Supporting Information

A comparative DFT mechanistic study of the [TBD]-catalyzed reactions of amines with CO_2 and hydrosilane: the effect of solvent polarity on the mechanistic preference and the origins of chemoselectivities

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SI 1: Computational Details

All geometries were optimized and characterized as minima (no imaginary frequency) or transition states (TS, having unique one imaginary frequency) at M05-2X[1]/6-31G(d,p) level. The right connections of a transition state to its forward and backward intermediates were confirmed by examining the vibrational mode of the imaginary frequency. In addion, we performed geometric optimizations with an initial geometreis obtained by displacing the structure of trastion states according to the vibratoinal mode of imaginary frequencies, confiming the geometric optimizations indeed led to the desired intermediates.

At the M05-2X/6-31G(d,p) geometries, the energies were further refined by M05-2X/6-311++G(d,p) single-point energy calculations with solvent effect accounted by SMD[2] solvent model. The M05-2X/6-31G(d,p) frequencies were used for thermal and entropic corrections at 298.15 K and 1 atm. It should be emphasized that such correctionapproach is based on the ideal gas phase model, which inevitably overestimates entropy contributions to free energies for reactions in solvent, in particular for reactions involving multicomponent change, because of ignoring the suppressing effect of solvent on the rotational and transitional freedoms of substrates. The entropy overestimationof the approch was also demonstrated experimentally.[3-4] While no standard quantum mechanics-based method is available to accurately calculate entropy in solution, approximate methods were proposed. According to the proposal of Martin et al.[5] We previously appllied a correction of (n-m)*4.3 kcalmol^{-1} for a process from m- to n-components and found such corrected free energies were more reasonable than enthalpies and uncorrected free energies,[6] although the protocol is by no means accurate. Other correction factors (e.g. 1.9[7], 2.6[7], and 5.4[8]kcal mol^{-1}) were adopted in the literatures depending on the approximate approaches based. As will be seen, our studied reactions involve multicomponent changes. As a conservative consideration, we applied a correction factor of 1.9 kcalmol^{-1} in this study. The corrected free energies are discussed. Note that using a correction factor of 4.3 kcalmol^{-1} does not alter our conclusions except for numerical values. Natural bond orbital (NBO) analyses were performed at M05-2X/6-311++G(d,p) level to assign partial atomic charges (Q).[9]

To verify the reasonability of using M05-2X gas phase geometries for energy corrections, we recalculated the selective-determining barriers in Scheme 2 of the main text at the other two levels shown in the table below. As compared, in spite of understandable numerical differences, overall, the energetic results agree with each other very well. Furthermore, the chemoselectvities were predicted the same at the three levels of calculations.

All calculations were carried out by using Gaussian 09.[10]

Table: Comparing the selectivity determining barriers (in kcal mol^{-1}) at the various levels.

	M05-2X(SMD)/ 6-311++G**)// M05-2X(gas)/6-31G**		M05-2X(SMD)/ 6-311++G**)// M05-2X(SMD)/6-31G**		M06-2X(SMD)/ 6-311++G**)// M06-2X(SMD)/6-31G**	
	modeCN	modeARE	modeCN	modeARE	modeCN	modeARE
1a	24.9	31.5	22.4	31.1	24.0	30.9
2a	32.6	29.8	31.7	30.1	31.2	30.0
3a	36.4	31.7	37.0	31.2	35.5	31.2

SMD calculations used acetonitrile as solvent.

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SI 3: Fig.S1-S14 in the main text

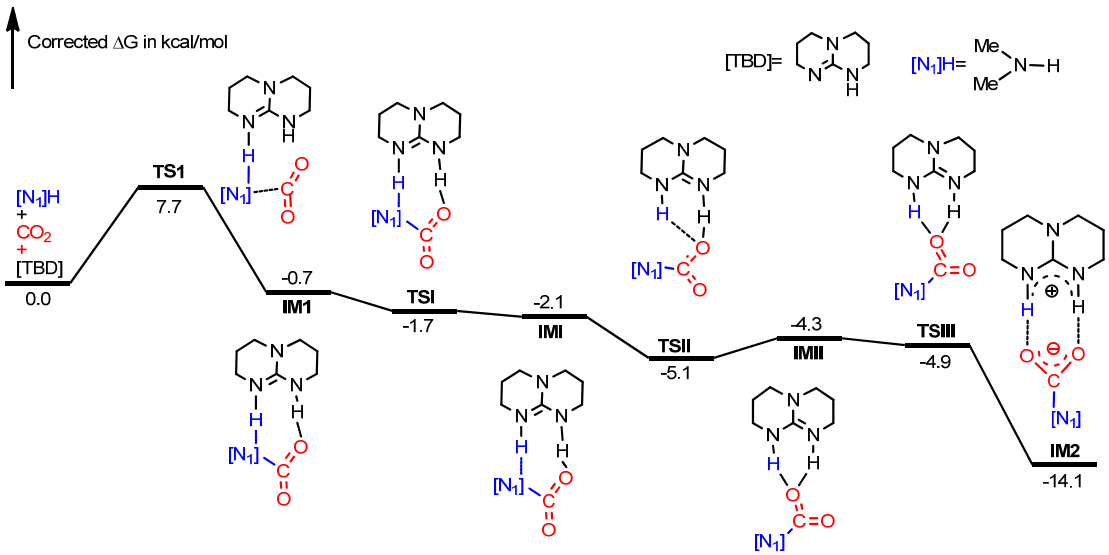


Fig. S1. Free energy profile for forming the carbamate [TBD]$HO_2C[N_1]$ in THF, omitted in Fig.1. Key optimized structures are given in Fig. S2.

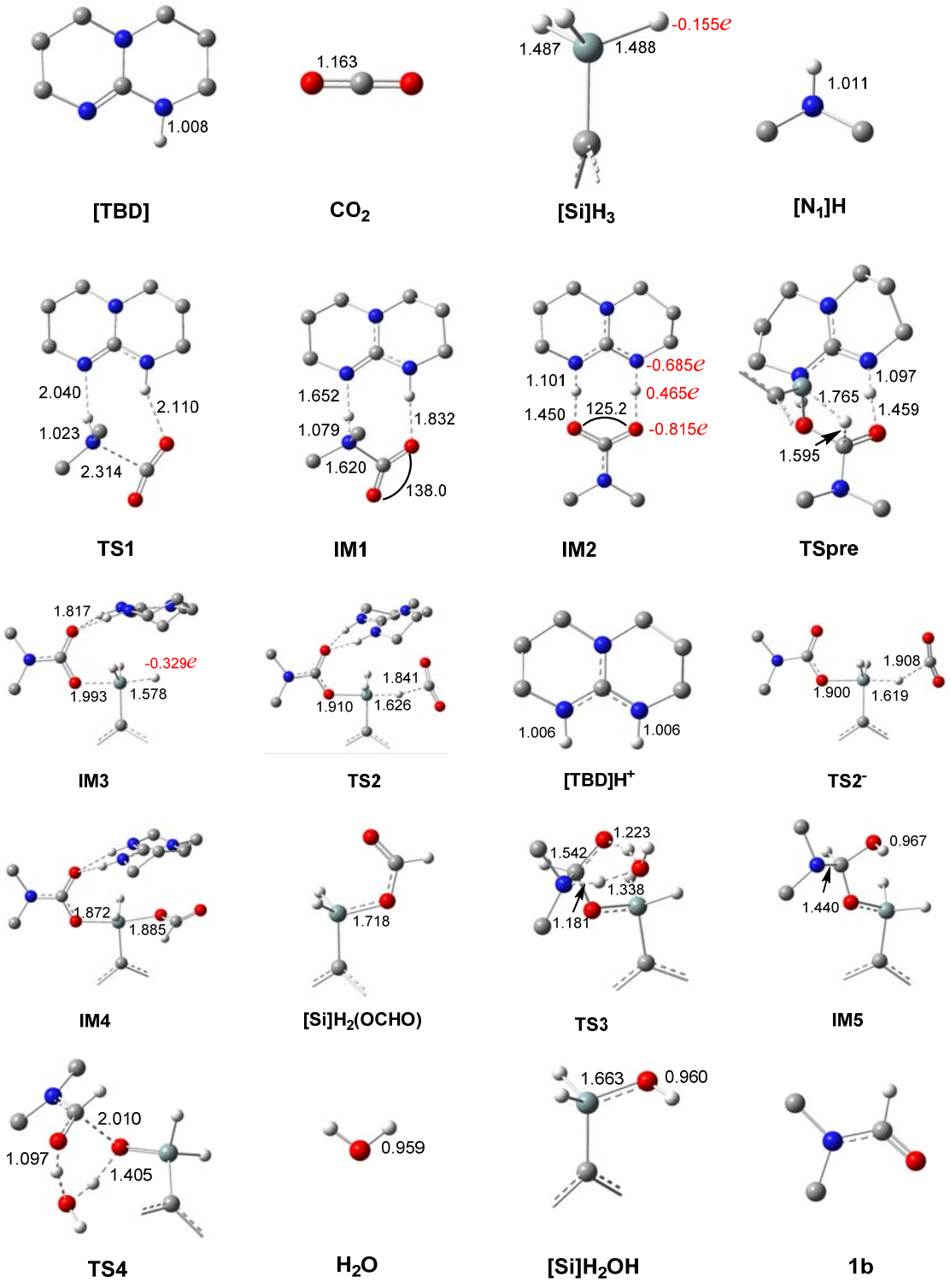


Fig. S2. Optimized structures of stationary points labeled in Fig. 1 and Fig. S1, along with key bond lengths in angstroms, and the NBO charges of [Si]H_3, IM2 and IM3. Trivial H atoms are omitted for clarity.

