Supporting Information for Unravelling the Mechanism of Tin-based Frustrated Lewis Pair Catalysed Hydrogenation of Carbonyl Compounds

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Table S1: Selected NBO interaction energies (computed at the second order pertubation level) in TS-H_2act(Sn/N)-dist and TS-H_2act(Sn/O)-dist. All energies are in kcal/mol

TS	$\Delta E^{int}_{N/O(LP)\rightarrow\sigma^*(H_2)}$	$\Delta E^{int}_{p(Sn)\leftarrow\sigma(H_2)}$
TS-H_2act(Sn/N)-dist	162.2	64.4
TS-H_2act(Sn/O)-dist	67.2	37.0

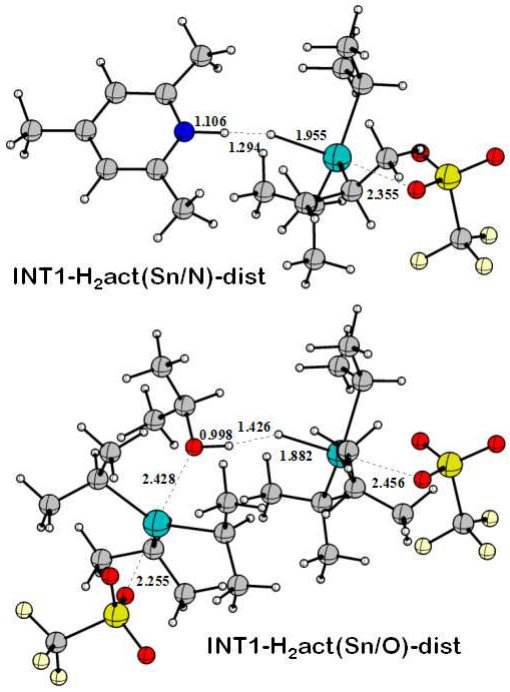


Figure S1: Geometry optimized structures of **INT1-H_2act(Sn/N)-dist** and **INT1-H_2act(Sn/O)-dist** during H_2 cleavage by Sn/N and Sn/O FLPs respectively. All distances shown in the figure are in Å unit.

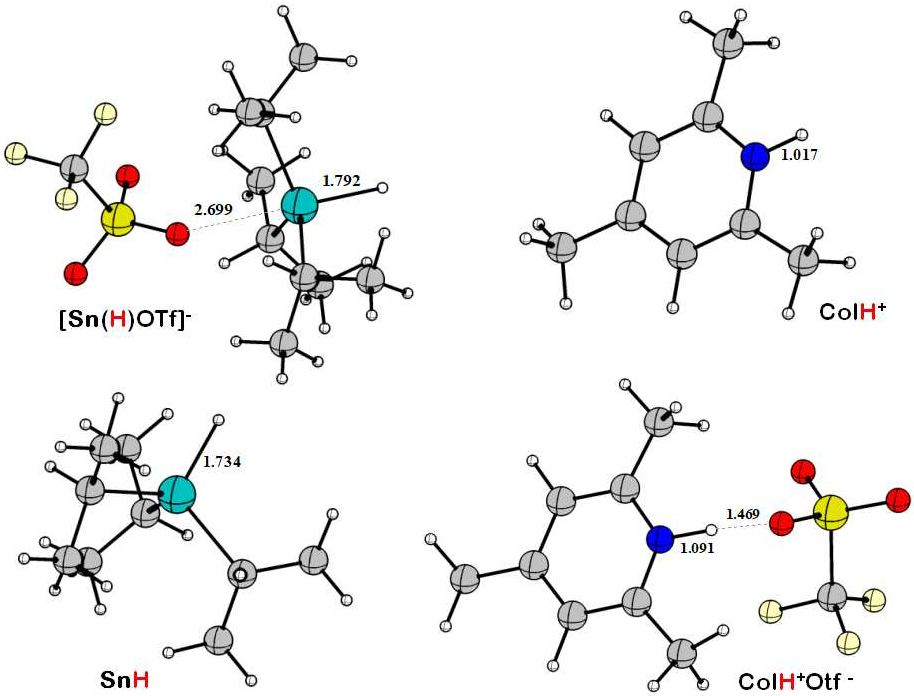
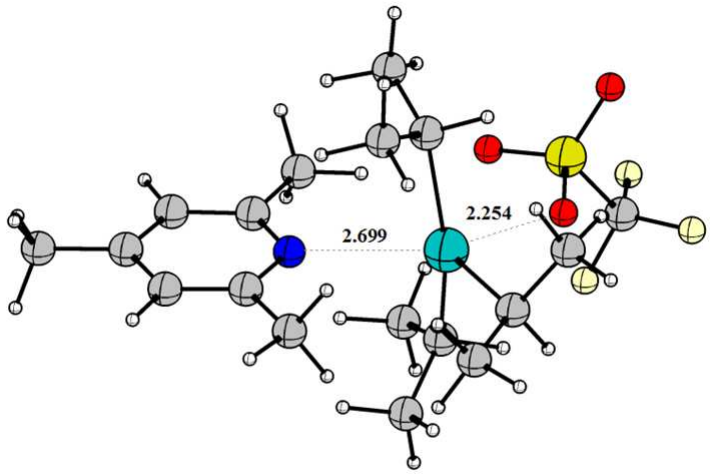
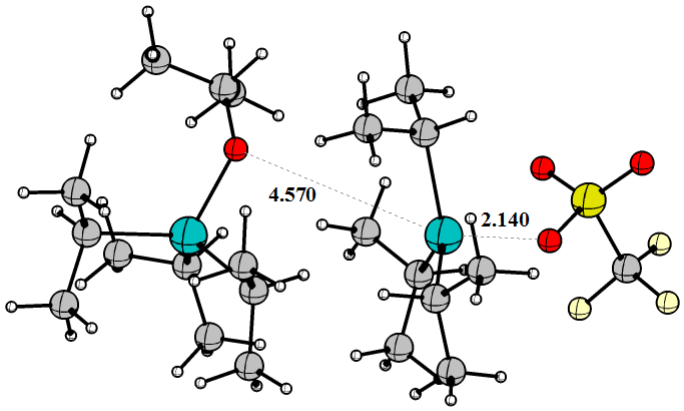


Figure S2: Geometry optimized structures of [**Sn**(H)OTf]$^{-}$, ColH^{+}, **Sn**H, and ColH^{+}OTf^{-}. All distances shown in the figure are in Å unit.



clp(Sn/N)-dist

Figure S3: Geometry optimized structures of a dative adduct between Col and **Sn**OTf. Formation of such dative adduct is found to be endergonic by 13.2 kcal/mol, presumably due to the high degree of strain caused by the steric repulsion between Me groups in Col and iPr groups in **SnOTf**. All distances shown in the figure are in Å unit.



flp(Me_2CHO**Sn**/**Sn**OTf)-dist

Figure S4: Geometry optimized structure of **Sn**OTf/Me_2CHO**Sn** EC. All distances shown in the figure are in Å unit.

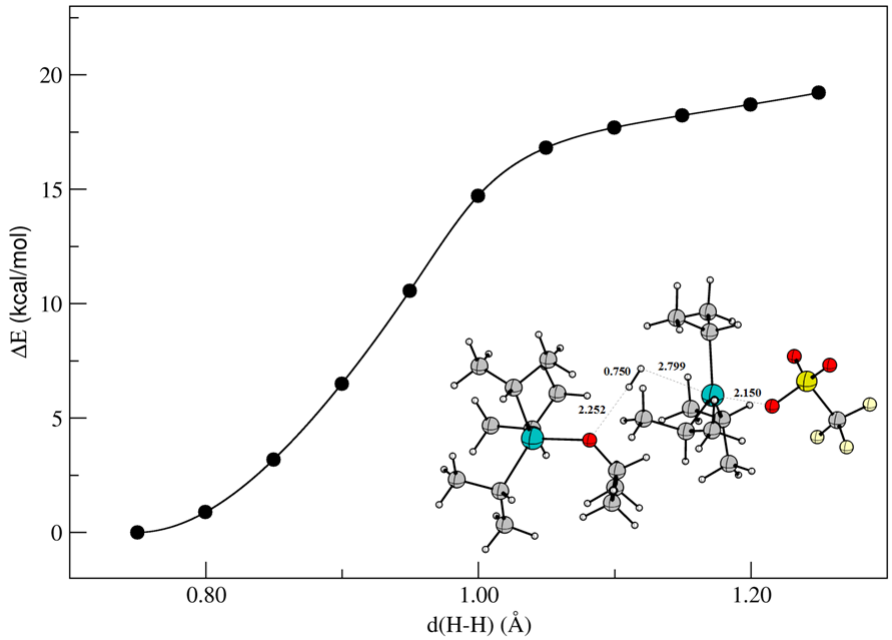


Figure S5: Potential energy profile for H_2 activation in the distal pathway for **Sn**OTf/Me_2CHO**Sn** Lewis pair. The data points are obtained by performing a relax PES scan with respect to H-H separation at M062X-D3/BSI level. A weak **Sn**OTf/Me_2CHO**Sn**/H_2-adduct (structure is shown in the inset) is chosen as the starting point for the scan calculation. All distances shown in the figure are in Å unit.

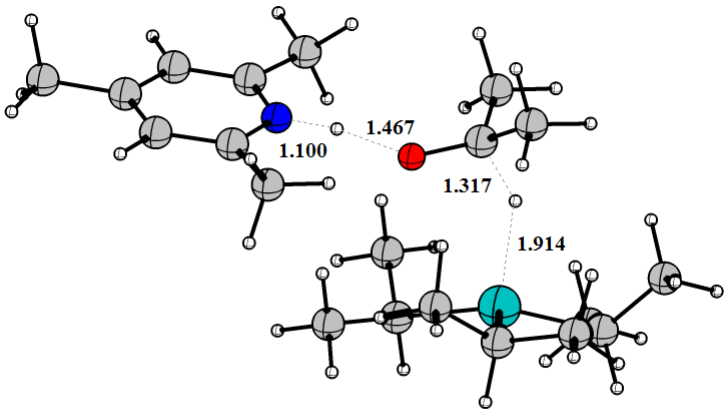


Figure S6: Geometry optimized structure for the alternative TS in BAA mode. All distances shown in the figure are in Å unit. Solvent-corrected Gibbs free energy is given in parenthesis.

