    1.48127946376412      1.19568034092214    -1.70330363604944
H    0.06722845020077      1.31649668668219    -2.88339019544329
H    1.40955225982020     -1.20937463432366    -5.20380741199375
H    1.92696806026787      0.42325274715689    -5.60356419253043
H    0.25121430845677      0.12540322234375    -5.10291372107517
H   -0.49031186562144     -0.96099777030119    -2.99030926725486
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H Oxydative Addition
M3
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O    3.00809909944055     -1.50481841010234    -1.03956606508854
Si   4.08537455756089     -2.56106207631373    -1.72985370904278
O    0.25727185974299     -2.62183394281300    -2.12915298827992
Si  -0.15829522283921     -3.91176116706886    -2.91423490104806
O    1.13441777487054     -4.53220024535378    -3.74606655770992
Si   2.71003738585617     -4.72135358752117    -3.49646517767782
O    3.38665263321019     -3.32623702921042    -2.96323462976600
Si   0.97148166203538     -3.42607279568499     1.35873123885757
O    0.11134082402120     -4.55609867529122     0.61391692344320
Si  -0.21598121347367     -5.72957544752750    -0.47804850520402
O    2.56981283079779     -3.59759128280206     1.12531788921594
Si   3.90403868780969     -4.41814169606289     0.66898558579339
O    1.12175402720221     -6.64538771921835    -0.64795183345438
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O    3.51713920752887    -5.91351055181525     0.20158890878269
Si   2.69972208039294    -6.65925459092021    -1.00254345218270
O    0.71228892283796    -1.90469324671759     0.77031621783832
O   -0.66488292235595    -5.10527137726908    -1.88939445282113
O    4.57183845224894    -3.58785173403751    -0.56455909570923
O    2.99758057275997    -5.87742618449964    -2.38736800035044
H    5.23597619998575    -1.80394983574057    -2.23513932662946
H    0.65589879996277    -3.46201323534285     2.79376621248111
H   -1.28688760209306    -6.57104381359517     0.06386234971989
H    3.37188228475551    -5.09908688828410    -4.74974760715068
H    4.85203503871729    -4.48013507737502     1.78407694051955
H   -1.23205731827525    -3.74809330707264    -3.91271903309402
H    3.16881721570935    -8.04356603810525    -1.09573691342423
H    2.88863683785487    -1.64957997558582    -0.09570574967779
H   -0.14524043087086    -1.47919835128899     0.86739938049959
Ni   0.72251878534776    -0.98399625041800    -1.36672152398842
H    2.12255377735378    -0.98526597181829    -3.78126444093134
C    1.33823664690609    -0.24230747061324    -3.66360207816868
C    0.17281940419879    -0.36448039341347    -4.57553510638682
C    1.49158416691910     0.72943814227187    -2.75024399533478
H    2.40803810420182     0.82263184164184    -2.17740894376827
H    0.75229875946730     1.51210488493322    -2.63647289970161
H   -0.26768032075873    -1.36035483701022    -4.50527733085198
H    0.49740182489680    -0.22784400474954    -5.61095659309678
H   -0.59371169125760     0.37624966738651    -4.34891804737085
H   -0.42338170266896    -0.08182732559069    -0.81874268924056
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H Oxydative Addition
M5
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O    2.82107600469413    -2.09509002449367    -3.65684273732112
Si   3.92278569685633    -3.11598197493463    -3.05097491544362
O    0.56448197177824    -3.06647865557462    -2.47757667402740
Si  -0.01974716571244    -4.53331011274572    -2.76516162259007
O    1.12664250176437    -5.46585054387913    -3.47046231879741
Si   2.67649961433685    -5.92777979154244    -3.42565879035587
O    3.65195057503385    -4.63887130355459    -3.56185615516594
Si   0.83826196279062    -3.09565629481904     1.32185625811878
O    0.08879738599781    -4.49847359684110     1.10410393559692
Si  -0.04844663064409    -5.78774583738896     0.09924536492857
O    2.31410394692573    -3.03025330090512     0.71281447490251
Si   3.69909686755230    -3.63809177114477     0.08457205367417
O    1.36842697168039    -6.57536469100441     0.09253520763505
O    3.66120347110865    -5.25751483078293     0.13699966234079
Si   2.91506762694194    -6.60491380209737    -0.40024938909510
O   -0.01530123503337    -1.91456932182982     0.48686762425261
O   -0.45956990689014    -5.28839654258856    -1.37554390966026
O    3.81604275510675    -3.08968303519208    -1.41657678442252
O    2.98576748116707    -6.68405307772770    -2.01226213773531