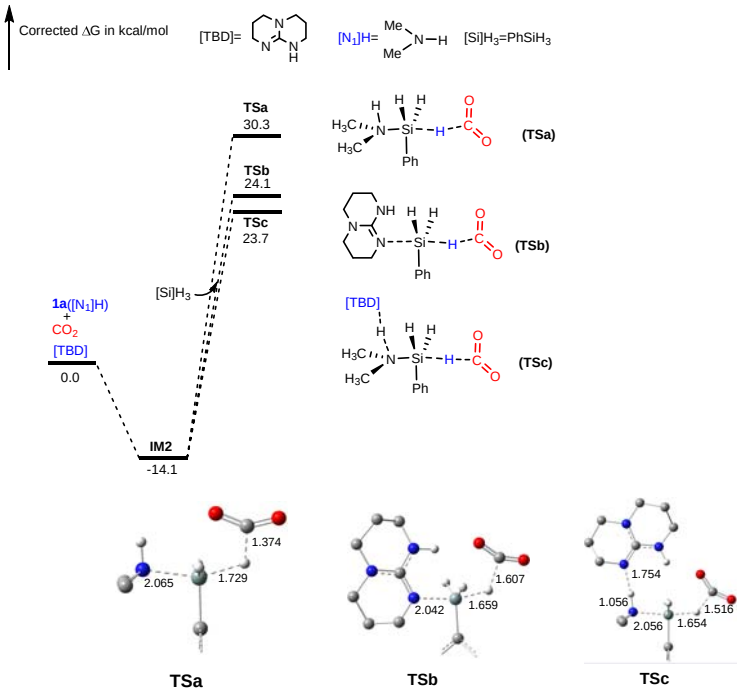


Fig. S3. Free energy results when using TBD, amine, and TBD-amine complex as activator to promote CO_2 reduction by $[Si]H_3$, along with the optimized structures of transition states. Key bond lengths are given in angstroms. Free energies in kcal mol^{-1} are relative to [**TBD**], **1a**, $[Si]H_3$ and CO_2, and are mass balanced.

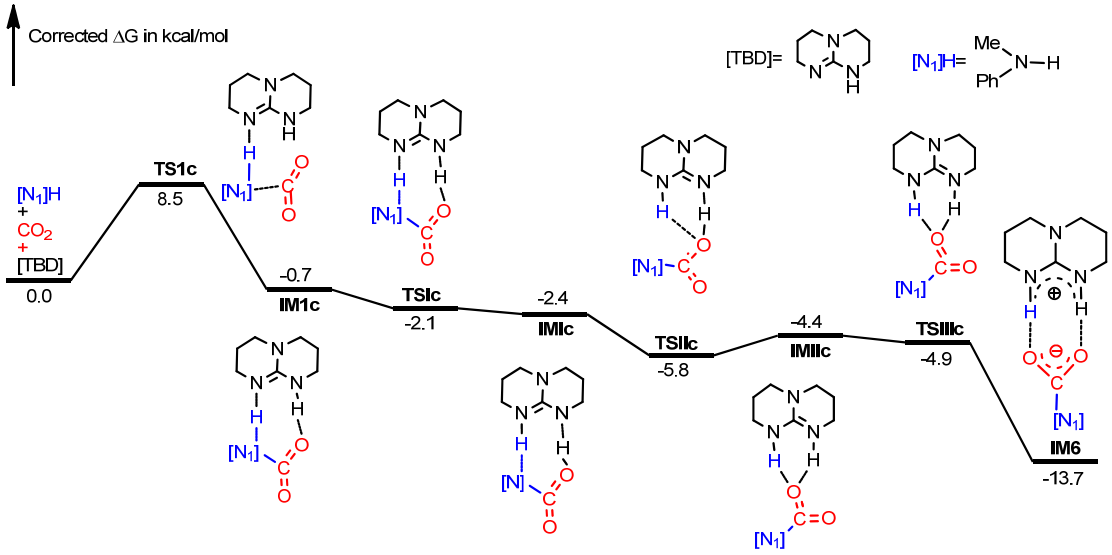


Fig.S4. Free energy profile for forming the carbamate $[TBD]HO_2C[N_1]$ in the CH_3CN solvent. The corresponding structures optimized in gas phase and displayed in Fig. S2 were used for the solvation-corrected energy calculations. Energies are relative to **TBD**, **1a** and CO_2, and are mass balanced.

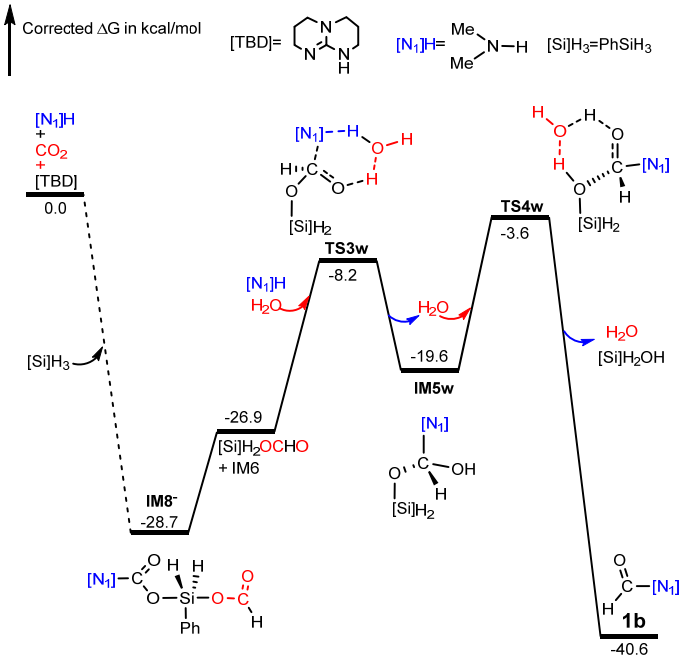


Fig. S5. Free energy profile for the C-N bond formation using water as a mediator in the anionic mechanism. Free energies are relative to TBD**, 1a**, $[Si]H_3$, water, and CO_2 and are mass balanced.

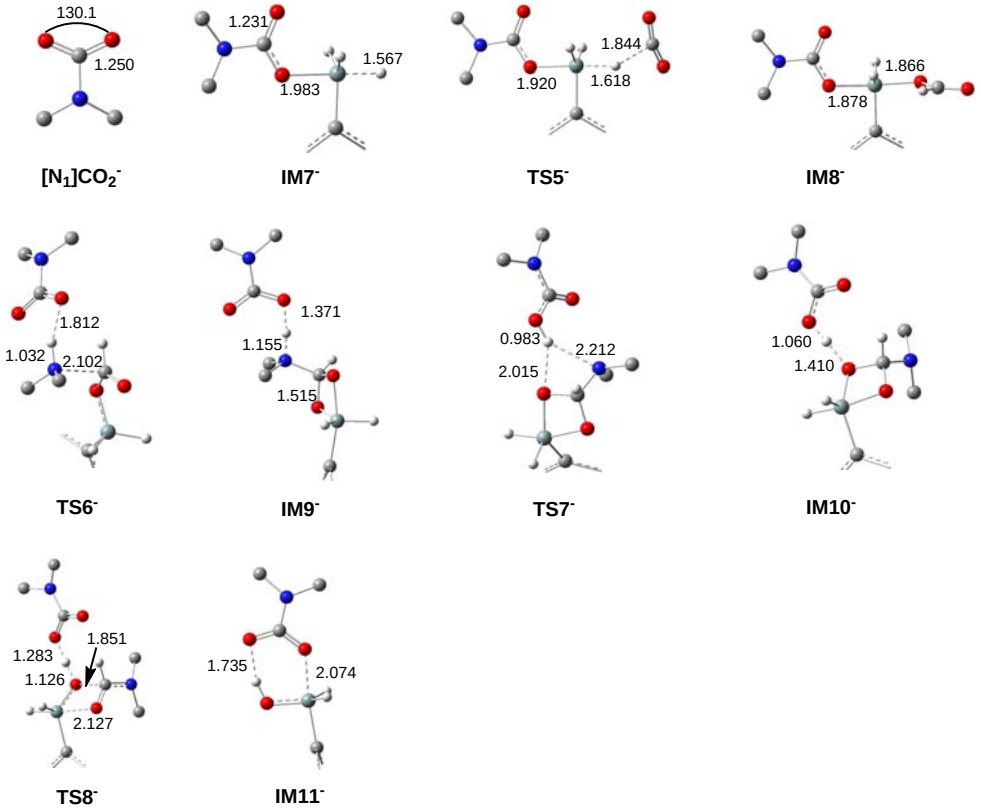


Fig. S6. Optimized structures of stationary points in Fig. 2, along with key bond lengths in angstroms. Trivial H atoms are omitted for clarity.

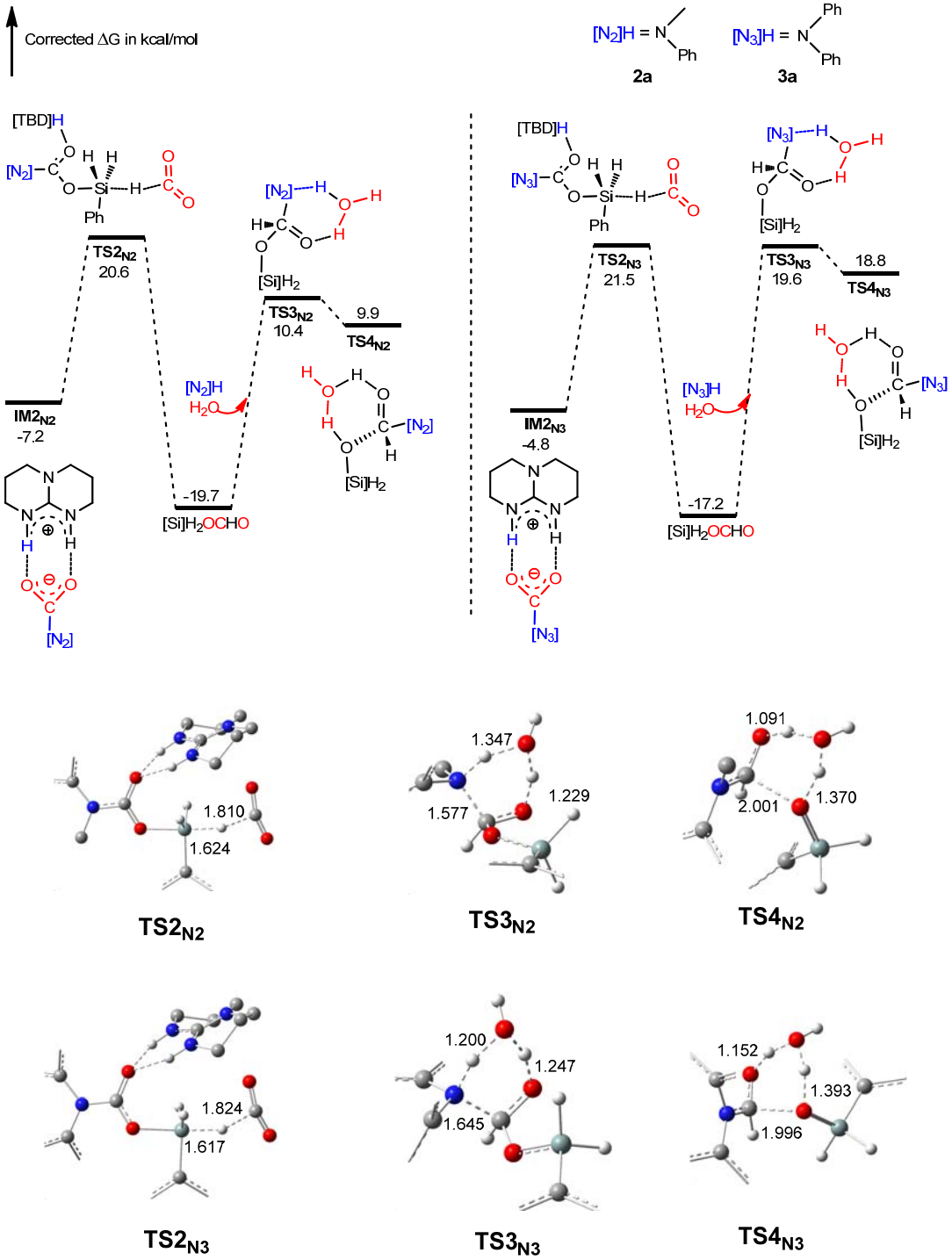


Fig. S7. Energetic and geometric results of the counterparts of **TS2**, **TS3,** and **TS4** for **2a** and **3a,** along with the optimized structures of transition states. Key bond lengths are given in angstroms. Free energies in kcal mol^{-1} are relative to [**TBD**], **2a/3a**, $[Si]H_3$, water and CO_2, and are mass balanced.