A note on the possibility of a radical mechanism in Tin-based FLP-catalysed hydrogenation reaction

We have also considered the possibility of a radical mechanism as this is quite common in the Sn-based reactions. This is particularly relevant because R_3SnH species (one of the reaction intermediates) are susceptible for homolytic Sn-H cleavage giving rise to radical chain mechanisms. However, the homolytic cleavage usually occurs in the presence of a radical initiator or UV radiations, the lack of which rules out the possibility of radical mechanism in the present case. This was also addressed in the experimental works of Ashley et al. While studying the hydrogenation of imines catalysed by iPr_3SnOTf, Ashley et al. deliberately used a bromoaryl imine substrate (see ref 24 of the main manuscript) to check whether a radical mechanism is operative or not. The NMR study showed a clean hydrogenation reaction with no experimental evidence of any side reaction such as hydrodebromination, the formation of $iPr_3Sn\text{-}SniPr_3$ or $iPr_3Sn\text{-}Br$. This suggests that the radical Sn species is not involved during the iPr_3SnOTf catalysed hydrogenation reaction. So, it was proposed that the reaction follows a normal polar FLP-hydrogenation mechanism. Also, during their mechanistic study of the carbonyl hydrogenation process, Ashley et. al. reported no evidence in favour of a radical mechanism. Therefore, considering these experimental observations, we ruled out possibility of a radical mechanism and did not further explore along this route. Instead, we focussed on the polar mechanism for hydrogenation of the carbonyl compound.

A note on the conformational complexity of the stationary points involved in the reaction pathway

This is a discussion regarding the conformational space of the molecular models investigated in the present study. Admittedly, we have not performed exhaustive conformational searches

as these are not expected to affect our chemical interpretation for the present reaction. However, care has been taken while constructing the input structures for the geometry optimization of the reaction intermediates (RIs)/TSs.

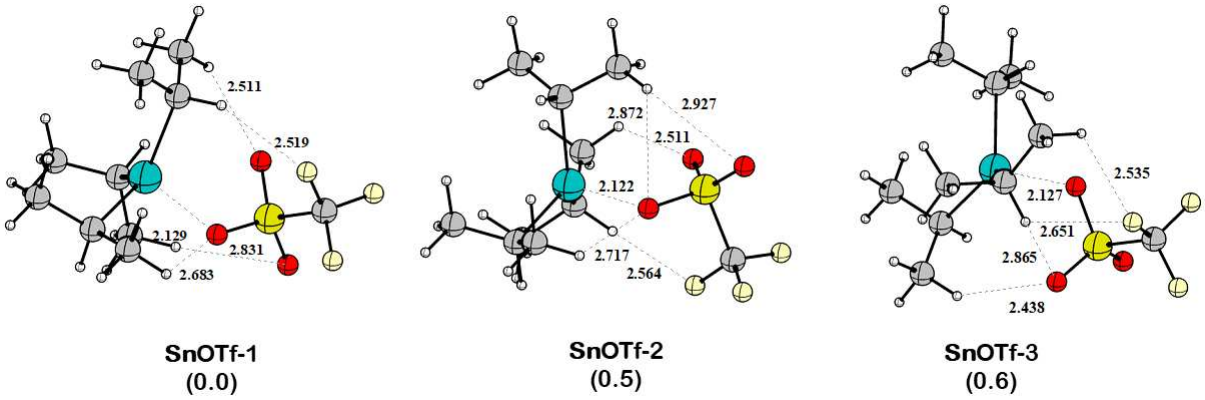


Figure S7: Geometry optimized structures of the three conformers of **Sn**OTf. All distances shown in the figure are in Å unit. The relative electronic energies (kcal/mol) of the conformers are shown in the parenthesis. The lowest energy conformer is considered as the reference.

In this context, the relative orientations of the iPr groups and counteranion OTf^- play an important role. Both the methine and the methyl hydrogens of the iPr groups can weakly interact with F and O atoms of the counterion. Based on their mutual positioning, it is possible to envisage a few possible conformations of the **Sn**OTf. For example, while optimizing **Sn**OTf, we manually constructed several input structures, which mainly differ from each other in the different relative orientations of the iPr methine hydrogens with respect to the OTf^- counterion. After geometry optimizations, we have been able to locate three structures as the local minimum which slightly differs in the relative orientation of the iPr groups and OTf^- although the relative energy difference between these three conformations lies within 1 kcal/mol. In these structures, we found a series of noncovalent interactions such as C-H$\cdots$O and C-H$\cdots$F contacts involving the methyl/methine hydrogens of the iPr groups and F/O atoms of OTf^-. In fact, the methine hydrogens are found to be more or less pointing towards the OTf^-. Note that, the input structures for the other intermediates/TSs are prepared with the lowest enrgy conformer of the sub-unit **Sn**OTf

(**Sn**OTf-1). However, from the relative stabilities of the three conformers, the estimated uncertainty arising due to diffrent orientation of the iPr groups relative to OTf^- can be roughly estimated to be within 1 kcal/mol. Geometry optimized structures of the three conformers of **Sn**OTf are depicted in Figure S7.

After geometry optimization, for each of the intermediate or TS structures, we have again carefully looked at the relative orientation of the iPr groups in the LA fragment. Mostly, what we found is that the iPr groups are locked in similar conformations (i.e. maintaining the minimum energy arrangements as mentioned in the previous paragraph) with methine hydrogens more or less pointing towards the OTf^- counterion. However, in some of the cases, slightly different situations were observed. For example, in the transition state for hydride transfer (**TS-HT-LAA-1**), there are two iPr_3Sn moieties; one from which the hydride is being transferred and the one, which is coordinated with the carbonyl oxygen (used for LA-activation of the substrate). Interestingly, the iPr groups of the LA unit, which coordinate with the carbonyl substrate, were found to exist in a different conformation; in this case the methine hydrogens point in the opposite direction of the counterion. Our natural response was to look for a structure that features this LA unit in the favorable conformation (i.e. methine hydrogens pointing towards the OTf^-). Unfortunately, all efforts to optimize a TS structure by rotating these methine hydrogens towards OTf^- were unsuccessful. Nevertheless, a close inspection of the structure of **TS-HT-LAA-1** reveals that most probably this conformation was assumed specifically to avoid the steric conflict with the iPr groups of the other iPr_3Sn moiety from which the hydride is transferring to the carbonyl carbon.

Cartesian coordinates and absolute energy data for the computed structures involved in the reaction pathway

We have used the following notations,

NImag= Number (and size, if any) of imaginary frequencies

$\mathbf{E}^{gas}$= gas-phase absolute electronic energy (hartree) at M062X/BS-I level of theory

$\mathbf{E}^{gas}_{sp}$= gas-phase absolute single point energy (hartree)

$\mathbf{E}^{sol}_{sp}$= solvent-phase absolute single point energy (hartree)

$\mathbf{G}^{gas}_{298.15}$= gas-phase absolute Gibbs free energy (hartree) at 298.15 K

$\mathbf{G}^{sol}_{393.15}$= solvent-phase absolute Gibbs free energy (hartree) at 393.15 K

SnOTf

NImag= 0

$\mathbf{E}^{gas}$= -1320.2932

$\mathbf{E}^{gas}_{sp}$= -1320.3086

$\mathbf{E}^{sol}_{sp}$= -1320.3087

$\mathbf{G}^{gas}_{298.15}$= -1320.0384

$\mathbf{G}^{sol}_{393.15}$= -1320.0936

Sn -1.04327200 0.01537500 -0.01465300

C -2.03696600 -0.82784300 -1.74283900

C -3.44830700 -1.32102600 -1.39990000

C -1.18692100 -1.94068000 -2.36390500

H -2.11508700 -0.00262600 -2.45862900

H -4.07440700 -0.53719700 -0.96433000

H -3.95543300 -1.68214400 -2.30090500

H -3.41724900 -2.15472800 -0.69280200

H -0.19438200 -1.58545800 -2.64726400

H -1.05793400 -2.77674400 -1.66889900

H -1.67388900 -2.33847300 -3.26084200

C -0.72806400 -1.28228200 1.68929100

C -1.69966700 -2.46686100 1.69802200

C -0.81938300 -0.46458100 2.98162400

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H -1.61843200 -3.07923700 0.79639800

H -1.49993500 -3.11540300 2.55746400

H -2.73916800 -2.13364500 1.78341200

H -0.08859300 0.34592800 2.99473900

H -1.81670500 -0.03097600 3.11294000

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C -1.57040300 2.06027700 0.43408100

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C 3.15936000 -0.61200300 -0.09771400

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F 3.55431100 -0.92010400 -1.31980800

F 2.53756900 -1.66110500 0.43357900

S 2.00249600 0.82723800 -0.14401500

O 1.55695500 1.02726700 1.22511900

O 2.68144100 1.87929300 -0.84754700

O 0.85650700 0.21234800 -0.95596600

H_2

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$\mathbf{E}^{gas}_{sp}$= -1.1684

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$\mathbf{G}^{gas}_{298.15}$= -1.1697

$\mathbf{G}^{sol}_{393.15}$= -1.1701

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H 0.00000000 0.00000000 -0.37024800

Col

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$\mathbf{E}^{gas}_{sp}$= -366.1670

$\mathbf{E}^{sol}_{sp}$= -366.1760

$\mathbf{G}^{gas}_{298.15}$= -366.0274

$\mathbf{G}^{sol}_{393.15}$= -366.0564

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H -2.16773600 2.42324400 0.88104600

C -1.52224000 -2.40589900 0.00229300

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(Sn/N)-dist

NImag= 0

$\mathbf{E}^{gas}$= -1686.4714

$\mathbf{E}^{gas}_{sp}$= -1686.4900

$\mathbf{E}^{sol}_{sp}$= -1686.4962

$\mathbf{G}^{gas}_{298.15}$= -1686.0566

$\mathbf{G}^{sol}_{393.15}$= -1686.1329

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C -1.00844000 2.29122000 -2.14715100

C -0.51594600 -0.13597900 -2.64380100

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$\mathbf{G}^{gas}_{298.15}$= -1686.0625

$\mathbf{G}^{sol}_{393.15}$= -1686.1346

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C -2.84222300 2.12834700 -1.25988600

C -1.98726500 3.71053500 0.52950500

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H -2.96376800 1.08776800 -1.56989600

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C 1.68266000 -2.70650800 -2.40739900

H 1.47180300 -3.75312000 -2.18943500

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TS-H_2act(Sn/N)-dist

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$\mathbf{E}^{gas}_{sp}$= -1687.6331

$\mathbf{E}^{sol}_{sp}$= -1687.6497

$\mathbf{G}^{gas}_{298.15}$= -1687.1880

$\mathbf{G}^{sol}_{393.15}$= -1687.2771

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C 0.23317800 2.10315400 -2.08633400

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H -0.13123000 4.34108400 -0.57694400

H -1.22195200 3.15144000 0.14244600

H 0.86413600 1.35654600 -2.57210600

H -0.81052100 1.78001200 -2.15883400

H 0.32223500 3.03943900 -2.64951000

C 0.32956800 -1.44097600 -0.62307500

C -0.98170000 -1.61733700 -1.38621400

C 0.58627800 -2.60644800 0.33598000

H 1.15131500 -1.38809600 -1.34237000

H -1.18375000 -0.77575600 -2.05615600

H -0.95846600 -2.52848200 -1.99489400

H -1.83311600 -1.70856900 -0.70388300

H 1.54387100 -2.50008300 0.85085600

H -0.19782700 -2.67779300 1.09982900

H 0.60488300 -3.56145500 -0.20172000

C 0.68045900 0.38778400 2.61791100

C -0.59934000 0.04490500 3.37376800

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H -0.96555800 -0.95191000 3.11402200