H    5.26888774514422    -2.71665894006399    -3.47596903296286
H    0.80036252810339    -2.73495284835531     2.74460987266667
H   -1.08422021857234    -6.66777966224231     0.64488839139164
H    2.94646593266119    -6.86157022769433    -4.52175977007536
H    4.81500843107416    -3.16693606871619     0.90949027713071
H   -1.20360050406415    -4.53150960427641    -3.63756743867010
H    3.58102111383702    -7.77483746238388     0.17555006103808
H    1.91487445802712    -2.33795439288714    -3.36621011743352
H   -0.90529045472749    -1.76310316028749     0.81766950707774
Ni  -0.17317224712829    -1.63364486856892    -1.55204657165310
H   -0.02333416810137     0.22734785012618    -3.74791819935437
C    0.83614720125908     0.54742164630150    -3.16903801197954
C    1.71308367660410     1.62089356060608    -3.70816488154316
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 C   1.07265526145332     0.00737729202408    -1.83378010832939
 H   2.01758135506703    -0.52399022131321    -1.67500690123095
 H   0.82981939400445     0.66375032772842    -0.98875390655464
 H   1.51036373074764     1.82011728358021    -4.76002324245487
 H   2.76745820061570     1.34238289005437    -3.60907947048641
 H   1.58101854408391     2.56045165528895    -3.15454231261104
 H  -1.72283987554374    -1.51118653987391    -1.58284729080020
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3 TS I B
M1
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 O   2.63536764546243    -1.30693258800890    -0.49101223407615
 Si  3.85324097139521    -2.25113064878301    -1.09858214184010
 O   0.19939774705633    -2.26714783624647    -1.23140556265807
 Si -0.26266417943899    -3.38863424085274    -2.28015248121713
 O   0.96941095826480    -3.76943031809345    -3.30330491447496
 Si  2.55314598107199    -4.08003330652165    -3.31391219947042
 O   3.36889631808465    -2.93280034816944    -2.48180125850054
 Si  1.07600472971598    -3.96584265806243     1.84551078178596
 O   0.13325763964007    -5.02574756202525     1.05508462738227
 Si -0.16596595659281    -5.79611606734991    -0.34519744564415
 O   2.62742662868043    -4.46590100550733     1.79482006252174
 Si  3.93239113791758    -4.70345105163618     0.86756445238675
 O   1.19438248456069    -6.53837503650986    -0.84300031077550
 O   3.68427001516253    -5.93558217197070    -0.15647293425657
 Si  2.73003424595911    -6.49440058447993    -1.34985016835767
 O   0.96817164073106    -2.49972120155860     1.14183955295339
 O  -0.67731218543318    -4.74778253710760    -1.46571528695585
 O   4.25178086684406    -3.35062768127931     0.01386180379835
 O   2.86480262815832    -5.52733494777630    -2.64728267602382
 H   4.99826522825029    -1.38106665066759    -1.38761626059280
 H   0.67246441002902    -3.90597991477361     3.25425376443674
 H  -1.19894526865462    -6.80953835624725    -0.11737871838482
 H   3.04542606625537    -4.07355789456068    -4.69427941354797
 H   5.08826475716603    -5.00439060827297     1.71490984937884
 H  -1.40646525087924    -2.99969722833839    -3.11946742766851
 H   3.17042321063782    -7.84385818529326    -1.71031348021742
 H   2.14699050269885    -1.70682359322652     0.27607326180196
 H   0.48544886109110    -2.45972569637210     0.25000046278020
 Ni  1.12758794689993    -0.73264093188616    -1.76864559692303
 H   2.89747524036625     0.97552887354327    -1.51156317283778
 C   2.30178282081267     0.77967522172189    -2.39775717118287
 C   3.05190768334916     0.46089588799322    -3.65268098705246
 C   0.98236320464083     1.18536574972362    -2.39919053353434
 H   0.54855013181824     1.67402203968796    -1.53282462817762
 H   0.46031776488928     1.36043982265477    -3.33217571778226
 H   3.73868936187787    -0.37591186743954    -3.51905084008657
 H   3.65365521507877     1.32294390884478    -3.95798690939163
 H   2.37353101667743     0.21603162187806    -4.47077878821869
 H   0.04686777975474    -0.43739040703042    -2.63793935937650
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3 TS I L
M1
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 O   2.40632158091208    -1.35016767400356    -0.87192798351378
 Si  3.69011113860468    -2.28816535014601    -1.33479656608048
 O   0.00947424714142    -2.53543463494310    -1.46803980371712
 Si -0.35372116035866    -3.82048642909544    -2.35854680381217
 O   0.90434832800351    -4.22345487695225    -3.34196760884857
 Si  2.50034116717869    -4.46519512900240    -3.32118232815452