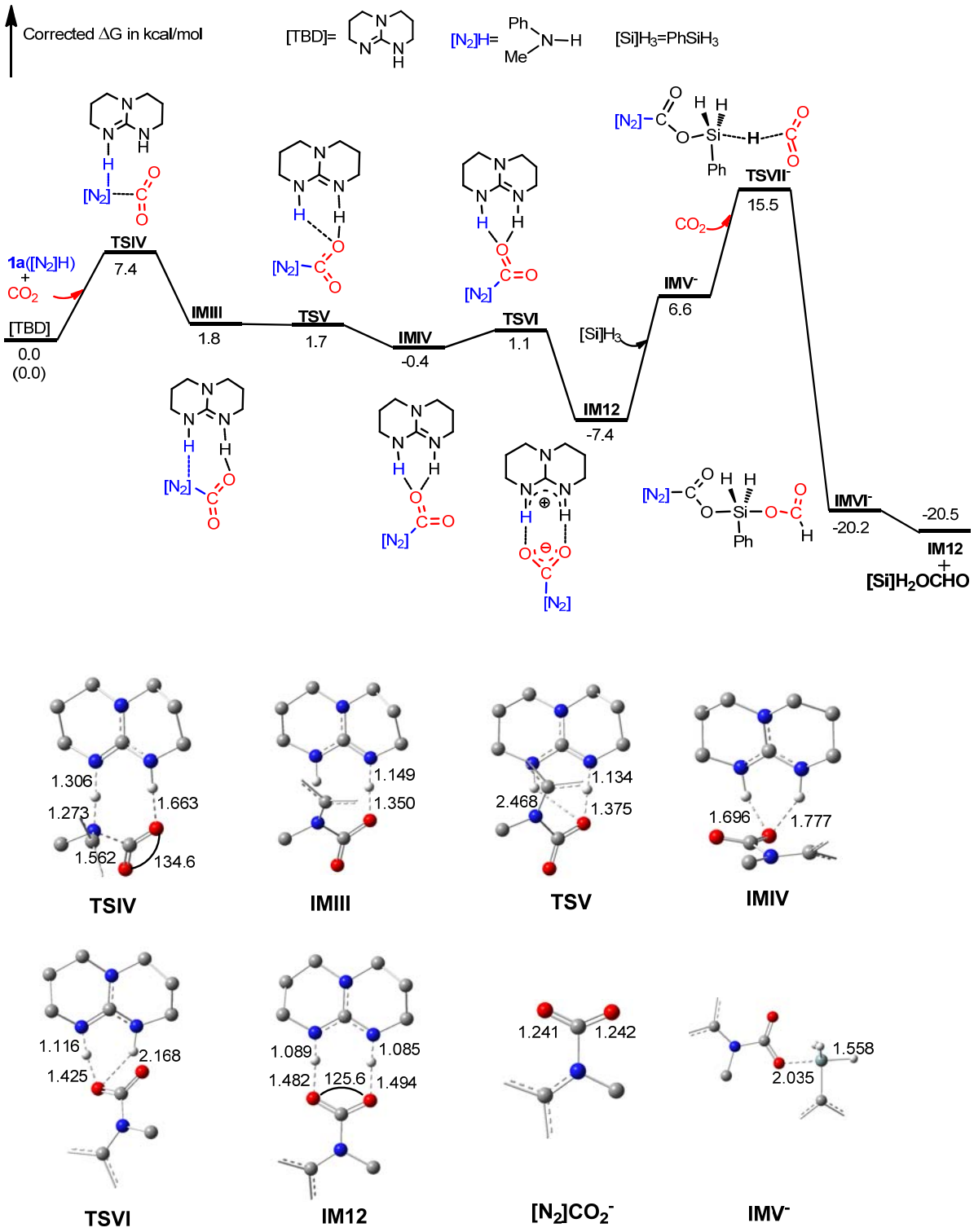


Fig. S8. Free energy profile for forming **IM13**$^-$, omitted in Fig. 3. along with the optimized structures of key stationary points. Key bond lengths are given in angstroms. Energies are relative to [**TBD**], **2a** and CO_2, and [Si]H_3 are mass balanced.

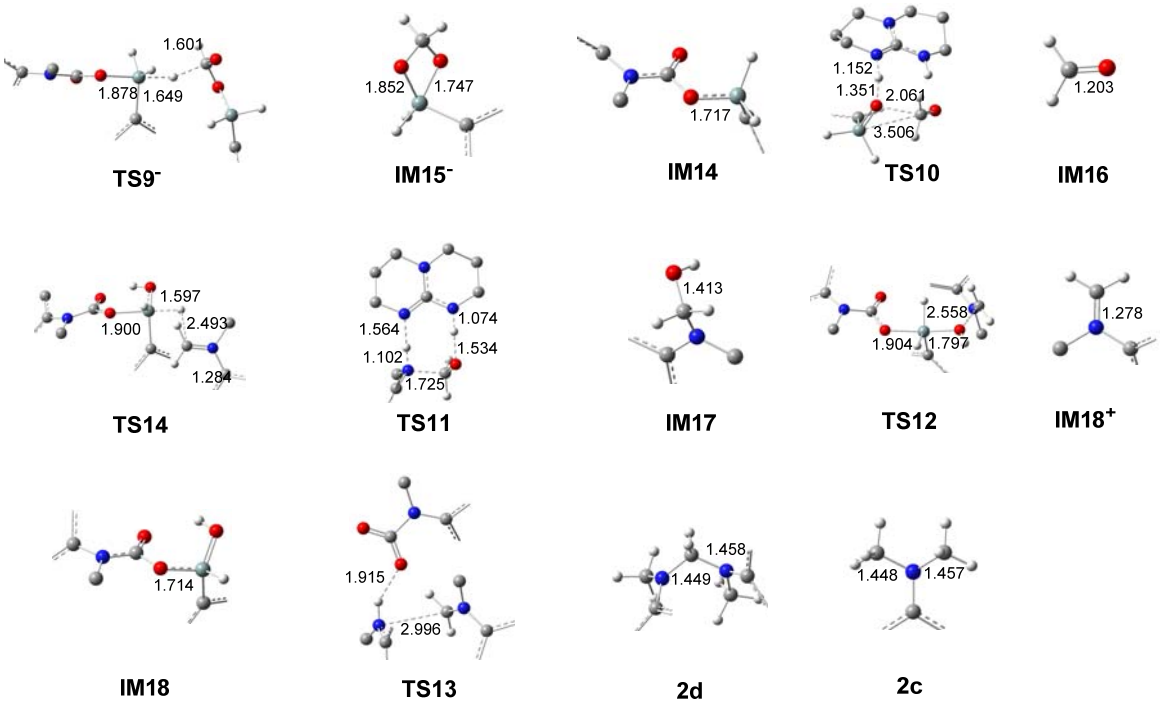


Fig. S9. Optimized structures of key stationary points labeled in Fig.3, along with key bond lengths in angstroms. Trivial H atoms are omitted for clarity.

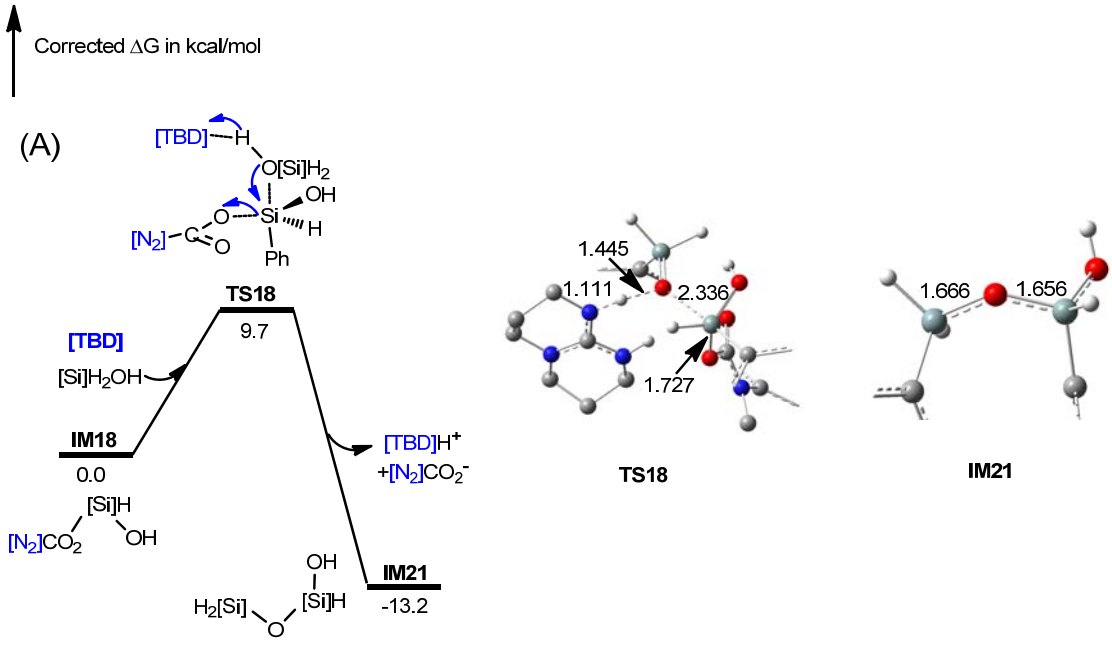


Fig. S10: Free energy profiles for the regeneration of $[TBD]H^+$ and $[N_2]CO_2^-$ active species, along with optimized structures of stationary points, along with key bond lengths in angstroms. Trivial H atoms are omitted for clarity.