H -0.42886000 0.06174600 4.45673900

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H 2.20348800 1.95390800 2.56508200

H 0.58706100 2.52797900 3.01807900

H 1.55893600 1.62388600 4.17715900

C 4.46528700 -1.38020100 -0.63545700

F 5.08452000 -1.62751600 0.51055500

F 5.34494200 -1.45204900 -1.62440600

F 3.53810700 -2.32017300 -0.82490900

S 3.67489900 0.28703100 -0.60634900

O 2.74495600 0.12585500 0.56835600

O 4.74608500 1.22400100 -0.36756100

O 2.94202700 0.36647200 -1.86187200

C -4.37924100 0.66862200 -1.01350600

C -5.68504700 0.30805200 -1.31876600

C -6.32451900 -0.68918000 -0.58839000

C -5.61813500 -1.29407000 0.45223400

C -4.32157800 -0.89885900 0.73510100

N -3.74329600 0.06443900 -0.00148500

H -6.19491200 0.80940800 -2.13261100

H -6.07692300 -2.07290100 1.04955900

C -3.62065900 1.69809600 -1.79466300

H -4.30568700 2.38128000 -2.29468400

H -2.94916100 2.26525100 -1.15035400

H -3.01151700 1.20478900 -2.55677500

C -3.50948900 -1.48446500 1.84965800

H -2.53093300 -1.80279700 1.48383100

H -3.33717000 -0.73505900 2.62488800

H -4.02101300 -2.33856300 2.28981900

C -7.72261100 -1.12448800 -0.92066400

H -7.69106200 -2.03757200 -1.52107000

H -8.28953300 -1.34241300 -0.01491100

H -8.25044500 -0.36202500 -1.49257900

H -2.56017600 0.38289200 0.26100900

H -1.56324500 0.65685000 0.50851800

TS-H_2act(Sn/N)-prox

NImag= 1 (i440.65)