 O   3.25706121577710    -3.21975371526573    -2.58194096159055
 Si  1.03138177578431    -3.82740903667224     1.79042279402663
 O   0.16283165776469    -5.04984027319547     1.16356353974417
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Si -0.08807022538460    -5.98253233860246    -0.14501197475865
O   2.61186269648796    -4.23364592447289     1.80284696760004
Si  3.92634904423364    -4.46699216257927     0.88767317813892
O   1.31388584402042    -6.69757642681936    -0.56111708390463
O   3.75237525249270    -5.78267536417732    -0.04416400084252
Si  2.83415226909428    -6.60206050007696    -1.10699335825300
O   0.83706070943889    -2.48195321243065     0.89263688247224
O  -0.64710010113841    -5.09912366945725    -1.37938245017487
O   4.16535796073685    -3.16169723116900    -0.06274548824321
O   2.87048513383045    -5.84079010492684    -2.54240172919701
H   4.76629695392206    -1.39521038475050    -1.77839156259961
H   0.61744876292166    -3.59946932918843     3.17882683026472
H  -1.06637569852173    -7.01850952188378     0.19489314160079
H   2.99657287855917    -4.54714022625031    -4.69817148740627
H   5.09833555781120    -4.63626073098782     1.74895193844662
H  -1.52616757414120    -3.63544135450050    -3.22793839306079
H   3.38148577706442    -7.95045693560024    -1.26983076195302
H   1.93818011488234    -1.68343709213981    -0.06192994065962
H   0.33895809751232    -2.56448253571596     0.01194335647116
Ni  0.92459261364379    -1.11874100554280    -2.28443761519591
H   1.97897066022507    -0.96098747117947    -4.53054571621448
C   1.37006711739671    -0.17786308551135    -4.08176204359909
C   0.30681362181889     0.37972463191130    -4.97901776720303
C   1.88563343037284     0.49061714739910    -2.99258570100695
H   2.90407164471951     0.32870727354838    -2.66543286750546
H   1.41199356962895     1.40349418552932    -2.64453567823311
H  -0.31804135389534    -0.40126905296355    -5.41077500917715
H   0.79564495055868     0.90764800394736    -5.80374922978763
H  -0.33067843505449     1.08917853254191    -4.45177907997793
H  -0.14900122404487    -1.05789699467456    -3.20188763409412
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3 B
M1
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O   2.70574969094803    -1.38493033940969    -0.50879163373445
Si  3.89153626618652    -2.32840186837366    -1.18935186531822
O   0.10075047468324    -2.16391551280460    -1.13497318139243
Si -0.35571380305585    -3.32096929500553    -2.13914575125959
O   0.84222376745672    -3.66899704281780    -3.21607309076698
Si  2.39759597283483    -4.07914321249620    -3.33400317650908
O   3.33492805781580    -2.99112319695438    -2.55304331948260
Si  1.19087329489076    -4.00538451386017     1.86129486467443
O   0.17225284573892    -5.06807190172097     1.17172553315961
Si -0.20576524439871    -5.78755631872217    -0.23853375146469
O   2.72547762719287    -4.54210856789857     1.72514133895544
Si  3.98573850512694    -4.80047490803195     0.74404055292356
O   1.10843870027398    -6.57138604552996    -0.79442546163126
O   3.65878603422034    -6.00583609253202    -0.28938511809590
Si  2.60518852157174    -6.53622245968890    -1.41035248657394
O   1.08372155435142    -2.55633531970558     1.12469187588862
O  -0.70804959399768    -4.69302420438062    -1.31737755702353
O   4.31013251960428    -3.44202022408137    -0.09776715609660
O   2.65825194763215    -5.54694905145607    -2.69521550734309
H   5.04047957891677    -1.47821905104223    -1.50664074970889
H   0.87885092235540    -3.89877863229816     3.29007904315380
H  -1.27109914389422    -6.76476790698373    -0.00103662373990
H   2.79630648776715    -4.08961553639349    -4.74433205193203
H   5.16544346284710    -5.15137729401902     1.53745389372801
H  -1.53787893551669    -2.97239121443556    -2.94681479211223
H   2.99556641065593    -7.88539500918611    -1.82476427167878
H   2.22999980909389    -1.80391037111728     0.26516029172660
H   0.51878118610471    -2.45946460815568     0.27681089726682
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Ni  1.28074782540052    -0.71531266347946    -1.64540925001310
H   2.15745679261525     1.58393294912055    -1.51585394887260
C   2.06679312584761     0.84915659693139    -2.31625914730488
C   3.30041917770995     0.74273286065685    -3.16965794917912
C   0.74386743788842     0.80853711649399    -2.96386857993087
H   0.04511781660600     1.59590422369018    -2.68590754477132