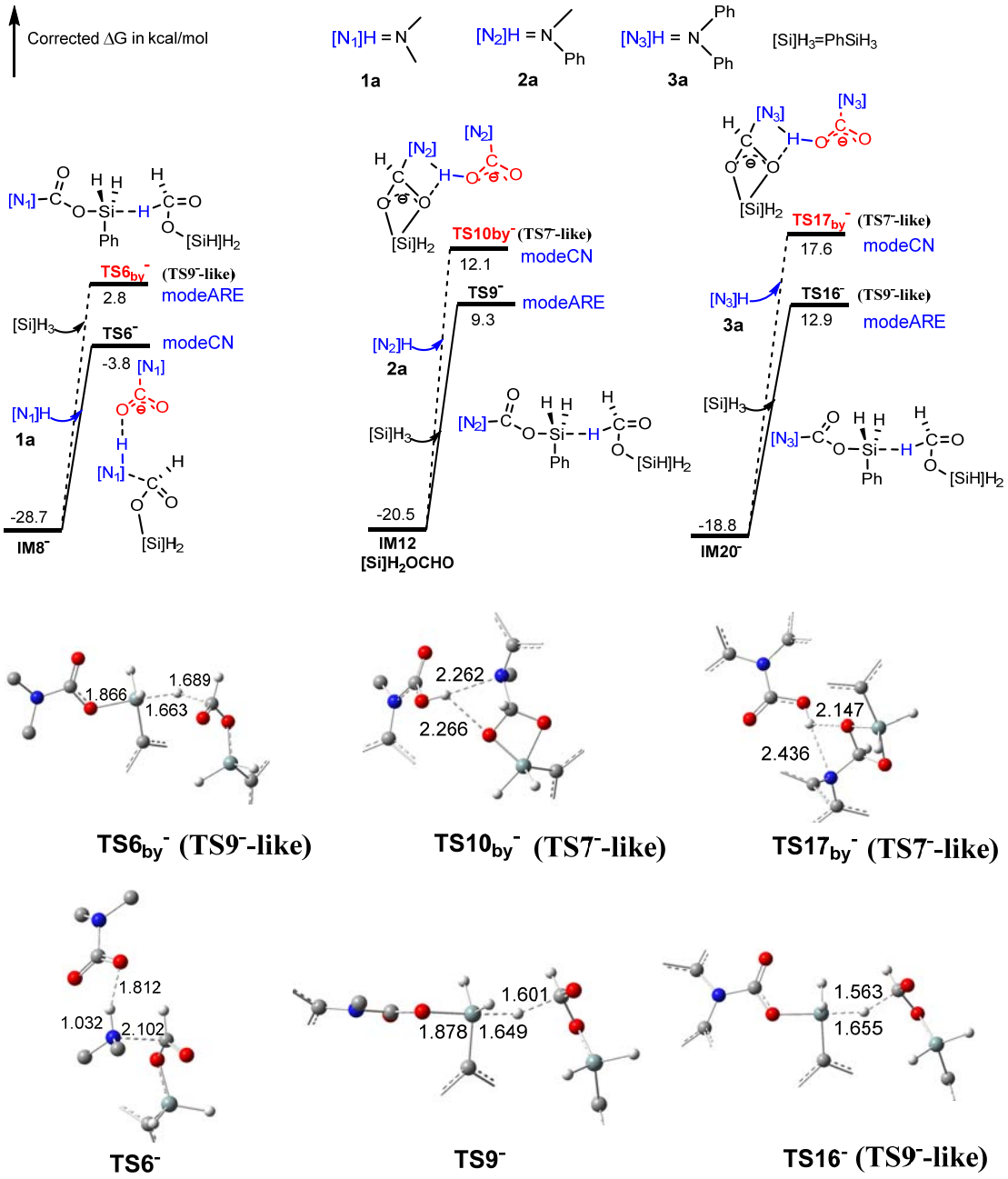


Fig. S11: Comparing the barriers (in kcal mol^{-1}) of selectivity-determining steps, leading to formamides (modeCN) and aminal (modeARE), respectively, along with the key optimized structures with key bond lengths in angstroms. Trivial H atoms are omitted for clarity.

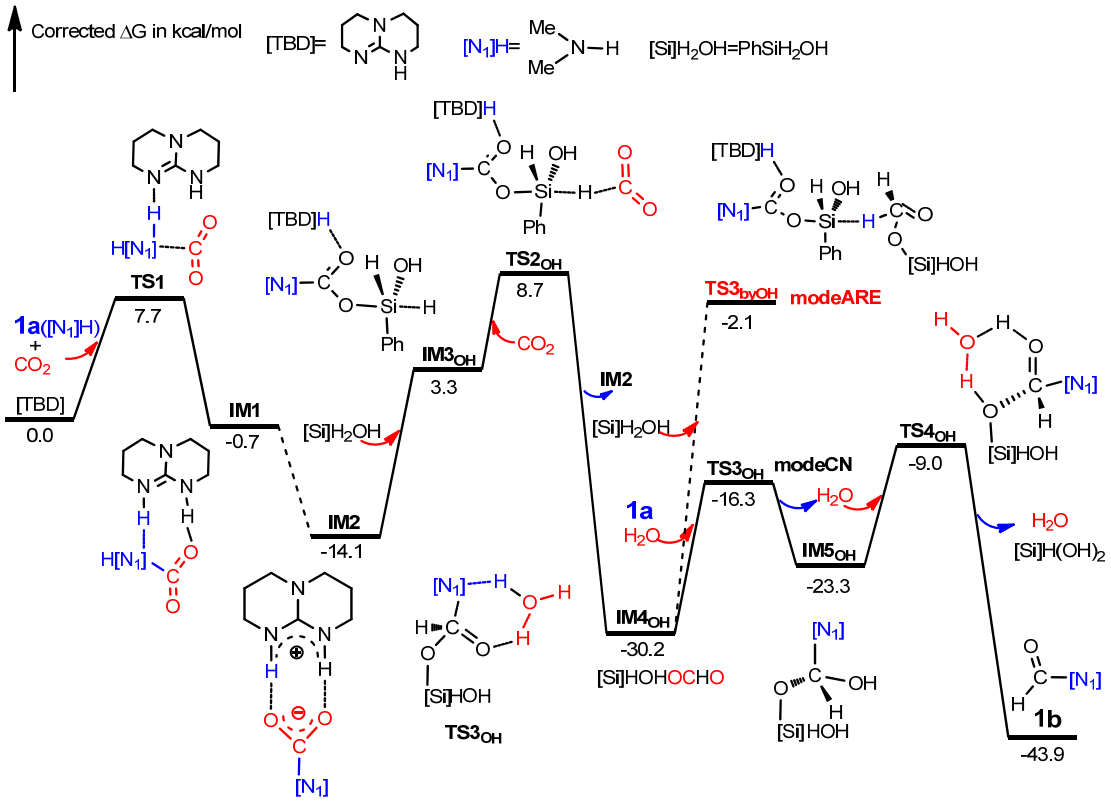


Fig. S12. Free energy profile for leading **1a** to **1b** via the neutral mechanism, when using $[Si]H_2OH$ as a reducing agent. Energies are relative to [**TBD**], **1a**, $[Si]H_2OH$, water and CO_2, and are mass balanced. Trivial H atoms are omitted for clarity.

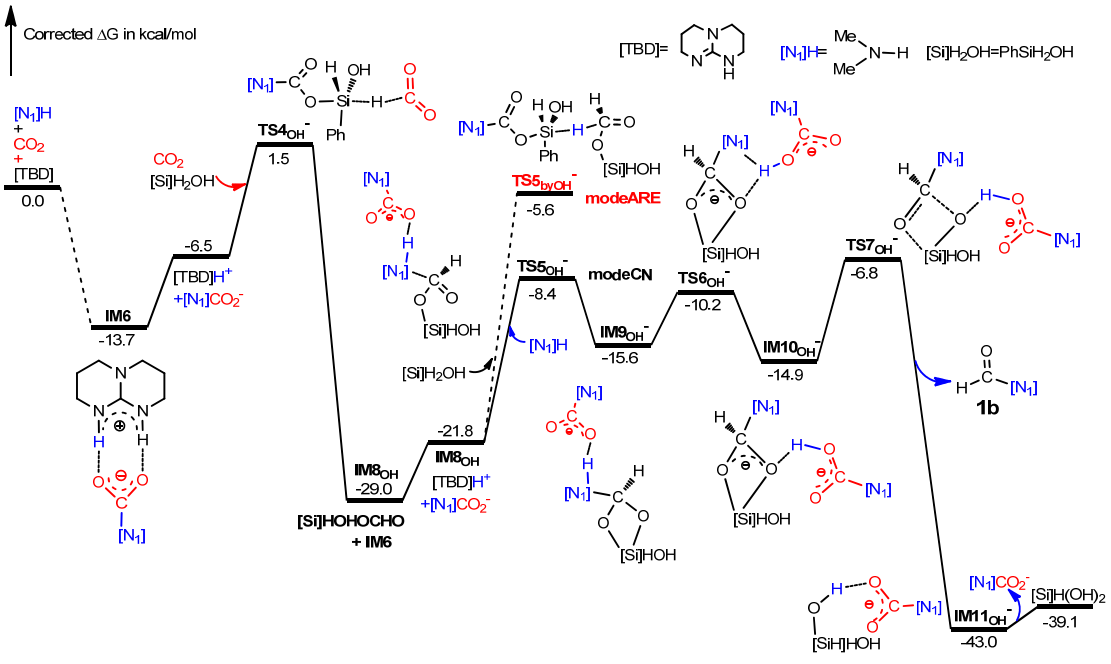


Fig. S13. Free energy profile for leading **1a** to **1b** via anionic mechanism, when using $[Si]H_2OH$ as a reducing agent,. Energies are relative to [**TBD**], **1a**, $[Si]H_2OH$, and CO_2, and

are mass balanced.