$\mathbf{E}^{gas}$= -1687.6078

$\mathbf{E}^{gas}_{sp}$= -1687.6275

$\mathbf{E}^{sol}_{sp}$= -1687.6304

$\mathbf{G}^{gas}_{298.15}$= -1687.1795

$\mathbf{G}^{sol}_{393.15}$= -1687.2550

Sn -1.83470800 -0.36283600 -0.00086000

C -2.07789200 -1.00030700 2.05616600

C -1.82118900 -2.49987300 2.22386500

C -3.44810900 -0.60050600 2.61564400

H -1.30295700 -0.44017800 2.58725200

H -0.86328500 -2.80565000 1.79596200

H -1.81624500 -2.77450300 3.28482000

H -2.60105600 -3.09525700 1.74113100

H -3.60866500 0.47993600 2.57182100

H -4.26418200 -1.08462400 2.06946600

H -3.53766600 -0.90377200 3.66480400

C -2.63814500 1.54902900 -0.64975200

C -4.17047300 1.49011500 -0.64002800

C -2.13514700 1.93465500 -2.04445500

H -2.29449900 2.28420900 0.08089200

H -4.58453200 1.20821200 0.33273300

H -4.58780200 2.46838300 -0.90366700

H -4.54026400 0.77746400 -1.38422600

H -1.04768600 1.98510800 -2.10361500

H -2.48089600 1.21401200 -2.79330200

H -2.53398100 2.91417400 -2.33223700

C -2.75383400 -1.79566800 -1.41618900

C -4.11395800 -2.21781500 -0.83946100

C -1.90469100 -3.01629300 -1.75263400

H -2.92928000 -1.21760300 -2.32994700

H -4.75143300 -1.36882400 -0.57714200

H -4.66733300 -2.82701500 -1.56349700

H -3.99104100 -2.82683900 0.06066000

H -0.97306000 -2.73975900 -2.25023400

H -1.63893800 -3.57761700 -0.85062000

H -2.44960100 -3.69832700 -2.41572200

C 0.83617100 3.26064600 0.29552500

F 1.82604900 3.98046300 -0.21105700

F 0.71770000 3.53638400 1.58692100

F -0.29491100 3.60478700 -0.31593100

S 1.19012900 1.46324600 0.05689800

O 1.15209800 1.24740600 -1.38281400

O 2.43997600 1.25760000 0.75523200

O 0.01439500 0.82304900 0.74535100

H -0.20454400 -1.53146000 -0.42074700

C 2.84395300 -1.50839200 -1.32286000

C 4.22075000 -1.34270300 -1.28852700

C 4.88561500 -1.29942700 -0.06510800

C 4.12888400 -1.43910100 1.09280900

C 2.75163000 -1.58227500 1.00432000

N 2.14429400 -1.62636200 -0.18645800

H 4.76829100 -1.23634600 -2.21754400

H 4.59917500 -1.39787900 2.06792700

H 0.66242100 -1.55377800 -0.29190000

C 1.87179800 -1.67047700 2.21599500

H 1.05219600 -0.95350900 2.12273000

H 1.44989000 -2.67413700 2.31033700

H 2.43418200 -1.44157800 3.11994500

C 2.06662500 -1.55675200 -2.60578700

H 1.49223100 -2.48374500 -2.66512300

H 1.37700500 -0.71023500 -2.64009900

H 2.73366400 -1.50195000 -3.46494300

C 6.36746300 -1.06050000 0.00208500

H 6.87166400 -1.44541100 -0.88484000

H 6.56004800 0.01415400 0.05938700

H 6.80348500 -1.52651600 0.88620700

INT1-H_2act-dist

NImag= 0

$\mathbf{E}^{gas}$= -1687.6148

$\mathbf{E}^{gas}_{sp}$= -1687.6345

$\mathbf{E}^{sol}_{sp}$= -1687.6587

$\mathbf{G}^{gas}_{298.15}$= -1687.1853

$\mathbf{G}^{sol}_{393.15}$= -1687.2827

Sn 0.41645700 0.52454000 0.42253200

C 0.70502100 2.25243700 -0.86495000

C -0.05368200 3.47647700 -0.35111700

C 0.29064000 1.90109100 -2.29567500

H 1.77802000 2.46282300 -0.85371900

H 0.31542900 3.81123200 0.62109200

H 0.04455200 4.31577300 -1.04970800

H -1.12365000 3.26552800 -0.23943800

H 0.88605400 1.07509400 -2.68888500

H -0.76857700 1.62217900 -2.33850200

H 0.42422800 2.76183100 -2.96170000

C 0.29955600 -1.46232100 -0.45285500

C -1.00804700 -1.73454800 -1.19378000

C 0.56470600 -2.51649400 0.62473300

H 1.12149800 -1.47991700 -1.17290200

H -1.22191000 -0.96626500 -1.94438600

H -0.97633100 -2.70166000 -1.70906900

H -1.85780900 -1.77094200 -0.50237700

H 1.52131900 -2.34404800 1.12276800

H -0.21808500 -2.51113800 1.39428900

H 0.59205600 -3.52500900 0.19531300

C 0.73005100 0.67446000 2.56885000

C -0.51979100 0.40984200 3.40320600

C 1.36060900 2.02533500 2.91583300

H 1.46919800 -0.10864000 2.76198100

H -0.90181400 -0.60343700 3.24682500

H -0.30926100 0.52031900 4.47379200

H -1.32025400 1.11485900 3.15118200

H 2.25229900 2.21680100 2.31374300

H 0.65242400 2.84465700 2.75350400

H 1.65633600 2.05892200 3.97093200

C 4.45201500 -1.48444800 -0.49258800

F 5.09772900 -1.58905900 0.66218500

F 5.31231100 -1.68415600 -1.48275000

F 3.52479200 -2.44368600 -0.54193700

S 3.65613200 0.17234300 -0.65416800

O 2.73945900 0.15321300 0.53250900

O 4.73207000 1.13111200 -0.54596400

O 2.92517300 0.09592300 -1.91280900

C -4.36910300 0.54478700 -1.10523500

C -5.66209500 0.12260400 -1.37141200

C -6.29442900 -0.78386800 -0.52323100

C -5.59675100 -1.24064600 0.59756800

C -4.31170500 -0.79764400 0.84815700

N -3.75113400 0.07545800 -0.01012300

H -6.16909100 0.50480000 -2.24869400

H -6.05475300 -1.94299000 1.28299400

C -3.60034900 1.47632200 -1.98755000

H -4.27928500 2.08534500 -2.58209900

H -2.94549700 2.12218700 -1.40184800

H -2.96953300 0.89706300 -2.66732200

C -3.49044400 -1.21822500 2.02505100

H -2.53487600 -1.63206700 1.69360000

H -3.26492000 -0.35700300 2.65716500

H -4.02082900 -1.96569200 2.61165000

C -7.67999500 -1.28115500 -0.81396500

H -7.62288900 -2.26091900 -1.29593300

H -8.25442100 -1.39657000 0.10563600

H -8.21253500 -0.60576600 -1.48244300

H -2.71651300 0.40608700 0.19635300

H -1.51795700 0.79994600 0.48357300

[**Sn**(H)OTf]$^{-}$

NImag= 0

$\mathbf{E}^{gas}$= -1320.9541

$\mathbf{E}_{sp}^{gas}$= -1320.9740

$\mathbf{E}_{sp}^{sol}$= -1321.0145

$\mathbf{G}^{gas}_{298.15}$= -1320.6945

$\mathbf{G}^{sol}_{393.15}$= –1320.7995

Sn 1.58736400 0.21663900 -0.19964600

C 1.48401500 -1.90290600 -0.69991500

C 2.77833500 -2.62416800 -0.31987000

C 1.19642700 -2.04918200 -2.19648300

H 0.64795500 -2.32758500 -0.13949700

H 2.96692700 -2.59208800 0.75697500

H 2.74232500 -3.68037400 -0.61869800

H 3.64182000 -2.17173100 -0.81994800

H 0.22847800 -1.61283800 -2.45194900

H 1.97687900 -1.56478600 -2.79692200

H 1.17317000 -3.10734200 -2.48926400

C 0.29962800 1.52543700 -1.37382700

C 0.99109300 2.01781500 -2.64499700

C -0.18278800 2.69534400 -0.51360900

H -0.56200600 0.90956100 -1.64469800

H 1.29556900 1.18785400 -3.28938100

H 0.32765600 2.66888400 -3.22989100

H 1.89371800 2.59180900 -2.40898800

H -0.70854400 2.33978300 0.37543600

H 0.65738600 3.32096400 -0.18688700

H -0.87246200 3.34011600 -1.07397800

C 1.71688900 0.73032300 1.91969800

C 2.93931900 1.59412700 2.22842500

C 1.68342200 -0.52387500 2.79512800

H 0.80424900 1.30164500 2.11189500

H 2.94502400 2.51984600 1.64506400

H 2.97689700 1.86741300 3.29179300

H 3.86730100 1.06246500 1.99226100

H 0.79951100 -1.12788000 2.57910000

H 2.57415400 -1.14237700 2.63565200

H 1.66240800 -0.26112900 3.86144000

C -3.28917900 0.33090500 0.18477600

F -3.50624100 0.89898800 1.37265500

F -4.44530400 -0.18315200 -0.23964300

F -2.93927400 1.29813900 -0.66820900

S -1.98154500 -0.97076000 0.29241000

O -0.85312000 -0.21412300 0.86945300

O -2.56193300 -1.96920400 1.17605500

O -1.78643300 -1.35816400 -1.10162000

H 3.22441600 0.62123800 -0.80604800

ColH$^+$

NImag= 0

$\mathbf{E}^{gas}$= -366.1630

$\mathbf{E}^{gas}_{sp}$= -366.1671

$\mathbf{E}^{sol}_{sp}$= -366.1760

$\mathbf{G}^{gas}_{298.15}$= -366.3971

$\mathbf{G}^{sol}_{393.15}$= -366.4971

C -0.65162800 -1.20045400 -0.00104900

C 0.72731000 -1.20224700 0.00887500

C 1.44355400 -0.00057600 0.01288800

C 0.72816900 1.20165200 0.00995300

C -0.65073400 1.20089200 -0.00020600

N -1.27882300 0.00043700 -0.00542200

H 1.24741400 -2.15161800 0.01557300

H 1.24899600 2.15062600 0.01749400

C -1.50767100 -2.42536400 -0.00162000

H -2.12855500 -2.45910800 0.89701400

H -2.16323400 -2.43633300 -0.87564300

H -0.88817300 -3.31884300 -0.02497600

C -1.50591000 2.42641000 -0.00221400

H -0.88554900 3.31957800 -0.00767600

H -2.14733300 2.44584300 -0.88658900

H -2.14113200 2.45247000 0.88653600

C 2.93966100 -0.00095400 -0.00704500

H 3.34234900 -0.89148100 0.47422200

H 3.28326900 0.00305600 -1.04617400

H 3.34266200 0.88578300 0.48098300

H -2.29546400 0.00081400 -0.01031000

Me_2CO

NImag= 0

$\mathbf{E}^{gas}$= -193.1152

$\mathbf{E}^{gas}_{sp}$= -193.1196

$\mathbf{E}_{sp}^{sol}$= -193.1239

$\mathbf{G}_{298.15}^{gas}$= -193.0594

$\mathbf{G}_{393.15}^{sol}$= -193.0802

C 0.00000000 0.18769800 0.00000000

O -0.00000400 1.39098400 0.00000000

C 1.28608800 -0.61228000 -0.00150900

H 1.28840200 -1.33047500 -0.82491100

H 2.13555100 0.06165300 -0.08895000

H 1.36431100 -1.18449800 0.92678100

C -1.28608400 -0.61228600 0.00150900

H -1.36430200 -1.18450900 -0.92677800

H -1.28840100 -1.33047400 0.82491600

H -2.13555000 0.06164600 0.08894300

$[Me_2CO\cdots HCol]^+$

NImag= 0

$\mathbf{E}^{gas}$= -559.6950

$\mathbf{E}_{sp}^{gas}$= -559.6998

$\mathbf{E}_{sp}^{sol}$= -559.7697

$\mathbf{G}_{298.15}^{gas}$= -559.4723

$\mathbf{G}_{393.15}^{sol}$= -559.5705

C 3.46804900 0.03126400 -0.04691600

O 2.28871000 0.32423500 -0.13501900

C 4.53804900 0.99550100 -0.46895300

H 4.11087200 1.81308200 -1.04483600

H 5.01661200 1.39638300 0.42997700

H 5.31449800 0.48514800 -1.04183100

C 3.91310600 -1.30256200 0.48419100

H 4.74761500 -1.18232200 1.17736800

H 3.09005500 -1.82199100 0.97088600

H 4.27983600 -1.90534500 -0.35228800

C -1.09103700 1.19744300 0.12067200

C -2.47355800 1.19831600 0.07336300

C -3.18082700 0.00072400 -0.03408900

C -2.45728000 -1.19656700 -0.09179600

C -1.07989200 -1.18347800 -0.04553400

N -0.45409700 0.01026400 0.05980800

H -2.99718300 2.14485200 0.11961500

H -2.97185100 -2.14546900 -0.17720400

C -0.21330000 -2.40186600 -0.08710900

H -0.79077300 -3.27085300 -0.39492800

H 0.61485200 -2.26094800 -0.78420700

H 0.20324200 -2.59794100 0.90423200

C -0.25134900 2.42641100 0.26189600

H -0.07297100 2.62763000 1.32174200

H 0.71466600 2.29361000 -0.22538900

H -0.76442200 3.28609200 -0.16536200

C -4.67658100 -0.01186800 -0.11526900

H -5.10472000 0.91964600 0.25149400

H -4.98204900 -0.14026500 -1.15766600

H -5.09041400 -0.84414600 0.45488900

H 0.57885700 0.01719600 0.07227000

TS-HT/PT-BAA

NImag= 1 (i334.28)

$\mathbf{E}^{gas}$= -1880.7441

$\mathbf{E}^{gas}_{sp}$= -1880.7666

$\mathbf{E}^{sol}_{sp}$= -1880.7878

$\mathbf{G}^{gas}_{298.15}$= -1880.2303

$\mathbf{G}^{sol}_{393.15}$= -1880.3336

C -2.36448100 2.97852600 -0.11520000

O -3.37266900 2.29187300 -0.37596200

C -2.23034000 3.61525300 1.24998100

H -2.63491300 2.96507900 2.02340300

H -1.19818300 3.87245100 1.48221300

H -2.83042400 4.53307500 1.22853400

C -1.66304300 3.67941900 -1.25370100

H -0.67118700 4.02882700 -0.97381000

H -1.60283500 3.02321400 -2.11992600

H -2.28216900 4.54498100 -1.51801500

Sn 0.56647600 0.67918700 0.14132600

C 0.60443900 0.19562200 2.26788600

C -0.00388000 -1.17719500 2.56653900

C 0.03894500 1.30131500 3.15865200

H 1.68049900 0.13562500 2.45537100

H 0.53644800 -1.96388800 2.03526500

H 0.04732400 -1.40124700 3.63916100

H -1.05745500 -1.23876200 2.26843200

H 0.53103600 2.26063000 2.97516800

H -1.03170900 1.45897400 3.00617700

H 0.18243800 1.05524300 4.21747100

C 2.05781900 2.11975600 -0.49723800

C 2.06151000 3.36957800 0.38420300

C 1.92604800 2.45217200 -1.98474100

H 3.00250200 1.59639300 -0.33776500

H 2.30055300 3.11887700 1.42115900

H 2.81442000 4.08790800 0.03927900

H 1.09474400 3.88568800 0.37780300

H 1.99141500 1.55288800 -2.60410700

H 0.97628200 2.94679600 -2.21296000

H 2.72814000 3.12811700 -2.30363900

C -0.21535000 -0.58270600 -1.46004100

C -1.17405000 0.17509700 -2.37299200

C -0.83616900 -1.86531300 -0.90889000

H 0.68457700 -0.85535300 -2.01808700

H -0.66564400 0.98798600 -2.90000500

H -1.60359900 -0.49031000 -3.13497000

H -1.99711000 0.62538200 -1.80808500

H -0.10230900 -2.43757900 -0.33774600

H -1.68146200 -1.64722900 -0.24717600

H -1.21230500 -2.50416300 -1.72044800

C 4.50909500 -1.24970100 -0.91739200

F 4.22475200 -2.31048400 -1.66548800

F 5.80416900 -1.26638300 -0.63079800

F 4.25228400 -0.15397000 -1.63828800

S 3.49383100 -1.24407200 0.62451000

O 2.11983900 -1.15395600 0.03981500

O 3.76881300 -2.51030800 1.26786600

O 3.88952100 -0.02132800 1.30993700

H -1.01089600 1.81110800 0.19096800

C -4.37471500 -0.86018900 -1.23469800

C -4.49445700 -2.23908100 -1.16662600

C -4.27173500 -2.90788600 0.03475200

C -3.95331000 -2.15419400 1.16929500

C -3.82572600 -0.78376300 1.07530200

N -4.03827300 -0.19388200 -0.11846200

H -4.74805800 -2.78774600 -2.06535000

H -3.76856300 -2.63720700 2.12071700

C -3.42418900 0.12673200 2.18761500

H -3.22473500 -0.43045200 3.10060600

H -2.51556100 0.65741900 1.88954200

H -4.20372400 0.86952000 2.37206000

C -4.62224100 -0.05876300 -2.47442700

H -5.69109500 -0.06155300 -2.70111100

H -4.29057100 0.97084800 -2.33898600

H -4.09185200 -0.49969300 -3.31852600

C -4.31413200 -4.40472700 0.10484600

H -4.92751500 -4.82464400 -0.69154600

H -3.29748600 -4.79301100 -0.00820000

H -4.69526000 -4.74438900 1.06799100

H -3.84602200 0.85076500 -0.18091300

Me_2CO-**Sn**OTf

NImag= 0

$\mathbf{E}^{gas}$= -1513.4349

$\mathbf{E}^{gas}_{sp}$= -1513.4526

$\mathbf{E}^{sol}_{sp}$= -1513.4579

$\mathbf{G}^{gas}_{298.15}$= -1513.1024

$\mathbf{G}^{sol}_{393.15}$= -1513.1729

Sn 0.72649000 0.08637300 0.01277200

C 0.56625600 1.23733900 1.82994100

C 0.59574100 0.34831700 3.07605300

C -0.65781000 2.15626300 1.83159200

H 1.47602100 1.84724500 1.80287200

H 1.49182300 -0.27860000 3.11128100

H 0.58632500 0.96342100 3.98276500

H -0.28404100 -0.29990200 3.10442000

H -0.73711700 2.75998300 0.92295500

H -1.57581100 1.57548500 1.92912000

H -0.60816100 2.84311500 2.68366000

C 1.06778400 -2.05521100 -0.06158300

C 0.71238700 -2.56379000 -1.46460400

C 0.33939000 -2.86620900 1.01523900

H 2.14531900 -2.16279000 0.10141700

H 1.24295600 -2.02378200 -2.25686600

H 0.95855900 -3.62661100 -1.56342500

H -0.36001800 -2.45834200 -1.65256300

H 0.55103000 -2.50631000 2.02429300

H -0.74273800 -2.84394200 0.87602300

H 0.64822400 -3.91606000 0.95900900

C 1.31824900 1.22416300 -1.73994800

C 1.80304000 2.61709700 -1.32062900

C 0.19769000 1.31367200 -2.77929700

H 2.16219000 0.68280400 -2.18251700

H 2.62106300 2.57158000 -0.59647800

H 2.15301700 3.18499400 -2.18981000

H 0.99245300 3.19334800 -0.86443900

H -0.14483200 0.32828900 -3.10186800

H -0.67501200 1.83175700 -2.37473300

H 0.53971000 1.86620600 -3.66144400

C 4.30732100 -0.09691500 0.11487900

O 3.24781300 0.27344400 0.58159900

C 5.60735200 0.34104300 0.73165800

H 5.42483600 0.80612200 1.69757400

H 6.29156800 -0.50361800 0.83190800

H 6.08220800 1.06527900 0.06307000

C 4.38914500 -0.99563800 -1.08993000

H 4.77029600 -1.97147900 -0.77405000

H 3.41456700 -1.12732500 -1.55552600

H 5.10229400 -0.59113400 -1.81165700

C -3.85469800 0.43514800 -0.22408300

F -4.95961400 -0.02724800 0.33931900

F -4.05474800 0.57717300 -1.52508100

F -3.56625300 1.62058400 0.29897000

S -2.46784600 -0.74578000 0.08070600

O -2.25657300 -0.76473100 1.51660800

O -2.82898400 -1.97079200 -0.59171100

O -1.34866200 -0.00069200 -0.62768100

TS-HT-LAA-1

NImag= 1 (i170.94)