H   0.75820913308863     0.66045272683909    -4.04313138196584
H   4.18734011399696     0.57359578532012    -2.55758473182127
H   3.47546990479157     1.66464282490060    -3.73586214958684
H   3.22937167655726    -0.07536282913127    -3.89030975404415
H   0.12423907809137    -0.14161489224038    -2.61577130812267


3 L
M1
O   0.17416546641573    -2.33501871285521     2.53967282548553
Si -0.02830895745161    -3.73270325206702     3.41124624685484
O   1.51178153920394    -2.57933458323792     0.11689867800259
Si  2.12920924104188    -3.91689154391752    -0.50435698961001
O   2.38427318861137    -5.04791775510403     0.66366738954660
Si  1.77198391943578    -5.84930366532603     1.92205886287893
O   1.10009989823734    -4.80916812575132     2.98841290430189
Si -2.12293971741720    -3.02957133175651    -0.39354777870127
O  -1.51457373094083    -4.06082199811739    -1.49121657296237
Si -0.37555171700536    -5.17023043103854    -1.83667896395122
O  -2.82674089536372    -3.85269838097300     0.82866006059708
Si -2.55625561267220    -4.91636542759630     2.02023358085882
O  -0.59439112997099    -6.47041782479398    -0.88150245782543
O  -1.92801391598755    -6.27885126865300     1.41249218569711
Si -0.75222228532582    -7.06858068378010     0.61566109451339
O  -0.93538141304378    -2.10918139284928     0.23572718787174
O   1.10172848794824    -4.55389655618131    -1.60945173291070
O  -1.52004144785833    -4.27921814502038     3.10916296964364
O   0.64139023127180    -6.90888539757897     1.43431213301291
H   0.12616323873075    -3.41326147481462     4.83214934100423
H  -3.15702601284683    -2.20397035662085    -1.02559587557509
H  -0.52602505702254    -5.58167240823561    -3.23445390153795
H   2.84132543098196    -6.57673285438718     2.61117117060470
H  -3.81596304620103    -5.21698928394681     2.70335485927509
H   3.42682393836928    -3.71176908821770    -1.17123749063278
H  -1.09945542708091    -8.48894741083997     0.53654478581487
H  -0.42966196464082    -2.20802931035246     1.75039588430892
H   0.04261206805238    -2.27855072729598    -0.00996971802446
Ni  1.94334681331933    -1.92757633603230     1.87780163188047
C   3.76691696904975    -1.02792789965284     2.41698897452966
C   4.12486116384732     0.38652954707704     1.99798009716156
C   2.71050358947352    -1.20102844003350     3.42156804039479
H   2.88580386209601    -1.92964131933391     4.21011381381107
H   2.21824775543957    -0.29827955476423     3.77685410148326
H   4.73209803985616     0.40500587224994     1.09252260682640
H   3.22528113969222     0.97630867209090     1.81892673456584
H   4.69082127126865     0.86708969431438     2.79734434881321
H   3.41543918805773    -1.54444540109467     1.38748646013597
H   4.65011989042878    -1.64411044351159     2.59312451185609
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4 B
M2
O   1.71431712335963    -1.43899381257867     2.46057759378708
Si  2.77589639009810    -2.06965926021022     3.57069241919403
O   2.16312058305261    -0.95743652234832    -0.45692823293479
Si  3.67338891456653    -1.30804918392631    -0.89025440066178
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O    4.54540751621183    -1.07713008692867     0.50167185206197
Si   5.30031075899857    -1.79310075350045     1.75757877776931
O    4.27923797692910    -1.82898490882808     3.02254392310557
Si   0.96505192491812    -4.47363343559256     0.29169372769179
O    2.03342818213988    -4.69844213741087    -0.91181593267823
Si   3.57728127497118    -4.42674539827211    -1.34828770205824
O    1.52793561310765    -5.10828201305060     1.67994618364245
Si   2.59477666753146    -5.06862463978475     2.90221556880272
O    4.58481174664119    -5.08895439811133    -0.25917691032499
O    4.10964267234969    -5.20470294683579     2.34073176010472
Si   5.22657640753659    -4.85861763213674     1.21373892314752
O    0.72452418999688    -2.87103411684382     0.52380384486112
O    3.85245593906979    -2.83215046864563    -1.41898426305825
O    2.44965630226336    -3.65350450395988     3.69630355619561
O    5.70617129137000    -3.31313402534872     1.36328661046084
H    2.59671068566327    -1.40525622925471     4.85982703259406
H   -0.29173579470140    -5.14888753990017    -0.04363857940800
H    3.81475411403701    -5.03505174634651    -2.65858618337135
H    6.49968343713503    -1.03770242441858     2.11697040938527
H    2.31035367805076    -6.16567633288944     3.82841076500824
H    4.22974353203096    -0.41335294058524    -1.91595354429961