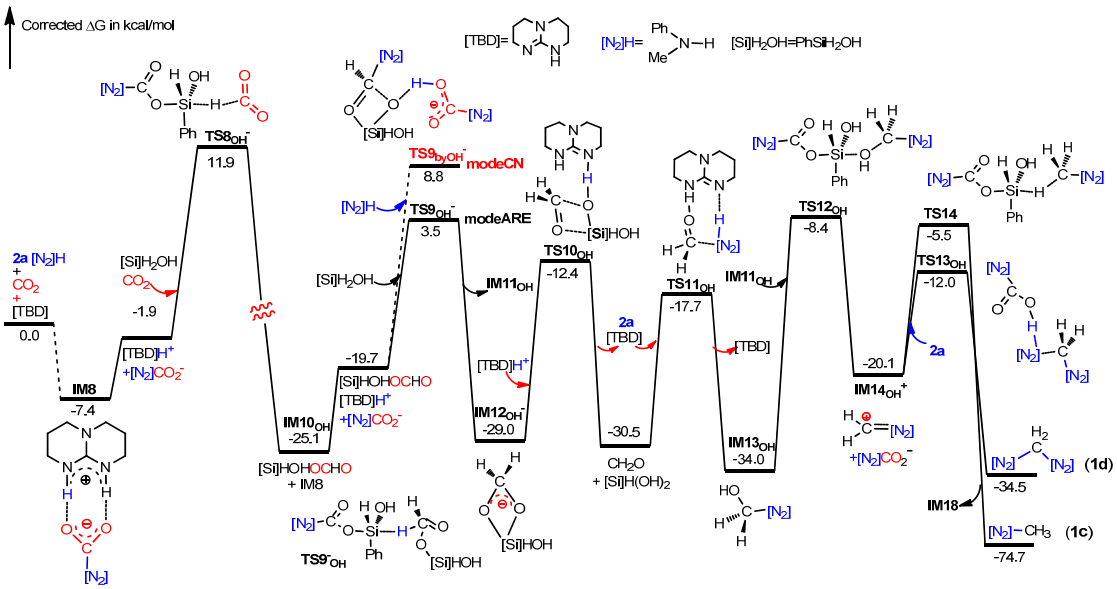
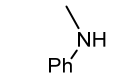
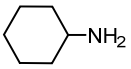
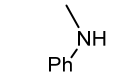
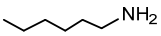
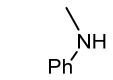
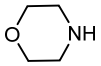
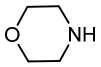
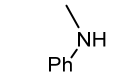
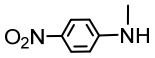
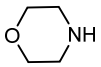
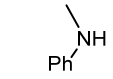
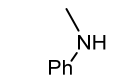
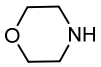
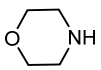
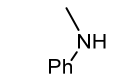
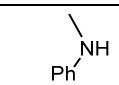
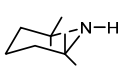
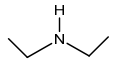
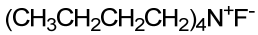


Fig. S14. Free energy profile for leading **1a** to **1d/1c** via ionic mechanism, when using [Si]H_2OH as a reducing agent. Energies are relative to [**TBD**], **2a**, [Si]H_2OH, and CO_2, and are mass balanced.

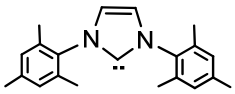
SI 4: Table S1. Experimental yields of the reactions of amine, CO_2, and hydrosilane, catalyzed by various catalysts, giving formamides or N-methylated amines. It can be observed that except for the yields in bold, aliphatic amines result in formamides via formylation, while aromatic amines give N-methylated amines via methylation.

Substrate	Catalyst	Solvent	Formylation (yield)	Methylation (yield)	Reference
	**[TBAF]**	CH_3CN	4%	95%	(1)
		CH_3CN	96%	-	(1)
	**[NHC]**	DMF	-	91%	(2)
	**[NSC]**	DMF	73%	-	(2)
		DMF	-	81%	(2)
	**[TMG]**	CH_3CN	98%	2%	(3)
	**$NaBH_4$**	DMSO	97%	-	(4)
		DMSO	**78%**	-	(4)
		DMSO	0%	-	(4)
	**Cs_2CO_3**	CH_3CN	95%	-	(5)
		CH_3CN	-	92%	(5)
	**[GB]**	CH_3CN	-	98%	(6)
		CH_3CN	98%	-	(6)
		CH_3CN	96%	-	(6)
	**[TBD]**	CH_3CN	93%	-	(7a)
		CH_3CN	-	97%	(7b)
	**[NHP]H**	CH_3CN	**95%**	-	(8)
		CH_3CN	-	**53%**	(8)

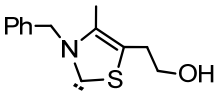
		CH_3CN	95%	-	(8)



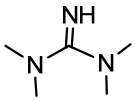
[TBAF]



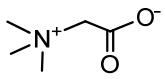
[NHC]



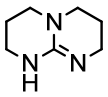
[NSC]



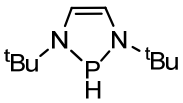
[TMG]



[GB]



[TBD]



[NHP]H

References for Table S1:

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(6) X. F. Liu, X. Y. Li, C. Qiao, H. C. Fu and L. N. He, *Angew Chem Int Ed ,*2017, **56,** 7425-7429.

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(8) C. C. Chong and R. Kinjo, *Angew. Chem., Int. Ed.,* 2015, **54**, 12116-12120.

SI 5: Cartesian Coordinates in Å, SCF Energies and Free Energies (in a.u.) at 298.15 K and 1 atm for the Optimized Structures [BS1= 6-31G(d,p), BS2=6-311++G(d,p)]

[TBD]

M05-2X/BS1 SCF energy in gas phase: -438.779479a.u.
M05-2X/BS2 SCF energy in THF solution: -438.909562 a.u.
M05-2X/BS2 SCF energy in Acetonitrile solution: -438.911792 a.u.
M05-2X/BS2 Free energy in THF solution: -438.733143 a.u.
M05-2X/BS2 Free energy in Acetonitrile solution: -438.735373 a.u.

C	-0.063853	-0.718488	-0.046217
C	2.393953	-0.761623	0.213110
C	2.423188	0.669749	-0.296537
C	1.190639	1.388725	0.226878
H	2.496094	-0.761751	1.308481
H	3.224070	-1.337175	-0.198506
H	3.324406	1.183375	0.041561
H	2.406594	0.662086	-1.387792
H	1.266783	1.504064	1.319799
H	1.120289	2.392291	-0.200026
N	-0.023000	0.671126	-0.134432
N	1.152011	-1.366602	-0.232115
C	-2.432940	0.607845	-0.372400
C	-2.409634	-0.815889	0.177669
C	-1.252244	1.366452	0.210550
H	-2.740628	-0.807781	1.223847
H	-3.128443	-1.436240	-0.364144
H	-2.331341	0.587389	-1.460015
H	-3.369710	1.110992	-0.125218
H	-1.361046	1.456767	1.302066
H	-1.189415	2.377372	-0.200067
N	-1.106764	-1.447953	0.094846
H	1.031965	-2.348014	-0.036398

CO_2

M05-2X/BS1 SCF energy in gas phase: -188.550523 a.u.
M05-2X/BS2 SCF energy in THF solution: -188.619248 a.u.
M05-2X/BS2 SCF energy in Acetonitrile solution: -188.618334 a.u.
M05-2X/BS2 Free energy in THF solution: -188.627974 a.u.
M05-2X/BS2 Free energy in Acetonitrile solution: -188.62706 a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.162854
O	0.000000	0.000000	-1.162854

$[N_1]H$

M05-2X/BS1 SCF energy in gas phase: -135.136551 a.u.
M05-2X/BS2 SCF energy in THF solution: -135.178553 a.u.
M05-2X/BS2 SCF energy in Acetonitrile solution: -135.179822 a.u.
M05-2X/BS2 Free energy in THF solution: -135.109732 a.u.
M05-2X/BS2 Free energy in Acetonitrile solution: -135.111001 a.u,

N	-0.000002	0.573344	-0.150005
H	-0.000002	1.325553	0.525800
C	1.201858	-0.224701	0.020311
H	1.256070	-0.964039	-0.782244
H	2.083716	0.412271	-0.054446
H	1.243522	-0.769511	0.976931
C	-1.201848	-0.224698	0.020310
H	-2.083712	0.412281	-0.054331
H	-1.256158	-0.963977	-0.782297
H	-1.243478	-0.769588	0.976894

$[N_2]H$

M05-2X/BS1 SCF energy in gas phase: -326.873835 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -326.967382 a.u.
M05-2X/BS2 Free energy in Acetonitrile solution: -326.850563 a.u,

N	-1.785953	0.620077	-0.147242
H	-1.992400	1.538077	0.207007
C	-2.808933	-0.370393	0.106532
H	-3.779662	0.122409	0.105752
H	-2.818522	-1.118341	-0.688909
H	-2.677184	-0.889740	1.064411
C	-0.443547	0.279172	-0.062863
C	-0.012218	-1.053711	-0.058890
C	0.523635	1.296353	-0.009951
C	1.347838	-1.348381	-0.011089
H	-0.730690	-1.860975	-0.095500
C	1.873094	0.987850	0.043740
H	0.200912	2.331906	-0.018084
C	2.301171	-0.339428	0.042108
H	1.659168	-2.386265	-0.010914
H	2.598136	1.791709	0.086354
H	3.355670	-0.578092	0.083053

$[N_3]H$

M05-2X/BS1 SCF energy in gas phase: -518.606038 a.u.
M05-2X/BS2 SCF energy in Acetonitrile solution: -518.746356 a.u.
M05-2X/BS2 Free energy in Acetonitrile solution: -518.581915 a.u,

N	-0.000043	1.071320	-0.000930
H	-0.000069	2.075791	-0.000039
C	-1.254032	0.461889	0.022830
C	-1.459802	-0.814701	0.561400
C	-2.356239	1.176969	-0.462266
C	-2.737443	-1.360970	0.584929
H	-0.625060	-1.362456	0.977008
C	-3.630125	0.627476	-0.414884
H	-2.202174	2.163141	-0.885701
C	-3.831265	-0.650388	0.099354
H	-2.877896	-2.349508	1.004930
H	-4.468413	1.199045	-0.793970
H	-4.822932	-1.082237	0.125994
C	1.253985	0.461956	-0.023453
C	2.355843	1.176955	0.462597
C	1.460170	-0.814472	-0.562182
C	3.629776	0.627549	0.415935
H	2.201407	2.163023	0.886153
C	2.737867	-1.360706	-0.584971
H	0.625739	-1.362202	-0.978462
C	3.831311	-0.650188	-0.098519
H	4.467792	1.199038	0.795732
H	2.878584	-2.349151	-1.005101
H	4.823040	-1.081930	-0.124658

$[Si]H_3$

M05-2X/BS1 SCF energy in gas phase: -522.881939 a.u.
M05-2X/BS2 SCF energy in THF solution: -522.968774 a.u.
M05-2X/BS2 SCF energy in Acetonitrile solution: -522.969658 a.u.
M05-2X/BS2 Free energy in THF solution: -522.882723 a.u.
M05-2X/BS2 Free energy in Acetonitrile solution: -522.883607 a.u.