$\mathbf{E}^{gas}$= -2834.4181

$\mathbf{E}^{gas}_{sp}$= -2834.4552

$\mathbf{E}^{sol}_{sp}$= -2834.4797

$\mathbf{G}^{gas}_{298.15}$= -2833.7965

$\mathbf{G}^{sol}_{393.15}$= -2833.9444

Sn -2.87820400 0.52757600 -0.10172600

C -3.85328300 1.92736500 1.23255300

C -3.56942100 1.59194000 2.69966000

C -5.35332700 2.08724500 0.98451300

H -3.34580700 2.86668200 0.98206800

H -2.49577500 1.53747900 2.89916100

H -3.99650100 2.35789700 3.35845600

H -4.02456400 0.63393600 2.96694500

H -5.59659900 2.23889500 -0.07059000

H -5.89374900 1.20472000 1.32735100

H -5.73746800 2.94831800 1.54461900

C -1.69858400 -1.18455100 0.47710300

C -1.81598700 -2.30386700 -0.56164900

C -2.00673600 -1.68559500 1.89039400

H -0.67867800 -0.78459900 0.46563400

H -1.48102900 -1.97522400 -1.55064700

H -1.18759800 -3.15398800 -0.27250400

H -2.84194600 -2.67024600 -0.64744600

H -1.82975000 -0.91258500 2.64261400

H -3.04261600 -2.02141600 1.98995500

H -1.36123100 -2.53817500 2.13262600

C -2.77435600 1.17043700 -2.17549600

C -3.26759100 2.61445600 -2.31147100

C -3.53361400 0.23817000 -3.12335800

H -1.71106200 1.13059200 -2.43316100

H -2.74959600 3.29818600 -1.63282900

H -3.12262600 2.98512300 -3.33328200

H -4.33714300 2.68162900 -2.09040400

H -3.18058100 -0.79319200 -3.05352100

H -4.60112000 0.22345600 -2.89305800

H -3.41177700 0.57068100 -4.16116800

C -0.06327900 2.61608500 0.39680500

O -0.97729000 1.80605300 0.59232600

C 0.55257000 3.30486200 1.58969900

H 0.60050700 2.61509600 2.43054900

H 1.54249800 3.69897100 1.36529900

H -0.11459500 4.13387600 1.85734900

C 0.09080900 3.28224000 -0.94822100

H 1.11016400 3.62528400 -1.11264200

H -0.21016000 2.60327600 -1.74386100

H -0.57845600 4.15178700 -0.95500200

C -7.19351400 -1.30901500 -0.31902400

F -8.07157900 -2.06762900 0.32668400

F -7.24855200 -1.60110600 -1.61298100

F -7.53822400 -0.03488300 -0.15942700

S -5.49560300 -1.61708900 0.33908200

O -5.52278400 -1.17027200 1.72084400

O -5.23901200 -3.01424700 0.07144400

O -4.71175900 -0.68480200 -0.54797900

Sn 2.92138700 0.37865400 0.02380500

C 2.80042000 -0.28381700 2.09226400

C 1.35706900 -0.60719000 2.48533400

C 3.39348200 0.81043100 2.98460100

H 3.41535400 -1.18221000 2.18694300

H 0.98086100 -1.48938600 1.96006600

H 1.27917300 -0.80909600 3.56124300

H 0.67513400 0.22113700 2.25565000

H 4.44492400 0.98411700 2.74402400

H 2.84623600 1.75441500 2.87136700

H 3.33140600 0.52643400 4.04250100

C 4.48770000 1.79879600 -0.49546000

C 4.18337500 3.22176800 -0.03107600

C 4.74404100 1.74191900 -2.00260000

H 5.37396800 1.43719000 0.03095200

H 4.03986200 3.27305600 1.05245800

H 5.00197300 3.90513600 -0.29032300

H 3.27547400 3.61034200 -0.50563000

H 5.00497300 0.72986500 -2.32109300

H 3.85899400 2.05845300 -2.56875900

H 5.57022900 2.40476300 -2.28956000

C 2.08968100 -0.83546000 -1.58203500

C 0.87807300 -0.15822400 -2.22201000

C 1.75689800 -2.24086400 -1.07693100

H 2.89801100 -0.91396900 -2.31534400

H 1.14474300 0.80129300 -2.67754100

H 0.42974300 -0.78742600 -3.00249000

H 0.10171100 0.04500200 -1.47526500

H 2.64279600 -2.72692000 -0.66286400

H 0.98629200 -2.21246500 -0.29980100

H 1.36720100 -2.86948600 -1.88803500

C 7.30868900 -1.17792200 -0.62593300

F 7.27241500 -1.99613200 -1.67493400

F 8.47005900 -1.35456700 0.00037900

F 7.27315500 0.07688200 -1.08146300

S 5.89381700 -1.49812600 0.51687300

O 4.73698800 -1.25766700 -0.38734900

O 6.06017200 -2.88005800 0.92130100

O 6.03958600 -0.47232700 1.54333100

H 1.49622500 1.58340200 0.13818600

TS-HT-LAA-2

NImag= 1 (i155.94)