H    6.37896224152185    -5.74447572339866     1.38693408902574
H    1.23487600619303    -2.08575707831423     1.88082238132592
H    1.21823842709500    -2.20323918609754    -0.03684999494506
Ni   2.32255363089389     0.09149909129381     1.17108136304426
H    0.11103969503514     0.11897419879043     0.44743007830665
C    0.50618614096787     1.00704963531073     0.94446231995465
C   -0.14430826044536     1.32497246704205     2.24493529094281
C    0.81285460370993     2.13412921745140     0.01685318583889
H   -0.15770325652843     0.46618753590048     2.91448172742609
H   -1.18969867676164     1.59345165216578     2.03699756448987
H    0.33278667935838     2.16373861636423     2.74781067808518
H    1.39260157873606     1.81029866282233    -0.84884475937073
H    1.32645112598328     2.94954944879971     0.52571860708900
H   -0.13885436700172     2.52551768977026    -0.36864097865530
C    2.90430273481346     1.37313941994842     2.44498468472850
N    3.29395056910092     2.13919180985941     3.21861656369628
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4 L
M2
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O    3.26704035753699    -0.76038762285120     0.08088355028739
Si   4.90686779657301    -0.98483402910536    -0.02485892110240
O    1.24765744643903    -0.11110566116469    -2.05758559793121
Si   2.01273656924156     0.04801539726372    -3.46646542548279
O    3.53947285428845     0.52103854644573    -3.01814537233254
Si   5.12063119169403     0.13094138883864    -2.89344434322184
O    5.43931920215889    -0.18448273262721    -1.33052228941306
Si   1.88837482651332    -3.86177201889316    -1.63009113174075
O    1.77543945751313    -3.73450316640338    -3.24519868999783
Si   2.33970062623735    -2.91288157951085    -4.52929811530225
O    3.40094230182827    -4.27323184384993    -1.19958213362865
Si   4.97608559872691    -3.88751443352447    -1.12941318468997
O    3.93558830006601    -3.16968192411342    -4.68168898457712
O    5.54452785896672    -3.56774147836965    -2.61559521636230
Si   5.37092644581236    -2.78634277907363    -4.02823834145240
O    1.54489641587179    -2.42488264534428    -0.92845269533022
O    2.07081381557743    -1.32880323869153    -4.32113995065722
O    5.16602471345181    -2.57664669603798    -0.18225104494638
O    5.44086472453086    -1.18089179092613    -3.78997850170284
H    5.56564002977645    -0.47379573453521     1.17505686245162
H    0.97537700416465    -4.90852344861516    -1.16320863229308
H    1.65876146932867    -3.37876431842474    -5.73833086306782
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H    5.95032621389005      1.24926810956304     -3.34169690434921
H    5.72427277622813     -5.00503514046435     -0.55235687169315
H    1.46089149414374      1.09469636920541     -4.33933946559464
H    6.44483800081696     -3.19000719978090     -4.93717983850747
H    2.68569787451825     -1.52985964984045     -0.14971350612795
H    1.26828939130537     -1.62771727796134     -1.46443013147715
Ni   2.30085015637654      0.89649232471002     -0.78741383626323
H    0.39356740854270      0.17578262235048      0.36368350177667
C    0.80630603717979      1.17931173581870      0.47586883919800
H    1.24009678292049      1.35668190951203      1.45472512801774
C   -0.04427936440702      2.28299023933070     -0.06352632939220
H   -0.28519463732571      2.09336714015716     -1.11253625469551
H    0.49021634131953      3.23251647904579     -0.00367056798005
C   -1.34589709126896      2.37411255857809      0.73900110347609
C    3.23828113587011      2.22807386690321      0.14789670326311
N    3.83611266033057      3.03727496945730      0.71753918982726
H   -1.97091944787658      3.17607441703291      0.34340079748910
H   -1.14606487123815      2.58797118285606      1.79017153261112
H   -1.91215986762361      1.44320715304005      0.68013593291515
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5 TS II B
M2
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O    1.34900711316621     -1.48990718831920      2.08984301178781
Si   2.45698988132291     -1.96967444140734      3.23539162453127
O    2.27158259185598     -1.30399311884706     -0.69321357741102
Si   3.80623914278069     -1.58976193485838     -1.09080189798424
O    4.77548284988705     -1.37484955301352      0.21103331583852
Si   5.21923010582013     -1.78385803994475      1.70648992168005
O    3.94606697986479     -1.65681663114694      2.71578535166826