Si	0.030850	2.337469	0.000000
H	-0.652810	2.854308	1.215709
H	-0.652810	2.854308	-1.215709
H	1.425837	2.856472	0.000000
C	-0.008710	0.463786	0.000000
C	-0.013669	-0.253481	1.202318
C	-0.013669	-0.253481	-1.202318
C	-0.013669	-1.645148	1.205072
H	-0.022389	0.277907	2.148021
C	-0.013669	-1.645148	-1.205072
H	-0.022389	0.277907	-2.148021
C	-0.012527	-2.341781	0.000000
H	-0.018453	-2.184536	2.144192
H	-0.018453	-2.184536	-2.144192
H	-0.014952	-3.424867	0.000000

H_2O

M05-2X/BS1 SCF energy in gas phase: -76.403595 a.u.
M05-2X/BS2 SCF energy in THF solution: -76.448784 a.u.
M05-2X/BS2 SCF energy in Acetonitrile

solution: -76.450547 a.u.
M05-2X/BS2 Free energy in THF solution: -76.444676 a.u.
M05-2X/BS2 Free energy in Acetonitrile solution: -76.446439 a.u.

O	0.000000	0.000000	0.116888
H	0.000000	0.760566	-0.467554
H	0.000000	-0.760566	-0.467554

TS1

M05-2X/BS1 SCF energy in gas phase: -762.493723 a.u.
M05-2X/BS2 SCF energy in THF solution: -762.72177 a.u.
M05-2X/BS2 Free energy in THF solution: -762.452473 a.u.

C	1.179224	0.049563	-0.112239
C	1.139625	2.378256	-0.553126
C	2.520201	2.435609	0.092024
C	3.297808	1.201592	-0.334841
H	1.230477	2.599160	-1.624236
H	0.498357	3.158123	-0.133231
H	3.053454	3.341977	-0.200379
H	2.422588	2.429697	1.180118
H	3.477290	1.221437	-1.419633
H	4.270955	1.159153	0.160312
N	2.554850	0.012561	0.048721
N	0.478253	1.098415	-0.378112
C	2.514319	-2.381366	0.570311
C	1.131702	-2.425391	-0.056819
C	3.289252	-1.239245	-0.066858
H	1.219345	-2.694179	-1.118904
H	0.502262	-3.174958	0.423037
H	2.420291	-2.205855	1.643506
H	3.042273	-3.322500	0.410540
H	3.497347	-1.474378	-1.121398
H	4.251821	-1.102288	0.431623
N	0.505994	-1.129659	0.128954
H	-0.465818	-1.075982	-0.138345
N	-2.458412	0.792709	0.298534
H	-1.541749	0.980429	-0.115205
C	-2.264463	0.590170	1.728324
H	-1.919848	1.498723	2.240141
H	-3.207463	0.279612	2.186239
H	-1.524791	-0.195674	1.882866
C	-3.380462	1.879787	0.013974
H	-3.438547	2.037486	-1.062905
H	-4.378227	1.609095	0.364890
H	-3.085087	2.822143	0.495404
C	-3.337279	-1.175537	-0.543289
O	-4.397714	-0.775203	-0.833527
O	-2.405948	-1.873552	-0.365958

IM1

M05-2X/BS1 SCF energy in gas phase: -762.500575 a.u.
M05-2X/BS2 SCF energy in THF solution: -762.738675 a.u.
M05-2X/BS2 Free energy in THF solution: -762.465939 a.u.

C	1.072875	0.009283	-0.055662
C	0.533315	2.313265	-0.364709
C	1.919683	2.625074	0.183271
C	2.890567	1.598892	-0.375953
H	0.501717	2.563713	-1.432821
H	-0.212127	2.948538	0.122693
H	2.233370	3.632938	-0.093543
H	1.913440	2.551527	1.273184
H	2.988709	1.721250	-1.463313
H	3.883735	1.723628	0.061347
N	2.427160	0.261673	-0.042808
N	0.153543	0.925442	-0.169543
C	2.928596	-2.072108	0.488460
C	1.547942	-2.419543	-0.038718
C	3.399413	-0.808947	-0.212843
H	1.619049	-2.708300	-1.095421
H	1.119115	-3.262345	0.503397
H	2.876745	-1.893856	1.564298
H	3.630040	-2.885841	0.300248
H	3.572196	-1.013516	-1.278654
H	4.344641	-0.462709	0.211262
N	0.672039	-1.278000	0.143480
H	-0.319947	-1.441520	-0.037437
N	-2.470433	0.376877	0.319536
H	-1.448531	0.578205	0.036431
C	-2.428463	0.052167	1.756485
H	-2.028490	0.901740	2.310888

H	-3.435643	-0.178850	2.104387
H	-1.784765	-0.813751	1.885222
C	-3.316773	1.539259	0.025083
H	-3.264106	1.748371	-1.039761
H	-4.348044	1.302892	0.277588
H	-2.966379	2.397820	0.599859
C	-2.908905	-0.935637	-0.522612
O	-3.938749	-0.770538	-1.139228
O	-2.083799	-1.832228	-0.343436

TSI

M05-2X/BS1 SCF energy in gas phase: -762.497956 a.u.

M05-2X/BS2 SCF energy in THF solution: -762.737998 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -762.741249 a.u.

M05-2X/BS2 Free energy in THF solution: -762.46753 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -762.470782 a.u.

C	1.008530	0.005714	-0.064803
C	0.391461	2.341435	0.091206
C	1.779441	2.564469	0.672816
C	2.763259	1.697459	-0.096343
H	0.333904	2.810372	-0.899700
H	-0.362700	2.824839	0.716442
H	2.063810	3.615176	0.601330
H	1.792822	2.271303	1.724580
H	2.832447	2.031546	-1.139546
H	3.761526	1.762811	0.340054
N	2.341261	0.307324	-0.020419
N	0.067645	0.928368	-0.001530
C	2.883709	-2.033486	0.384983
C	1.546423	-2.403629	-0.234789
C	3.348401	-0.722863	-0.229993
H	1.695104	-2.706726	-1.277666
H	1.086062	-3.241050	0.289164
H	2.771061	-1.905067	1.463367
H	3.621201	-2.815643	0.201858
H	3.554362	-0.857845	-1.299687
H	4.270267	-0.380544	0.243902
N	0.633109	-1.279685	-0.154861
H	-0.380962	-1.488295	-0.015482
N	-2.408337	0.306971	-0.337728
H	-1.183276	0.599615	-0.119805
C	-3.266777	1.456580	-0.041993
H	-2.936109	2.309609	-0.638851
H	-4.307837	1.224771	-0.270374
H	-3.196355	1.684430	1.017843
C	-2.440659	-0.051274	-1.762797
H	-1.826550	-0.935762	-1.906871
H	-3.464116	-0.264893	-2.080859
H	-2.044685	0.778065	-2.352509
C	-2.707914	-0.907136	0.557844
O	-1.948964	-1.865707	0.292514
O	-3.594907	-0.739440	1.375960

IMI

M05-2X/BS1 SCF energy in gas phase: -762.508895 a.u.

M05-2X/BS2 SCF energy in THF solution: -762.742337 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -762.745525 a.u.

M05-2X/BS2 Free energy in THF solution: -762.468087 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -762.471275 a.u.

C	1.345594	-0.106952	-0.786643
C	0.726432	2.277993	-0.752069
C	1.560888	2.296409	0.522962
C	2.805547	1.446842	0.284895
H	1.073212	3.045295	-1.447654
H	-0.320569	2.459985	-0.508876
H	1.820931	3.322372	0.785838
H	0.983251	1.847907	1.332588
H	3.361345	1.806950	-0.585641
H	3.477653	1.449999	1.141588
N	2.376339	0.069361	0.058836
N	0.831429	0.973015	-1.420923
C	1.645091	-2.048351	1.078842
C	1.365456	-2.446895	-0.366959
C	2.688939	-0.940907	1.077445
H	2.277358	-2.816395	-0.848339
H	0.615478	-3.234465	-0.423564
H	0.716597	-1.668963	1.508693
H	2.010097	-2.890600	1.668196

H	3.687037	-1.344449	0.883346
H	2.707084	-0.441106	2.048827
N	0.846063	-1.295332	-1.086043
H	-0.275327	-1.174466	-1.190569
N	-3.130703	0.119576	0.270419
H	-0.001590	0.705037	-1.931816
C	-3.499290	0.617765	1.573014
H	-4.201217	1.452018	1.474426
H	-3.983301	-0.160614	2.176692
H	-2.598284	0.951468	2.077816
C	-4.207986	-0.357892	-0.563397
H	-3.797863	-0.677562	-1.515313
H	-4.731029	-1.201176	-0.094542
H	-4.938487	0.440715	-0.727258
C	-1.807415	-0.157302	-0.017990
O	-1.589530	-0.706602	-1.169400
O	-0.920948	0.153784	0.809268

TSII

M05-2X/BS1 SCF energy in gas phase: -762.503666 a.u.

M05-2X/BS2 SCF energy in THF solution: -762.746203 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -762.749906 a.u.

M05-2X/BS2 Free energy in THF solution: -762.472971 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -762.476674 a.u.

C	-1.062399	-0.004564	0.139075
C	-0.411860	2.379102	0.086003
C	-1.735315	2.611192	-0.623672
C	-2.791964	1.734497	0.030696
H	-0.454112	2.796500	1.098584
H	0.408227	2.867543	-0.440630
H	-2.027896	3.659332	-0.555554
H	-1.641862	2.341606	-1.677319
H	-2.975299	2.065303	1.060739
H	-3.735966	1.802598	-0.512590
N	-2.372734	0.339754	0.004530
N	-0.123638	0.957945	0.127477
C	-2.907527	-1.990408	-0.442749
C	-1.599066	-2.380356	0.227006
C	-3.394916	-0.685984	0.170347
H	-1.790673	-2.725757	1.248484
H	-1.110323	-3.195450	-0.306987
H	-2.750295	-1.844051	-1.513219
H	-3.654860	-2.772670	-0.306655
H	-3.635940	-0.826917	1.231025
H	-4.295901	-0.333041	-0.333719
N	-0.678207	-1.257835	0.252358
H	0.441408	-1.474133	0.368249
N	2.730097	0.330092	0.132464
H	0.868038	0.676541	0.113664
C	3.673963	1.084689	-0.676417
H	3.591965	2.145604	-0.426757
H	4.707241	0.761952	-0.500281
H	3.445404	0.927102	-1.725871
C	2.932556	0.512077	1.564725
H	2.237323	-0.128092	2.099231
H	3.956021	0.252234	1.864215
H	2.755161	1.557974	1.831503
C	2.494961	-1.026151	-0.312885
O	1.758930	-1.703657	0.499161
O	2.938958	-1.364898	-1.399998

IMII

M05-2X/BS1 SCF energy in gas phase: -762.51917 a.u.