$\mathbf{E}^{gas}$= -1872.8554

$\mathbf{E}^{gas}_{sp}$= -1872.8754

$\mathbf{E}^{sol}_{sp}$= -1872.8886

$\mathbf{G}^{gas}_{298.15}$= -1872.2477

$\mathbf{G}^{sol}_{393.15}$= -1872.3421

Sn -1.23642800 0.17806500 -0.32916700

C -1.60424300 2.29835100 -0.04469000

C -1.26893200 2.72296600 1.38834700

C -3.00189600 2.77934200 -0.43797500

H -0.87608600 2.75279800 -0.73002400

H -0.26524400 2.40528900 1.68844800

H -1.32349100 3.81311000 1.49501000

H -1.99044000 2.28555600 2.08420200

H -3.30394600 2.44113300 -1.43115800

H -3.74337200 2.42309500 0.27678500

H -3.03496200 3.87519900 -0.43047400

C -0.69166200 -1.21159400 1.24575200

C -1.14801300 -2.64701200 0.97166200

C -1.10693100 -0.76077800 2.64963500

H 0.39900800 -1.15940800 1.17602600

H -0.73648600 -3.04032100 0.03795800

H -0.81646500 -3.30784300 1.78254800

H -2.23703600 -2.72142600 0.92006800

H -0.75443000 0.24693300 2.88367200

H -2.19159900 -0.76668000 2.77429000

H -0.69029700 -1.44465100 3.40001000

C -1.21978300 -0.45956100 -2.41100600

C -2.12071800 0.48590700 -3.21428600

C -1.67889900 -1.91002500 -2.58677200

H -0.19179000 -0.36756900 -2.77156200

H -1.79858500 1.53011800 -3.14495100

H -2.12835900 0.20874000 -4.27453800

H -3.15155200 0.43043700 -2.85143500

H -0.97768700 -2.62056700 -2.14330200

H -2.65688800 -2.06987000 -2.12653500

H -1.76647400 -2.15484700 -3.65194400

C 1.80956300 1.55405800 -0.79824800

O 1.02800500 0.71677200 -0.19292900

C 2.10067500 2.85803000 -0.06706600

H 2.23676500 2.66675700 0.99707600

H 2.97377600 3.37322000 -0.47230900

H 1.22352800 3.50328100 -0.18079300

C 1.65156300 1.71111900 -2.30460100

H 2.41959600 2.36057800 -2.72761900

H 1.67504300 0.74109200 -2.79844700

H 0.66880200 2.16110200 -2.48590000

C -5.91867600 -0.05359500 -0.03121300

F -6.91055400 -0.01692500 0.84683300

F -6.19936300 -0.95453300 -0.96271500

F -5.81463300 1.13820700 -0.60989100

S -4.34182200 -0.49038600 0.82439600

O -4.08701300 0.58767000 1.76551300

O -4.53872400 -1.82443200 1.34595800

O -3.39561200 -0.44644200 -0.35132700

Sn 3.86476000 -0.34763500 0.19379700

C 3.69539800 0.15484400 2.29949000

C 2.27335500 0.20508200 2.86122800

C 4.50790300 1.41313100 2.62724000

H 4.21153700 -0.70124600 2.75621600

H 1.78548000 -0.77017700 2.81159400

H 2.29964800 0.50838000 3.91330400

H 1.63601700 0.90474600 2.31690000

H 5.54383800 1.33895600 2.28473600

H 4.07154000 2.30926400 2.17913000

H 4.52965000 1.57163500 3.71015800

C 5.87253900 0.09157300 -0.55278900

C 5.98039100 1.58117900 -0.89623000

C 6.22190900 -0.78082000 -1.76109500

H 6.56301800 -0.13351800 0.26795600

H 5.73861300 2.22624200 -0.04671800

H 6.99470000 1.83085600 -1.22471000

H 5.30043500 1.84385100 -1.71350600

H 6.23553400 -1.84545500 -1.51604200

H 5.50428900 -0.63739900 -2.57625600

H 7.21078100 -0.52086200 -2.15387400

C 3.06587100 -2.24333100 -0.51033700

C 1.92383700 -2.13046400 -1.52070800

C 2.67922000 -3.13152500 0.67843200

H 3.93294900 -2.68777400 -1.01272800

H 2.20399000 -1.54617700 -2.40140800

H 1.63297800 -3.12907400 -1.86475000

H 1.04771000 -1.66017100 -1.07297500

H 3.49084100 -3.24871200 1.40260600

H 1.80905300 -2.73446200 1.20657400

H 2.41056000 -4.13200300 0.32347700

H 3.07090900 1.04195600 -0.82101900

$[Me_2CHO\text{-}(\mathbf{Sn}OTf)_2]^-$

NImag= 0

$\mathbf{E}^{gas}$= -2834.4669

$\mathbf{E}^{gas}_{sp}$= -2834.5038

$\mathbf{E}^{sol}_{sp}$= -2834.5265

$\mathbf{G}^{gas}_{298.15}$= -2833.8308

$\mathbf{G}^{sol}_{393.15}$= -2833.9748

Sn -2.05436400 0.39031000 -0.05262500

C -3.00749900 2.17979900 0.78029700

C -2.72591300 2.35648000 2.27721800

C -4.51865500 2.26771700 0.54488700

H -2.55268700 3.00055200 0.22261400

H -1.66981400 2.25855600 2.53803400

H -3.06249100 3.34363000 2.61774200

H -3.28393300 1.60903900 2.84715800

H -4.79867900 2.11356800 -0.49668800

H -5.05701900 1.53627800 1.14691900

H -4.86805300 3.26406800 0.84438200

C -1.42829200 -1.22442300 1.25342000

C -1.81508000 -2.62159700 0.75686800

C -1.97328800 -1.01375300 2.67136800

H -0.33769400 -1.13130300 1.27873900

H -1.41329800 -2.85687700 -0.23015200

H -1.42747100 -3.37654100 1.45215500

H -2.89770100 -2.74611300 0.71433300

H -1.60871100 -0.09150700 3.12727000

H -3.06811900 -0.98440600 2.67841300

H -1.66797000 -1.84664700 3.31600200

C -2.30744700 0.20130900 -2.21469700

C -3.37944500 1.18901100 -2.69184800

C -2.70534500 -1.20382700 -2.68270400

H -1.33842400 0.47157300 -2.64546700

H -3.20561500 2.21808300 -2.36416700

H -3.43511500 1.19371600 -3.78675800

H -4.35886000 0.87955700 -2.31580200

H -1.97063000 -1.96913900 -2.43273700

H -3.65848400 -1.49742300 -2.23986800

H -2.82630400 -1.20870400 -3.77308400

C 0.40259700 2.58217900 -0.35813900

O 0.13767600 1.19607900 -0.10092200

C 0.06090400 3.53362000 0.79147700

H 0.34654300 3.10101000 1.74976400

H 0.63497100 4.45613800 0.65955000

H -0.99045200 3.80601800 0.83660900

C -0.22307000 3.02246000 -1.67508800

H 0.06721500 4.04938900 -1.91356600

H 0.10657200 2.36837700 -2.48619000

H -1.31424700 2.98325300 -1.62719800

C -6.70250300 -0.83056700 -0.51148800

F -7.85182600 -1.35820800 -0.10176500

F -6.44158900 -1.29053200 -1.73429600

F -6.85493500 0.49032700 -0.59303800

S -5.33314500 -1.27204000 0.64661100

O -5.67923600 -0.63370100 1.90569700

O -5.29402300 -2.72089200 0.61228700

O -4.19095000 -0.62174700 -0.05674000

Sn 2.22603100 0.18338400 0.00347300

C 2.49192700 0.70894800 2.09429300

C 1.22774600 0.55691600 2.93912200

C 3.11891500 2.10553700 2.19550100

H 3.23517300 -0.01365500 2.44231500

H 0.94675300 -0.49355100 3.05420300

H 1.38387000 0.96975600 3.94303500

H 0.37348900 1.07067800 2.49118000

H 4.08057500 2.13923200 1.67930700

H 2.47152100 2.88295800 1.78098400

H 3.29982800 2.36077100 3.24640400

C 3.52209600 1.29430800 -1.40751300

C 3.35460100 2.76484100 -1.79049900

C 3.68940000 0.43869600 -2.66921100

H 4.45141100 1.22591700 -0.83406600

H 3.33899900 3.42506400 -0.91933400

H 4.20590000 3.07018100 -2.41053400

H 2.44987800 2.94576500 -2.37771100

H 3.99125200 -0.58264700 -2.43019500

H 2.76522500 0.39843400 -3.25599400

H 4.46998600 0.86180900 -3.31235600

C 1.76401800 -1.76492600 -0.82838300

C 0.58661600 -1.74063700 -1.78939300

C 1.68728000 -2.88024500 0.21642000

H 2.68130400 -1.93251600 -1.39775300

H 0.74247200 -1.03772800 -2.61375300

H 0.40713600 -2.73318700 -2.22205500

H -0.32724300 -1.44087300 -1.28296200

H 2.60427000 -2.91153100 0.80820700

H 0.83916000 -2.76971800 0.89394200

H 1.57431300 -3.85154900 -0.28078000

C 6.74189500 -1.08203100 -0.56777100

F 6.59053700 -2.29702300 -1.08765000

F 8.01067400 -0.93988200 -0.19525800

F 6.48945500 -0.18853100 -1.52686100

S 5.60865100 -0.82866500 0.86770100

O 4.28884900 -1.09485700 0.22828800

O 6.00723000 -1.83017400 1.83467200

O 5.79917500 0.57225400 1.21833000

H 1.48041300 2.67888500 -0.47936900

$[Me_2CHO\text{-}\mathbf{Sn}OTf]^-$

NImag= 0

$\mathbf{E}^{gas}$= -1514.1281

$\mathbf{E}^{gas}_{sp}$= -1514.1485

$\mathbf{E}^{sol}_{sp}$= -1514.1877

$\mathbf{G}^{gas}_{298.15}$= -1513.7791

$\mathbf{G}^{sol}_{393.15}$= -1513.8871

Sn -1.17436500 0.16451200 -0.26534400

C -1.17542500 -0.15480100 1.90224700

C -1.70996700 1.08210300 2.63544400

C 0.14795000 -0.60116000 2.52454100

H -1.90493400 -0.96656600 2.02243900

H -2.60268900 1.50115900 2.16219900

H -1.96100000 0.84447400 3.67769100

H -0.94346900 1.86164100 2.65850600

H 0.55294900 -1.49420300 2.04580200

H 0.90709400 0.17926300 2.43796900

H 0.00955000 -0.81917200 3.59244900

C -0.86708500 2.16652800 -1.04671100

C -0.00958200 2.19261900 -2.31429700

C -0.30056100 3.11495700 0.01429500

H -1.88635200 2.47806200 -1.29596000

H -0.46182100 1.61063700 -3.12174800

H 0.10545600 3.22357200 -2.67432600

H 0.99289700 1.79746600 -2.13145800

H -1.00286400 3.26094700 0.83877200

H 0.63818400 2.74499400 0.43781000

H -0.09297000 4.10025500 -0.42296300

C -0.68175200 -1.61762400 -1.43301900

C -0.07335600 -2.69240200 -0.52714900

C 0.23790200 -1.34783400 -2.62648400

H -1.64558600 -1.97246600 -1.80859600

H -0.71021400 -2.92322400 0.33383300

H 0.08929500 -3.62615900 -1.08116000

H 0.89660300 -2.36180000 -0.14664700

H -0.22765700 -0.68222100 -3.35728900

H 1.17598300 -0.89101700 -2.30379900

H 0.48189300 -2.28690100 -3.14139400

C -4.29074100 -0.50644300 -0.17655500

O -3.21610200 0.28756700 -0.56453700

C -4.80667200 -0.11227100 1.21104400

H -4.97738500 0.96581200 1.24393500

H -5.74412800 -0.62592200 1.44792900

H -4.07070700 -0.36438800 1.97968900

C -3.98409000 -2.00686100 -0.22225200

H -4.84669600 -2.59570300 0.10435700

H -3.71969300 -2.31345100 -1.23563500