Si   1.12593460607844     -4.82112762140945      0.13758982183374
O    2.36347362492532     -5.09993782429230     -0.87138945052475
Si   3.88680516404463     -4.70854374803378     -1.28957270341249
O    1.50281950939355     -5.32659014443938      1.63826419483719
Si   2.48984631989509     -5.06271434836845      2.89962899566183
O    4.88893245096817     -5.09101481139386     -0.06853028824505
O    4.03486066308593     -5.22870998266631      2.44520531684010
Si   5.29744547747635     -4.86669796686044      1.48553365551946
O    0.80494999048948     -3.21654349884758      0.20540214450117
O    3.97377229487237     -3.12828809713737     -1.61530563111407
O    2.23865460978486     -3.55589773734409      3.47261744508993
O    5.73795880342063     -3.32491182336807      1.73249378884997
H    2.18921347308362     -1.21998393169622      4.46449491926781
H   -0.05349826360644     -5.56893400157767     -0.30938973278848
H    4.26368471217318     -5.48177922663105     -2.47485840833468
H    6.29305409792341     -0.90907968844924      2.17576271410607
H    2.18172074752504     -6.02257464002243      3.96126314706185
H    4.29512830060962     -0.70207603808364     -2.15605460967548
H    6.41590104413061     -5.75009223058163      1.82064122302212
H    1.01473006362380     -2.23501007910948      1.52291905164949
H    1.35041492662196     -2.57385112818031     -0.33538430379441
Ni   1.82866950712645     -0.06541110952367      0.65738864245345
H   -0.01669418708882      0.63480181896853      0.84604757654158
C    0.60215116830259      1.42645066470911      1.31596026412294
C    0.19610848289115      1.59314029294103      2.75354166630104
C    0.58086177576903      2.67512097990142      0.47621250222505
H    0.30698958223081      0.66726617549046      3.31467639663552
H   -0.86191395818383      1.87460834684932      2.77790665312407
H    0.77476476038118      2.37620340271488      3.23973304477592
H    0.94092381604383      2.49935305995954     -0.53826060637734
H    1.18263624152462      3.46203558708013      0.92759928481784
H   -0.45406093017681      3.02502464215861      0.40297705226115
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C  2.60993647162691      1.29078629611657      1.60998659442836
N  3.35696598833380      1.99095931866516      2.15353188822774
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5 TS II L
M2
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O   2.99522588272340     -0.78728542710915      0.09833748048852
Si  4.63901981796128     -0.92984418275340     -0.10041685934046
O   1.49653291303431     -0.17809754500707     -2.36282074401824
Si  2.17382653064274     -0.03196632736236     -3.81433043515901
O   3.73021291212162      0.46171239196839     -3.67102867968777
Si  5.18030515761435      0.06033775367585     -3.08027203933749
O   5.06710105808223     -0.21131325539518     -1.47853761197943
Si  1.87928834095388     -3.91988745567950     -1.80304026949690
O   1.88914359617329     -3.84459335666689     -3.42296711508722
Si  2.53485266776983     -3.04105889019518     -4.68475215805161
O   3.35661883139876     -4.30342987120303     -1.23897728010296
Si  4.90679338596228     -3.86728283608848     -1.04175245241547
O   4.14775366200961     -3.24044516852561     -4.66929883620163
O   5.60271815249965     -3.58897775239556     -2.47677670538864
Si  5.55862662192065     -2.89697168199961     -3.94777251276879
O   1.45922219876828     -2.46699075040301     -1.17705606615274
O   2.15828642434709     -1.47402149280671     -4.58067296191203
O   4.97469685766427     -2.51414163833981     -0.13590572943710
O   5.72780093023329     -1.29149254014723     -3.79635991115933
H   5.30243122525568     -0.28281869468223      1.03095410368203
H   0.94191890798969     -4.95873805195849     -1.36649073883252
H   1.99709217606058     -3.59885849839797     -5.92757698164169
H   6.12785806215201      1.14990564730446     -3.31935820064080
H   5.62695335969521     -4.93593191515218     -0.34758171653633
H   1.48624064545284      0.94322400230155     -4.67426859361474
H   6.65811955114376     -3.42302207350631     -4.75919694899543
H   2.47246231587708     -1.56860807157144     -0.22007466631397
H   1.33805143374830     -1.67488019053770     -1.77525866154487
Ni  1.96793395745216      0.77164579806412     -0.80439148488420
H   0.63884135949692      0.47661413233068      0.78909611937484
C   0.97667500575726      1.52443525605240      0.75535723085443