M05-2X/BS2 SCF energy in THF solution: -762.744561 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -762.747205 a.u.

M05-2X/BS2 Free energy in THF solution: -762.487212 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -762.471666 a.u.

O	1.676060	0.247781	-1.273299
O	1.027143	-0.109584	0.860261
C	1.906531	-0.010358	-0.022754
C	4.302106	-0.036665	-0.642633
H	4.923859	-0.938203	-0.679633
H	4.948683	0.805010	-0.365986
H	3.870948	0.146773	-1.620960
N	-0.867541	-1.147149	-1.153086
H	0.069489	-1.061655	-1.539756
N	-0.681439	1.126161	-1.191694
H	0.395416	0.858561	-1.346665

N	-2.298469	0.129798	0.188292
C	-1.284514	0.057810	-0.691837
C	-1.111753	-2.315687	-0.321622
H	-0.501493	-2.264877	0.586135
H	-0.834824	-3.201712	-0.890926
C	-2.596001	-2.320950	0.008448
H	-3.165347	-2.358746	-0.921849
H	-2.864222	-3.186522	0.614734
C	-2.922106	-1.052165	0.781439
H	-4.001477	-0.882449	0.816588
H	-2.562345	-1.144315	1.811942
C	-2.597674	1.394644	0.863576
H	-2.842779	1.154040	1.900214
H	-3.479783	1.856172	0.407744
C	-1.398533	2.326416	0.800927
H	-1.662807	3.297831	1.220562
H	-0.572095	1.888862	1.364571
C	-0.973771	2.445868	-0.655713
H	-1.758177	2.930664	-1.246309
H	-0.067130	3.042271	-0.754086
N	3.232618	-0.199607	0.311334
C	3.615666	-0.460225	1.676124
H	4.221116	0.360857	2.078908
H	2.711894	-0.565962	2.267944
H	4.209565	-1.378720	1.741479

TSIII

M05-2X/BS1 SCF energy in gas phase: -762.516525 a.u.

M05-2X/BS2 SCF energy in THF solution: -762.745638 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -762.748314 a.u.

M05-2X/BS2 Free energy in THF solution: -762.472533 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -762.475209 a.u.

O	1.722114	-0.821900	-0.887717
O	1.522962	0.928935	0.518307
C	2.193370	0.033192	-0.030176
C	4.380846	-1.062326	-0.402285
H	4.937386	-1.645591	0.339530
H	5.110242	-0.571110	-1.058330
H	3.756723	-1.723933	-0.993197
N	-0.699575	-1.254756	-0.460889
H	0.433081	-1.141336	-0.666535
N	-0.746971	0.920342	-1.150687
H	0.233624	0.709606	-1.305970
N	-2.541413	0.095411	0.089799
C	-1.330504	-0.097338	-0.479552
C	-1.249651	-2.380630	0.266937
H	-0.916786	-2.364534	1.311416
H	-0.871263	-3.297612	-0.184870
C	-2.770774	-2.335429	0.207649
H	-3.094909	-2.444655	-0.829494
H	-3.208448	-3.144764	0.792890
C	-3.245245	-0.996054	0.751795
H	-4.314035	-0.863245	0.568526
H	-3.080109	-0.943213	1.834487
C	-3.048825	1.451348	0.272040
H	-3.668267	1.446783	1.170881
H	-3.680710	1.743948	-0.573752
C	-1.875424	2.409058	0.427290
H	-2.232525	3.429436	0.568926
H	-1.284516	2.114642	1.297384
C	-1.001611	2.319605	-0.812702
H	-1.486002	2.819136	-1.656051
H	-0.034865	2.784574	-0.625885
N	3.537927	-0.092291	0.252730
C	4.196509	0.862898	1.108508
H	4.938212	1.446537	0.549381
H	3.443325	1.529563	1.516272
H	4.717305	0.352611	1.925980

IM2

M05-2X/BS1 SCF energy in gas phase: -762.527412 a.u.

M05-2X/BS2 SCF energy in THF solution: -762.758447 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -762.760432 a.u.

M05-2X/BS2 Free energy in THF solution: -762.487212 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -762.489181 a.u.

N	-0.651897	1.131069	-0.145113
H	0.445529	1.097040	-0.054467
N	-0.654490	-1.131923	0.154042

H	0.443316	-1.098902	0.072794
N	-2.692865	0.000667	-0.004812
C	-1.331648	-0.000015	0.001361
C	-1.319500	2.391388	-0.382910
H	-1.526269	2.537524	-1.450412
H	-0.645933	3.186960	-0.065648
C	-2.622496	2.424464	0.403949
H	-2.396654	2.359861	1.470267
H	-3.173836	3.347509	0.221033
C	-3.469863	1.234145	-0.018613
H	-4.314151	1.103079	0.664668
H	-3.879884	1.397290	-1.022444
C	-3.471341	-1.231957	0.001454
H	-4.308859	-1.099940	-0.689920
H	-3.891154	-1.394666	1.001276
C	-2.621265	-2.423246	-0.412946
H	-3.175289	-3.345676	-0.235089
H	-2.385286	-2.359024	-1.477091
C	-1.325734	-2.391374	0.386172
H	-1.542790	-2.536662	1.451735
H	-0.650148	-3.187902	0.075683
O	1.888032	-1.126571	-0.046394
O	1.888084	1.125086	0.076551
C	2.472534	-0.001447	0.026256
C	4.600147	-1.225316	-0.088568
H	5.374016	-1.290961	0.682935
H	5.094138	-1.266499	-1.067354
H	3.920216	-2.065522	0.004299
N	3.848429	-0.003528	0.066497
C	4.600716	1.226821	0.023588
H	5.369674	1.225237	0.802899
H	5.100984	1.352612	-0.944675
H	3.919911	2.055753	0.185501

IM3

M05-2X/BS1 SCF energy in gas phase: -1285.411625 a.u.

M05-2X/BS2 SCF energy in THF solution: -1285.724713 a.u.

M05-2X/BS2 Free energy in THF solution: -1285.337783 a.u.

O	-0.295068	2.335307	-0.290796
O	1.631035	1.159283	-0.119048
C	0.965602	2.249209	-0.211928
N	-2.254226	0.543849	-1.202227
H	-1.506884	1.245576	-1.199421
N	-2.339807	1.001791	1.035184
H	-1.588134	1.655626	0.790261
N	-3.398830	-0.912745	0.222192
C	-2.654978	0.186404	0.022425
C	-2.385945	-0.339863	-2.351145
H	-1.521816	-1.007526	-2.402886
H	-2.406407	0.278635	-3.247452
C	-3.672699	-1.134579	-2.202977
H	-4.533538	-0.463789	-2.243537
H	-3.762597	-1.862152	-3.009504
C	-3.645224	-1.858157	-0.866975
H	-4.603671	-2.340299	-0.667591
H	-2.857022	-2.618634	-0.860098
C	-3.663985	-1.387740	1.581031
H	-3.680393	-2.477606	1.540351
H	-4.649975	-1.043832	1.908926
C	-2.574533	-0.909646	2.527087
H	-2.806533	-1.213050	3.548081
H	-1.622140	-1.351972	2.228506
C	-2.475199	0.604537	2.431432
H	-3.359621	1.075870	2.869498
H	-1.595443	0.966949	2.961699
Si	0.688326	-0.588399	-0.293599
H	0.008349	-0.175802	0.979066
H	0.363940	-0.085599	-1.671009
C	2.323229	-1.525178	-0.074255
C	2.376232	-2.886425	-0.401805
C	3.493768	-0.936352	0.425138
C	3.544840	-3.629240	-0.253738
H	1.481437	-3.369375	-0.777360
C	4.662499	-1.674759	0.589138
H	3.479934	0.112667	0.687957
C	4.693287	-3.023420	0.245823
H	3.557582	-4.679175	-0.522839
H	5.551900	-1.196673	0.983072
H	5.604489	-3.597116	0.368436
N	1.704482	3.402563	-0.239595
C	1.062860	4.695134	-0.164526
H	1.194294	5.147555	0.825495
H	1.496990	5.369908	-0.907161
H	0.004011	4.568781	-0.363456
C	3.140157	3.375568	-0.062320

H	3.423383	3.539254	0.984194
H	3.524219	2.413890	-0.387135
H	3.588535	4.167786	-0.666407
H	-0.229971	-1.860200	-0.463886

TS2

M05-2X/BS1 SCF energy in gas phase: -1473.968458 a.u.

M05-2X/BS2 SCF energy in THF solution: -1474.343171 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1474.346021 a.u.

M05-2X/BS2 Free energy in THF solution: -1473.948403 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1473.951253 a.u.

O	-0.077254	2.538935	-0.355299
O	1.833176	1.360934	-0.093898
C	1.173218	2.460069	-0.226927
N	-2.072772	0.778966	-1.262660
H	-1.245852	1.380061	-1.249650
N	-2.280514	1.423774	0.922508
H	-1.419780	1.943818	0.739304
N	-3.651034	-0.267852	0.098935
C	-2.663026	0.622359	-0.074259
C	-2.243822	-0.207138	-2.317608
H	-1.606715	-1.077320	-2.131066
H	-1.935122	0.251702	-3.255036
C	-3.714836	-0.593842	-2.347483
H	-4.313552	0.286666	-2.588695
H	-3.900325	-1.355698	-3.104677
C	-4.104644	-1.142015	-0.983346
H	-5.190444	-1.230848	-0.896973
H	-3.661385	-2.128714	-0.828028
C	-4.096606	-0.661634	1.437571
H	-4.152633	-1.751877	1.444375
H	-5.099273	-0.259718	1.614296
C	-3.122319	-0.191955	2.506393
H	-3.564137	-0.340618	3.491817
H	-2.204115	-0.775907	2.433161
C	-2.798709	1.275509	2.270838
H	-3.690754	1.895364	2.408211
H	-2.032665	1.625465	2.960525
Si	1.021267	-0.350127	-0.340962
H	0.118270	-0.081678	0.824431
H	0.637458	0.081647	-1.726110
C	2.689095	-1.206401	-0.055328
C	2.871451	-2.517571	-0.513519
C	3.760746	-0.598228	0.614493
C	4.077100	-3.189974	-0.330320
H	2.052547	-3.022829	-1.010767
C	4.962066	-1.271301	0.817838
H	3.647075	0.413309	0.980446
C	5.125740	-2.568512	0.339867
H	4.192499	-4.201168	-0.701880
H	5.772294	-0.782362	1.346352
H	6.062420	-3.091430	0.492603
N	1.923009	3.599502	-0.234663
C	1.291771	4.900393	-0.238861
H	1.416336	5.400357	0.728001
H	1.742761	5.530463	-1.010000
H	0.234609	4.773327	-0.446219
C	3.356772	3.570372	-0.033414
H	3.620688	3.807600	1.003176
H	3.736746	2.584832	-0.281897
H	3.823176	4.313096	-0.684821
H	0.265668	-1.767291	-0.598137
C	-0.750791	-3.056838	0.235036
O	-1.686582	-2.408893	0.558762
O	-0.058537	-3.990846	0.083692

TS_{pre}

M05-2X/BS1 SCF energy in gas phase: -1285.377521 a.u.