H -3.14101300 -2.24459000 0.43643200

C 3.61643200 -0.86987900 0.38217700

F 4.91090300 -0.63136900 0.59408300

F 3.51582000 -1.69105400 -0.66523200

F 3.13716600 -1.51173700 1.44907400

S 2.69035800 0.69816000 0.07577300

O 2.86526600 1.46112100 1.30278400

O 3.29954400 1.22899600 -1.13309300

O 1.32397800 0.16659600 -0.11717900

H -5.11303500 -0.32504700 -0.88880700

Me_2CHO**Sn**

NImag= 0

$\mathbf{E}^{gas}$= -552.5965

$\mathbf{E}^{gas}_{sp}$= -552.6000

$\mathbf{E}^{sol}_{sp}$= -552.6085

$\mathbf{G}^{gas}_{298.15}$= -552.2669

$\mathbf{G}^{sol}_{393.15}$= -552.3035

Sn -0.15084000 0.01203100 -0.16032900

C -0.61328900 -0.15409400 1.96262500

C -0.98349200 -1.59829500 2.31528100

C -1.71802000 0.82175300 2.38429400

H 0.30678900 0.11218500 2.49339700

H -0.20606700 -2.30605600 2.01555800

H -1.14572900 -1.71079300 3.39342600

H -1.91090900 -1.89901200 1.81670200

H -1.44926800 1.86325500 2.18669900

H -2.65621400 0.61806000 1.85931100

H -1.92485800 0.73505000 3.45722400

C -1.72803300 -0.75937000 -1.43547700

C -3.12383200 -0.37020700 -0.93608700

C -1.59638200 -2.27842100 -1.58829100

H -1.56534900 -0.29504900 -2.41485800

H -3.24590300 0.71147200 -0.82574400

H -3.89656100 -0.72123600 -1.62935200

H -3.33436800 -0.82809200 0.03566000

H -0.60361000 -2.56499500 -1.93852500

H -1.76220800 -2.78431200 -0.63176300

H -2.34175600 -2.66230900 -2.29428400

C 0.38214300 2.06302100 -0.68504600

C 1.17108700 2.77396100 0.41755600

C -0.90162700 2.83318400 -1.02324200

H 0.99985400 2.00301100 -1.58692600

H 2.13594600 2.29859500 0.61153800

H 1.36985400 3.81700800 0.14540100

H 0.61635200 2.78745500 1.36153700

H -1.45745600 2.36744600 -1.84192700

H -1.57311900 2.89185700 -0.15945900

H -0.67340200 3.86258900 -1.32155500

C 2.66295100 -1.22086700 -0.23895500

O 1.29833900 -1.28676700 -0.57907800

C 2.86813100 -0.88472600 1.23598300

H 2.29450400 -1.56916100 1.86527100

H 3.92229200 -0.95491500 1.51459800

H 2.53628400 0.13888400 1.44704300

C 3.39925800 -0.23387300 -1.14017300

H 4.47547000 -0.24736600 -0.94986200

H 3.22430800 -0.48403400 -2.18776900

H 3.03454100 0.78365200 -0.96412400

H 3.07249800 -2.22299500 -0.41897300

Me_2CHOH-**Sn**OTf

NImag= 0

$\mathbf{E}^{gas}$= -1514.6376

$\mathbf{E}^{gas}_{sp}$= -1514.6554

$\mathbf{E}^{sol}_{sp}$= -1514.6585

$\mathbf{G}^{gas}_{298.15}$= -1514.2778

$\mathbf{G}^{sol}_{393.15}$= -1514.3457

H -3.36625600 1.05446500 -1.13701000

Sn -0.67753000 0.12354800 -0.01329400

C -1.51606000 -0.02353300 1.97984700

C -2.07400800 1.33680500 2.41203300

C -0.51178100 -0.56160500 3.00285400

H -2.34520700 -0.73434000 1.89613900

H -2.79493400 1.73889200 1.69369300

H -2.57742400 1.26433300 3.38279300

H -1.26949400 2.07039700 2.51926500

H -0.11497500 -1.53853600 2.71587500

H 0.34073500 0.11182700 3.10743400

H -0.98719700 -0.66456500 3.98455300

C -0.83844100 2.08583300 -0.92728200

C -0.75224800 2.00029700 -2.45512500

C 0.15230700 3.11594400 -0.37666300

H -1.84455600 2.41398600 -0.63365200

H -1.47573800 1.29527200 -2.87758600

H -0.93352100 2.98085400 -2.90884500

H 0.24825900 1.67619500 -2.75327500

H 0.19550300 3.12691200 0.71515900

H 1.16049100 2.93011200 -0.74886000

H -0.13192400 4.11975700 -0.70992600

C -0.53777100 -1.71469700 -1.14166000

C -0.20432000 -2.86576100 -0.18573600

C 0.41737100 -1.68045000 -2.33676100

H -1.55588900 -1.84456700 -1.51746900

H -0.93034800 -2.95356100 0.62908100

H -0.19212400 -3.82021600 -0.72329000

H 0.78422600 -2.73032400 0.26121800

H 0.18962200 -0.86368000 -3.02472900

H 1.45333300 -1.55697200 -2.02287600

H 0.34498200 -2.62224700 -2.89245800

C -4.41675600 -0.52240000 -0.57020300

O -3.17447400 0.15856700 -0.84081700

C -5.10796000 0.09741000 0.63390100

H -5.27709500 1.16682600 0.48351300

H -6.07794600 -0.37589700 0.79881200

H -4.49948400 -0.03206700 1.53159000

C -4.09296700 -1.98994200 -0.36919900

H -4.99790700 -2.53640100 -0.09887500

H -3.68261500 -2.42901900 -1.27867400

H -3.36485800 -2.11266500 0.43693000

C 3.68525800 -0.76176900 0.25642100

F 4.82491300 -0.56055500 -0.38389400

F 3.11278300 -1.86456300 -0.22250400

F 3.93075500 -0.93547900 1.54448300

S 2.56879700 0.68809000 0.00576200

O 3.22907600 1.80216600 0.63545700

O 2.28615600 0.73303900 -1.41879400

O 1.34658800 0.21149600 0.77694600

H -5.05249100 -0.41515900 -1.45570400

Me_2CHOH

NImag= 0

$\mathbf{E}^{gas}$= -194.3171

$\mathbf{E}^{gas}_{sp}$= -194.3223

$\mathbf{E}^{sol}_{sp}$= -194.3239

$\mathbf{G}^{gas}_{298.15}$= -194.2354

$\mathbf{G}^{sol}_{393.15}$= -194.2547

H 0.88702400 1.75311100 0.09544800

C -0.00214800 0.04264000 0.36957000

O 0.05094600 1.35965000 -0.16498900

C 1.18903000 -0.78082100 -0.10296200

H 2.13032700 -0.33264400 0.22765100

H 1.14628600 -1.79897400 0.29031700

H 1.19491200 -0.82413900 -1.19451500

C -1.32318800 -0.54584000 -0.08957200

H -1.46171500 -1.55222500 0.30973700

H -2.14922000 0.08404600 0.24239300

H -1.34296500 -0.59208100 -1.18083400

H 0.00561300 0.08983400 1.46750000

(Sn/O)-dist

NImag= 0

$\mathbf{E}^{gas}$= -2834.4552

$\mathbf{E}^{gas}_{sp}$= -2834.4912

$\mathbf{E}^{sol}_{sp}$= -2834.5138

$\mathbf{G}^{gas}_{298.15}$= -2833.8272

$\mathbf{G}^{sol}_{393.15}$= -2833.9711

Sn -2.36694500 0.88661500 -0.20237500

C -3.98745800 2.18699800 0.46896100

C -3.76480200 2.66227500 1.90883900

C -5.39757000 1.61820700 0.31574500

H -3.88908300 3.05100800 -0.20016400

H -2.76228600 3.06719100 2.06813600

H -4.48976800 3.44167000 2.17663600

H -3.91046200 1.83245600 2.60655600

H -5.59245200 1.24619300 -0.69156700

H -5.56037000 0.78756800 1.00487400

H -6.14117900 2.39295900 0.54423100

C -1.05712600 -0.16856000 1.18851900

C -1.29847500 -1.66164900 1.38898300

C -1.02793200 0.57277200 2.52965600

H -0.08960200 -0.01308600 0.68180200

H -1.46303600 -2.20267900 0.45451300

H -0.45611100 -2.13119300 1.91601600

H -2.18586900 -1.82721900 2.00485400

H -0.83398100 1.63958600 2.39579300

H -1.98788400 0.46029600 3.04186600

H -0.26106400 0.17047100 3.20544100

C -2.40463800 0.25342800 -2.28721400

C -3.78015100 0.49893900 -2.91290000

C -1.99388500 -1.21097800 -2.45537700

H -1.66447300 0.88634800 -2.78571000

H -4.09597100 1.54426100 -2.82857700

H -3.77735000 0.23777900 -3.97873800

H -4.53401100 -0.12274900 -2.42220600

H -1.00285000 -1.40565100 -2.03774100

H -2.70469500 -1.87261000 -1.95517100

H -1.96511200 -1.48615200 -3.51793700

C -0.75937300 3.59146600 -0.83495300

O -0.84087400 2.31983800 -0.26532000

C -1.29247200 4.66597100 0.11581500

H -0.81375500 4.56206600 1.09275400

H -1.08946100 5.67050800 -0.26787400

H -2.37174700 4.55988100 0.25294600

C -1.44662000 3.67575000 -2.19909300

H -1.37188600 4.68379100 -2.61682600

H -0.98826100 2.97565900 -2.90047600

H -2.50909400 3.42263100 -2.10891900

C -6.17634000 -2.20567900 -0.33448800

F -6.96651700 -3.15160700 0.16957500

F -5.86106800 -2.55036100 -1.58355800

F -6.87257400 -1.07059200 -0.38644600

S -4.64877700 -2.01523500 0.68674800

O -5.12211100 -1.56182800 1.98593100

O -4.02627200 -3.32481500 0.61525200

O -3.94231200 -0.96493600 -0.08970500

H 0.30874500 3.81460900 -0.99962800

Sn 2.79513300 0.16491300 0.54574700

C 3.00922000 2.27667000 0.95139800

C 1.78663000 2.80431700 1.71078700

C 3.28153700 3.09356400 -0.31363800

H 3.89187100 2.31345200 1.60125200

H 1.63065900 2.27911100 2.65830800

H 1.91602300 3.86903500 1.94007200

H 0.87348000 2.69255200 1.11599800

H 4.13457000 2.71492700 -0.88155800

H 2.40673400 3.08637700 -0.96839800

H 3.48104700 4.13888500 -0.05060500

C 2.21311500 -0.56276000 -1.40983300

C 1.30931100 0.44469700 -2.13160900

C 1.58196000 -1.95334500 -1.29729100

H 3.15491000 -0.64070400 -1.95765200

H 1.86646600 1.34630000 -2.39837300

H 0.92565900 0.00191600 -3.05852700

H 0.44958200 0.76306600 -1.53459200

H 2.30119500 -2.68998200 -0.93220200

H 0.71646700 -1.96382400 -0.62634600

H 1.23246700 -2.28837700 -2.28021100

C 2.42372900 -1.03528800 2.30937700

C 3.24333000 -0.45191700 3.46637500

C 2.77738400 -2.50642000 2.07052400

H 1.35984800 -0.95680100 2.54118500

H 2.97531600 0.58596300 3.68297500

H 3.07882400 -1.03400300 4.38012800

H 4.31317100 -0.48343300 3.24048500

H 2.09801500 -2.97742000 1.35771200

H 3.80071500 -2.61537700 1.69708500

H 2.70958800 -3.06677600 3.01013700

C 6.09813800 -1.91899300 -1.01536700

F 6.53984500 -2.70695300 -0.04525200

F 6.94267700 -1.97389400 -2.03488500

F 4.91095800 -2.36862300 -1.41798300

S 5.93690300 -0.18132500 -0.41276400

O 4.88664300 -0.39280100 0.66400600

O 7.22347500 0.16889400 0.12976800

O 5.39670900 0.56684400 -1.53198700

TS-H_2act(Sn/O)-dist

NImag= 1(i329.08)