H   1.38633071999474      1.77704254086249      1.72730834233024
C  -0.07221434083101      2.48694986247102      0.26316259879908
H  -0.35955760417547      2.24817408216454     -0.76542014759180
H   0.33879227105518      3.49713646528272      0.25486984995160
C  -1.30485389177387      2.42275548132915      1.15883238232136
C   2.74564512203478      2.17989391068644      0.06165782272807
N   3.44157835409309      3.04825527846449      0.38664820639004
H  -2.05837331465495      3.13433498064882      0.81900262065730
H  -1.05333433458959      2.66902425339636      2.19217638399038
H  -1.75369692311668      1.42762583088108      1.14796336672603
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5 B
M2
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O   1.74146047094344     -1.56355714079792     -1.06201781798178
Si  2.98351058360862     -2.30455315460237     -1.84604622607156
O  -0.68242090472897     -3.30384853842202     -0.94567457998289
Si -0.83401344738608     -4.74553637413577     -1.62128262505390
O   0.21932941157570     -4.94344219433231     -2.87457879098897
Si  1.78359157385579     -4.87415599113873     -3.26100604222763
O   2.41567166587369     -3.42279917080093     -2.86973154100377
Si  1.53060738530322     -3.93755813497775      1.95506764912693
O   0.83941601284398     -5.38333626713041      1.69048830209431
Si  0.49166998498607     -6.51737822898235      0.57663979548102
O   3.10965086021561     -3.98817840671410      1.54591568350750
Si  4.21061137714358     -4.12757482059678      0.36005289406231
O   1.87533103593973     -7.01040408768326     -0.12746968056842
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O    4.10217229519179    -5.58110872668765    -0.34528991281561
Si   3.13288564564506    -6.65711591987492    -1.08452759666308
O    0.79350240802148    -2.79043227210307     1.06543906054819
O   -0.52503030227038    -5.93052052390235    -0.53141679886171
O    3.97704470955915    -2.96172926117871    -0.74728557316529
O    2.61734483398628    -6.03859620900426    -2.49293120257039
H    3.70216540726036    -1.29157793830627    -2.62836002806768
H    1.45871992808226    -3.62356707694275     3.38641434738626
H   -0.12095087132399    -7.66652780121077     1.24914179912353
H    1.93758677067960    -5.06352927060423    -4.70745191929663
H    5.55314204373832    -3.97023662372645     0.93146944955060
H   -2.17492160353354    -5.00388764603734    -2.17315417888280
H    3.89943407789745    -7.87739337653764    -1.35049911773207
H    1.53718442743808    -1.90674519418907    -0.15651098529249
H    0.09875081453903    -3.06714719457582     0.38343484610437
Ni  -0.17326204347996    -1.78332380759836    -1.96085751805354
H    1.50834992647650     1.57197901485381    -5.00624463445690
C    0.42907413369626     1.38427695421110    -5.01932388045882
C    0.03752176984147     0.84388566139820    -6.39495196993499
C   -0.30464434787727     2.67905936455829    -4.67128972853332
H    0.56653532917357    -0.08018588781193    -6.62609724843685
H    0.28437239719256     1.58505038727367    -7.15541647192552
H   -1.03447990302644     0.64898110510895    -6.44034071085607
H   -1.38290512787393     2.51656917340510    -4.65863605070481
H   -0.07931501916333     3.43383943267508    -5.42503577463346
H   -0.00095827423891     3.05980668867989    -3.69666183464437
C    0.18988456848044     0.37725003449879    -3.99666750054035
N   -0.00500000428633    -0.42325057605651    -3.19554588657932
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5 B
M2
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O    2.80035005057423    -1.08660973985039    -0.37833217803667
Si   3.97032087032459    -2.12060876298904    -0.93266671585055
O    0.15508860443984    -1.75956091227838    -1.42568758452725
Si  -0.15978189124580    -2.81926440531178    -2.57143523901908
O    1.17584527463346    -3.18930499941818    -3.46453204890971
Si   2.70867816278489    -3.67747430717273    -3.36126403423540
O    3.56930772833468    -2.68379275105394    -2.39295666450077
Si   0.75070934104073    -3.73292099901179     1.56177635102878
O   -0.18269870394441    -4.69225857030625     0.63698381076558
Si  -0.42560071660861    -5.36130463458135    -0.82450403801681
O    2.24811120386863    -4.37279813716988     1.70580109002306
Si   3.60214386879640    -4.67875756389367     0.87049902100844
O    0.89222687571913    -6.22585198130829    -1.23609586167627
O    3.33153340225236    -5.81805799805370    -0.25216272061263