E^{gas}= -2835.6217

$\mathbf{E}_{sp}^{gas}$= -2835.6578

$\mathbf{E}_{sp}^{sol}$= -2835.6788

$\mathbf{G}_{298.15}^{gas}$= -2834.9805

$\mathbf{G}_{393.15}^{sol}$= -2835.1233

Sn -2.51548400 0.65084400 -0.28244800

C -3.97077000 2.22100800 0.09507300

C -3.80500700 2.79100700 1.50773300

C -5.42620100 1.83270000 -0.15783000

H -3.68349500 2.99197600 -0.62956100

H -2.77227500 3.07839800 1.72221300

H -4.43785200 3.67693300 1.64548400

H -4.11500500 2.05034200 2.25082000

H -5.57402700 1.36138400 -1.13184000

H -5.77328200 1.13187600 0.60240200

H -6.06784200 2.72154800 -0.10770800

C -1.32270000 -0.31743900 1.25217600

C -1.68378900 -1.76105200 1.59144700

C -1.24558200 0.53859900 2.52047100

H -0.33593200 -0.30668900 0.76953300

H -1.84556900 -2.38354200 0.70895500

H -0.88526500 -2.21744900 2.19151000

H -2.59753400 -1.80883400 2.18824200

H -0.89022600 1.55082400 2.30801300

H -2.22818700 0.61262600 2.99547800

H -0.56571700 0.08851000 3.25494900

C -2.35003800 -0.14498600 -2.29930900

C -3.64985600 0.05544700 -3.08309300

C -1.95583700 -1.62467400 -2.26284600

H -1.54962500 0.41996400 -2.78332400

H -3.92901300 1.11204800 -3.15418900

H -3.55203300 -0.33135900 -4.10501300

H -4.47297300 -0.48022900 -2.60231200

H -1.01179600 -1.78481100 -1.73226400

H -2.72785800 -2.21693900 -1.76514300

H -1.83305500 -2.01734500 -3.28018200

C -0.58038400 3.24800800 -1.05176500

O -0.84286300 2.06560900 -0.33541600

C -1.05671400 4.47127400 -0.27188900

H -0.64123200 4.44618300 0.73826500

H -0.73584400 5.39632300 -0.75908900

H -2.14653700 4.48010700 -0.19122600

C -1.15673400 3.20399200 -2.46355300

H -0.96428000 4.14378400 -2.98764200

H -0.70474200 2.39145000 -3.03500400

H -2.23982300 3.04511300 -2.43625400

C -6.61324800 -1.89562200 -0.13176800

F -7.50586500 -2.58811100 0.57093400

F -6.39232500 -2.53760600 -1.27708900

F -7.14334500 -0.70881800 -0.42022700

S -5.03913100 -1.72707900 0.82288000

O -5.37453000 -0.91189200 1.98014900

O -4.63379700 -3.09934100 1.05004600

O -4.19772600 -1.00335900 -0.17587600

H 0.51669200 3.32590100 -1.14704800

Sn 2.96630300 0.46236200 0.52141900

C 3.98255000 2.37017900 0.29110600

C 3.49355400 3.44118800 1.26721400

C 3.85319600 2.84558400 -1.15834400

H 5.03444400 2.14644300 0.49504400

H 3.64728900 3.15569500 2.31019000

H 4.02894300 4.38247500 1.09547400

H 2.42645400 3.64275800 1.12974700

H 4.23936200 2.10386200 -1.86075700

H 2.80740200 3.05610000 -1.40660300

H 4.41435300 3.77571600 -1.30628400

C 2.33417900 -0.63528300 -1.23311300

C 1.29274300 0.10364200 -2.07294600

C 1.84330200 -2.02478200 -0.81266700

H 3.25327200 -0.74326900 -1.81624800

H 1.66254100 1.07311600 -2.42083700

H 1.01859300 -0.48984000 -2.95415000

H 0.37737500 0.29264100 -1.50815200

H 2.61191000 -2.57737600 -0.26603600

H 0.95316700 -1.96503300 -0.17589200

H 1.57125000 -2.61965600 -1.69254900

C 2.30315300 -0.29630600 2.44498000

C 2.22145500 0.81687500 3.49236300

C 3.14056700 -1.47363600 2.94763200

H 1.28836800 -0.65256900 2.23801400

H 1.61710100 1.66189700 3.15084700

H 1.77133400 0.44093400 4.41883200

H 3.21941000 1.19046500 3.74351700

H 3.18386600 -2.28815500 2.22165600

H 4.17081200 -1.17212000 3.14778900

H 2.71134300 -1.86754500 3.87645700

C 6.07928600 -2.38732000 -0.87840300

F 6.27357300 -3.23080900 0.12697800

F 7.06670300 -2.53197600 -1.75417100

F 4.93321000 -2.70128600 -1.47805500

S 6.02466700 -0.64603800 -0.26844000

O 4.86249400 -0.73611300 0.68829900

O 7.29073000 -0.43126600 0.39136600

O 5.70019700 0.15015700 -1.44054300

H 0.37823300 1.75004700 0.25607400

H 1.18163000 1.68158200 0.60067500

INT1-H_2act(Sn/O)-dist

NImag= 0

$\mathbf{E}^{gas}$= -2835.6355

$\mathbf{E}^{gas}_{sp}$= -2835.6719

$\mathbf{E}^{sol}_{sp}$= -2835.6958

$\mathbf{G}^{gas}_{298.15}$= -2834.9897

$\mathbf{G}^{sol}_{393.15}$= -2835.1360

Sn -2.60645100 0.44830700 -0.38554600

C -3.90242600 2.15441500 -0.05205000

C -3.74083500 2.71441500 1.36363300

C -5.37664700 1.91937900 -0.37727400

H -3.49835900 2.88193800 -0.76562100

H -2.69763200 2.93866700 1.59872300

H -4.31866700 3.64004100 1.47788200

H -4.11526500 1.99613500 2.09809900

H -5.52896500 1.42572500 -1.34001200

H -5.83886300 1.30151700 0.39223900

H -5.91279500 2.87580500 -0.39864700

C -1.29914700 -0.43445600 1.09986000

C -1.49895200 -1.93789100 1.29945500

C -1.35096000 0.31119100 2.43703400

H -0.30904500 -0.27944500 0.65260800

H -1.57059200 -2.48854100 0.35835800

H -0.65343100 -2.34723100 1.86560800

H -2.40358100 -2.15247100 1.87110900

H -1.05478700 1.35896200 2.33466100

H -2.35803200 0.27631800 2.86325700

H -0.66806600 -0.15377700 3.15726700

C -2.30881500 -0.15958800 -2.44362100

C -3.59234000 0.05959200 -3.24988900

C -1.85922200 -1.62275400 -2.50023600

H -1.51403900 0.46892900 -2.85089900

H -3.89163700 1.11257200 -3.26710300

H -3.45754700 -0.26459300 -4.28854800

H -4.41900400 -0.51917500 -2.82699500

H -0.91212800 -1.77909600 -1.97495600

H -2.61108500 -2.27799500 -2.05167100

H -1.71531700 -1.94029900 -3.53988300

C -0.48217200 3.31131500 -1.07716200

O -0.84668100 2.12096500 -0.36242900

C -0.97576800 4.53262300 -0.31639600

H -0.58558900 4.51885100 0.70332500

H -0.63860800 5.44966700 -0.80538000

H -2.06758700 4.54231200 -0.26830800

C -1.01384100 3.23301600 -2.49793200

H -0.80040500 4.16248100 -3.03008600

H -0.54342000 2.40968300 -3.03703500

H -2.09711100 3.07914700 -2.50062400

C -6.66691100 -1.76293400 0.09710000

F -7.54554000 -2.13064000 1.02249600

F -6.64185400 -2.68390400 -0.85810700

F -7.07456200 -0.61644100 -0.43785200

S -4.99138300 -1.60117500 0.86340000

O -5.09001000 -0.54216400 1.85548800

O -4.69072600 -2.94193800 1.30846600

O -4.18697400 -1.15925300 -0.33366500

H 0.61341000 3.33010700 -1.10946400

Sn 2.80651900 0.58530000 0.64519300

C 4.12972600 2.31415800 0.60529200

C 3.74936800 3.33135700 1.68183400

C 4.05788900 2.94287400 -0.78835600

H 5.14606000 1.95311700 0.77965500

H 3.87672000 2.93284500 2.69153300

H 4.36614400 4.23523300 1.59923600

H 2.70235300 3.63820800 1.57748600

H 4.38966600 2.24114300 -1.55663400

H 3.03363500 3.26350500 -1.01826000

H 4.69403500 3.83497000 -0.84739700

C 2.39727300 -0.48495700 -1.20590400

C 1.36581000 0.22099500 -2.08334500

C 1.97011000 -1.91975400 -0.88494400

H 3.35526500 -0.50886500 -1.73065000

H 1.68031600 1.23810100 -2.34188300

H 1.19749000 -0.32823300 -3.01963800

H 0.39865900 0.29817000 -1.57748900

H 2.73382000 -2.43927900 -0.30119300

H 1.03417600 -1.94429900 -0.31210600

H 1.80444400 -2.49722700 -1.80350100

C 2.28679000 -0.45989800 2.49057500

C 2.10123100 0.54848500 3.62913000

C 3.21841900 -1.59507400 2.91174900

H 1.30475100 -0.88852400 2.25160200

H 1.45840300 1.38593200 3.34101600

H 1.65404600 0.07062100 4.51009500

H 3.06730100 0.95883500 3.94046300

H 3.32831500 -2.34817100 2.13017200

H 4.22250900 -1.22258900 3.12481100

H 2.83327000 -2.08516100 3.81537300

C 6.04935100 -2.34582800 -1.04582500

F 6.14444800 -3.30810400 -0.13154100

F 7.09362500 -2.44421100 -1.86562100

F 4.94267800 -2.56289700 -1.75931900

S 5.99583800 -0.67973800 -0.25145800

O 4.81234900 -0.83252500 0.63754600

O 7.25882700 -0.56967100 0.45169300

O 5.76365800 0.23135400 -1.36578300

H -0.03575500 1.83056000 0.14133800

H 1.26750400 1.66669400 0.69725500

TS-HT/PT-BAA-alt

NImag= 1(i122.34)

$\mathbf{E}^{gas}$= -919.1182

$\mathbf{E}^{gas}_{sp}$= -919.1247

$\mathbf{E}^{sol}_{sp}$= -919.1927

$\mathbf{G}^{gas}_{298.15}$= -918.6224

$\mathbf{G}^{sol}_{393.15}$= -918.7337

C -0.45234700 -0.47808200 1.85212600

O 0.51562000 0.10247800 1.20220500

C -1.08398100 0.33737200 2.97498900

H -1.26995100 1.35947100 2.64878100

H -2.01288800 -0.10881600 3.33563200

H -0.36638200 0.37126600 3.80006500

C -0.27899900 -1.94879300 2.22128100

H -1.20342000 -2.38055300 2.60828900

H 0.05985900 -2.53323500 1.36620000

H 0.47737900 -2.00326500 3.01134800

Sn -2.15069300 0.11906700 -0.56940500

C -2.38508700 2.25110800 -0.23812000

C -1.09561300 2.99235900 0.12484100

C -3.52191300 2.54295900 0.74784800

H -2.70334800 2.59200500 -1.23267800

H -0.32146200 2.86043700 -0.63322200

H -1.29928800 4.06426500 0.21423600

H -0.68284600 2.64943600 1.07494300

H -4.46648700 2.09089200 0.43490300

H -3.29206400 2.17843500 1.75274400

H -3.68482500 3.62245200 0.82306600

C -3.98670100 -1.04343900 -0.54626300

C -4.52140400 -1.16100800 0.88520700

C -3.76254000 -2.42419100 -1.17000200

H -4.70669400 -0.48289000 -1.15268100

H -4.70525300 -0.18894300 1.34929400

H -5.46462200 -1.71571600 0.89456300

H -3.81863200 -1.70816300 1.52198300

H -3.38300000 -2.36893200 -2.19359700

H -3.05233200 -3.01091800 -0.57814000

H -4.70004500 -2.98817600 -1.19616900

C -0.63323700 -0.51128200 -1.98834500

C 0.04818200 -1.80519900 -1.53612000

C 0.39936300 0.58939200 -2.24608100

H -1.19218200 -0.70598800 -2.91117100

H -0.65898200 -2.62117400 -1.36626300

H 0.76546000 -2.14040300 -2.29338800

H 0.59376800 -1.61864500 -0.60894100

H -0.05348400 1.50688500 -2.63071800

H 0.92744200 0.83128200 -1.31986300

H 1.13686400 0.25194400 -2.98227200

H -1.50527000 -0.62037000 1.07414900

C 3.70537600 -1.21533000 0.44502000

C 5.00405200 -1.13767700 -0.01259200

C 5.55664000 0.09557000 -0.37630800

C 4.75979500 1.22795500 -0.25235700

C 3.45622400 1.12656000 0.21280800

N 2.96969500 -0.08505000 0.53633700

H 5.59276600 -2.04411100 -0.08314500

H 5.14570700 2.20633000 -0.51177300

C 2.56570900 2.32006000 0.37598600

H 2.36976200 2.76973800 -0.60071600

H 1.62087900 2.03799800 0.83787600

H 3.06667900 3.06988600 0.99066000

C 3.05379500 -2.49853800 0.85605900

H 3.79469600 -3.29204700 0.93168200

H 2.55852000 -2.38472800 1.82099400

H 2.30218900 -2.79760000 0.12176800

C 6.97372000 0.17997400 -0.85903400

H 7.16089200 -0.56689500 -1.63233500

H 7.20252500 1.16649200 -1.25880100

H 7.65863800 -0.02400400 -0.03204400

H 1.92506500 -0.14010200 0.87730500