Si   2.47626846016810    -6.23272689241532    -1.57232998062371
O    0.87533397857182    -2.26089587158783     0.88504341687705
O   -0.71905295449917    -4.22492928550552    -1.93505391884293
O    4.12460972661102    -3.31696448550462     0.14373486275754
O    2.79895799837302    -5.18766651753357    -2.77010288837737
H    5.22280094948653    -1.36756088502411    -1.05015611196581
H    0.17264176401252    -3.66501303838144     2.90925144123557
H   -1.57268376981263    -6.27064603186569    -0.74265851303714
H    3.31858660112615    -3.65510364083292    -4.69440579429550
H    4.64280612722905    -5.14831840173764     1.78818929126143
H   -1.17139376394687    -2.35604436036000    -3.54305180610327
H    2.87729608997447    -7.57967755376013    -1.98669357744859
H    2.18099340026498    -1.50362254719897     0.28812272858463
H    0.43153190856176    -2.10298814541483    -0.03955188632586
Ni   1.46588049581410    -0.27407735748135    -1.63949181020075
C   -2.63719238963430     0.83595222782663    -4.11169341386636
C   -3.12610606130278     0.61228924784041    -2.69291995292487
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C  -1.44402279954177     1.79844499919578    -4.19304601140827
H  -1.12122472828724     1.93964752423209    -5.22731424804025
H  -1.71467607146726     2.78215642683873    -3.79820276777136
H  -4.00046073966109    -0.03895988102470    -2.68739532365572
H  -3.40859133836681     1.55486581148651    -2.21770511472918
H  -2.35851415014855     0.13687266053163    -2.07850686177131
H  -3.43185629551123     1.25820042810631    -4.73084383551809
H  -2.35157984937582    -0.11635367262851    -4.56357444974639
C  -0.32335739796776     1.29738871509513    -3.42433379132714
N   0.50181073835963     0.82400628950334    -2.78120287017711
```
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3 (TS connecting 3L to 3B isomerization l to b)
M1
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O  -2.49091020349340    -1.02398248553091     1.61192599045800
Si -3.32697292398650    -1.62488650825628     2.90416746807416
O   0.26816210712949    -1.54660071231725     1.62171293300073
Si  1.09798409608633    -2.20418216108625     2.81911699649834
O   0.27276031589959    -2.12668720874931     4.24548663049259
Si -1.12781249742307    -2.41557620596544     4.98854786468008
O  -2.35831530614316    -1.68540174255256     4.19939601687844
Si -1.43791621035025    -4.37060262307599     0.04098962423308
O  -0.19586650700462    -5.09657060217455     0.80013763973558
Si  0.70633640716663    -5.20643591504141     2.14759624541427
O  -2.84304329752632    -4.77786664357618     0.76976074491414
Si -3.67754723398923    -4.65962097074393     2.15174659891704
O  -0.24164604109979    -5.69175561677440     3.37974139275236
O  -2.88413690464853    -5.39848526400850     3.35854606756154
Si -1.55282075991536    -5.42707241155827     4.29111912281739
O  -1.27373263172351    -2.75430814276998     0.09314762868574
O   1.38812991379655    -3.78502118906986     2.50259980699735
O  -3.89981423115857    -3.08735661762583     2.52438468760918
O  -1.42421038619994    -4.00899846090449     5.07158489148735
H  -4.43282475132070    -0.70845827849469     3.20362680661625
H  -1.50373759330734    -4.85753247575517    -1.34130130135201
H   1.75259300172056    -6.21057198702504     1.93817818010346
H  -1.08173775958426    -1.86557466761195     6.34770437216332
H  -4.99013429308203    -5.28797898341848     1.98670801515018
H   2.39649250089605    -1.55443953954903     3.07108805175029
H  -1.68495864944701    -6.50313459136565     5.27611494422999
H  -2.21096321621605    -1.69595193881769     0.93289025544425
H  -0.50982762228147    -2.33582966118304     0.63904867179353
Ni -0.78481604293325    -0.00195991500517     2.03264880411970
H  -1.67445005454099     2.29833052430283     1.76678406399026
C  -1.25843726316712     1.74290842104605     2.60710688533034
C  -1.98736003008990     1.85415186862103     3.92851387047749
C   0.30866690774796     1.37889628043528     2.53733847850865
H   0.90028877824584     1.79835589057384     1.72421667631552
H   0.82705468115743     1.31455958503820     3.49258906716772
H  -3.00993765289190     1.50083833650270     3.79322531733708
H  -2.04258808712827     2.87625610916359     4.31326845430594
H  -1.52724437396073     1.22164433996150     4.68762631304447
H  -0.30474618523275     2.51006216436290     2.76694572229538
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