M05-2X/BS2 SCF energy in THF solution: -1285.689696 a.u.

M05-2X/BS2 Free energy in THF solution: -1285.305796 a.u.

N	2.266344	1.015578	-0.738633
H	1.414131	1.649487	-0.462504
N	2.291068	0.136289	1.376580
H	1.371776	0.572208	1.463675
N	3.698664	-0.761009	-0.263431
C	2.745774	0.122420	0.105553
C	2.619087	1.028213	-2.147293
H	3.435396	1.734884	-2.329845
H	1.740373	1.378633	-2.688492
C	3.022063	-0.369692	-2.587277

H	2.155002	-1.030309	-2.520791
H	3.381703	-0.365447	-3.616389
C	4.118196	-0.869681	-1.659486
H	4.330923	-1.923599	-1.850498
H	5.044762	-0.306130	-1.812857
C	4.248591	-1.759965	0.649510
H	5.316696	-1.847998	0.436381
H	3.783960	-2.730460	0.442051
C	4.023321	-1.366787	2.100260
H	4.280296	-2.205492	2.747381
H	4.658920	-0.518505	2.361290
C	2.566712	-0.971741	2.275546
H	1.905487	-1.819668	2.064753
H	2.372526	-0.632409	3.291979
O	-0.433250	0.758929	0.973402
O	0.240458	2.504802	-0.324184
C	-0.709961	1.944509	0.289204
C	-2.845120	2.037589	1.418745
H	-3.476480	1.635748	0.615634
H	-3.427277	2.746174	2.008811
H	-2.528963	1.219017	2.059508
N	-1.684939	2.726284	0.885948
C	-2.019186	3.920768	0.130217
H	-2.586003	3.667489	-0.777290
H	-2.626584	4.575539	0.755541
H	-1.103366	4.428311	-0.155952
Si	-0.955431	-0.420091	-0.194763
H	-0.175625	-0.483468	-1.476441
H	-1.562746	1.128871	-0.783768
H	-0.282135	-1.562553	0.574865
C	-2.699252	-1.158560	-0.282691
C	-3.710809	-0.618151	-1.086981
C	-2.988364	-2.324276	0.435522
C	-4.961738	-1.219351	-1.175004
H	-3.507383	0.290627	-1.643479
C	-4.243239	-2.926167	0.364899
H	-2.217764	-2.764789	1.058558
C	-5.231520	-2.374651	-0.443566
H	-5.727863	-0.788271	-1.808587
H	-4.448524	-3.823221	0.937088
H	-6.208154	-2.840088	-0.503882

IM4

M05-2X/BS1 SCF energy in gas phase: -1474.038004 a.u.

M05-2X/BS2 SCF energy in THF solution: -1474.408407 a.u.

M05-2X/BS2 Free energy in THF solution: - 1474.005307 a.u.

O	0.126496	2.511620	0.217228
O	2.003752	1.265759	0.082536
C	1.375823	2.398599	0.147243
N	-2.134116	1.258179	-0.993596
H	-1.284660	1.803613	-0.850362
N	-2.073273	1.016819	1.282503
H	-1.229510	1.584479	1.221594
N	-3.537617	-0.293747	0.038190
C	-2.580249	0.634140	0.109450
C	-2.438867	0.736145	-2.314984
H	-1.795363	-0.116809	-2.555622
H	-2.247341	1.526290	-3.039244
C	-3.902138	0.320928	-2.323768
H	-4.523950	1.200325	-2.144127
H	-4.176043	-0.105574	-3.288731
C	-4.122662	-0.719441	-1.236521
H	-5.190445	-0.874242	-1.064410
H	-3.667841	-1.675608	-1.506035
C	-3.885151	-1.137689	1.186781
H	-3.950332	-2.157997	0.807200
H	-4.863931	-0.826702	1.566134
C	-2.816449	-1.075117	2.266023
H	-3.195159	-1.544004	3.174659
H	-1.936175	-1.613205	1.915665
C	-2.439298	0.373768	2.536357
H	-3.267116	0.915905	3.004007
H	-1.574243	0.431129	3.194997
Si	0.993106	-0.305246	0.199283
H	0.592823	0.074682	1.580320
H	0.328632	0.066181	-1.086314
C	2.497365	-1.429835	0.011122
C	2.460247	-2.756398	0.461877
C	3.681035	-0.981361	-0.591347
C	3.560271	-3.599077	0.325776
H	1.556840	-3.132196	0.925846
C	4.778815	-1.823132	-0.744949
H	3.739452	0.040403	-0.944133
C	4.722104	-3.134776	-0.282598
H	3.507847	-4.618121	0.690167
H	5.679630	-1.455149	-1.221802

H	5.577320	-3.790351	-0.396099
N	2.163989	3.508090	0.145393
C	1.576984	4.829723	0.119224
H	1.998315	5.441655	0.921381
H	1.781181	5.326521	-0.834989
H	0.504783	4.737039	0.256543
C	3.604616	3.433285	0.018803
H	4.065902	4.115193	0.737459
H	3.932589	2.419625	0.223241
H	3.927403	3.723325	-0.986676
H	-0.259441	-2.189660	-1.570534
C	-0.828503	-2.273728	-0.626150
O	-1.889741	-2.876584	-0.593266
O	-0.281907	-1.680156	0.393308

[Si]H_2(OCHO)

M05-2X/BS1 SCF energy in gas phase: -711.473028 a.u.
M05-2X/BS2 SCF energy in THF solution: -711.625526 a.u.
M05-2X/BS2 SCF energy in Acetonitrile solution: -711.626726 a.u.
M05-2X/BS2 Free energy in THF solution: -711.527448 a.u.
M05-2X/BS2 Free energy in Acetonitrile solution: -711.528648 a.u.

C	-3.245885	0.635531	-0.394171
O	-3.894557	-0.273351	0.054297
O	-1.910203	0.680090	-0.378066
H	-3.675395	1.526050	-0.866530
C	0.711210	-0.230726	0.134753
C	1.183014	1.079089	0.290073
C	1.629721	-1.242336	-0.167564
C	2.536319	1.367462	0.152445
H	0.486266	1.880686	0.508208
C	2.985934	-0.958446	-0.300950
H	1.284991	-2.261354	-0.308970
C	3.438486	0.347418	-0.140551
H	2.888031	2.384746	0.270722
H	3.684976	-1.751339	-0.535842
H	4.492487	0.571776	-0.248272
Si	-1.089233	-0.641554	0.350510
H	-1.502911	-0.704008	1.771262
H	-1.403886	-1.906651	-0.351768

TS3

M05-2X/BS1 SCF energy in gas phase: -923.030446 a.u.
M05-2X/BS2 SCF energy in THF solution: -923.256163 a.u.
M05-2X/BS2 SCF energy in Acetonitrile solution: -923.259516 a.u.
M05-2X/BS2 Free energy in THF solution: -923.046962 a.u.
M05-2X/BS2 Free energy in Acetonitrile solution: -923.050315 a.u.

Si	0.400074	1.081140	-0.629134
C	2.059856	0.327877	-0.207966
C	3.065230	1.116341	0.362854
C	2.340758	-1.019458	-0.466399
C	4.316848	0.583180	0.656988
H	2.866481	2.158505	0.592183
C	3.588266	-1.559880	-0.170162
H	1.569528	-1.650524	-0.893245
C	4.579031	-0.757295	0.389534
H	5.082657	1.208416	1.099562
H	3.788821	-2.604831	-0.373968
H	5.550727	-1.176635	0.620586
O	-2.343278	1.280713	-0.829595
C	-2.000598	-0.009137	-0.810048
H	-2.246539	-0.542197	-1.740962
O	-0.650427	-0.231019	-0.496754
N	-2.789604	-0.715292	0.310474
H	-2.691020	0.122153	1.137494
C	-4.207337	-0.779164	-0.077810
H	-4.800920	-1.116541	0.771009
H	-4.516591	0.216970	-0.384894
H	-4.336258	-1.475010	-0.909985
O	-2.479742	1.377447	1.548040
H	-3.234302	1.836525	1.925126
H	-2.404994	1.562689	0.358347
C	-2.254530	-2.034943	0.670714
H	-2.249258	-2.684147	-0.208524
H	-1.241118	-1.917039	1.038687
H	-2.888825	-2.474210	1.440139
H	0.389828	1.598592	-2.022038
H	0.150402	2.186122	0.325272

IM5

M05-2X/BS1 SCF energy in gas phase: -846.626127 a.u.

M05-2X/BS2 SCF energy in THF solution: -846.813972 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -846.816345 a.u.

M05-2X/BS2 Free energy in THF solution: -846.622743 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -846.625116 a.u.

Si	-0.241340	-1.280954	-0.206176
C	-1.867527	-0.380755	-0.072085
C	-3.038113	-1.066579	0.271140
C	-1.950525	0.991085	-0.338651
C	-4.261368	-0.406281	0.334363
H	-2.995997	-2.126717	0.500299
C	-3.170492	1.656783	-0.271997
H	-1.050152	1.540410	-0.589191
C	-4.327230	0.957246	0.061698
H	-5.158633	-0.950621	0.601712
H	-3.219912	2.719081	-0.477440
H	-5.277305	1.474651	0.114067
O	2.641555	-1.659545	0.040394
C	2.248026	-0.354653	-0.272873
H	2.317751	-0.283663	-1.370727
O	0.925088	-0.124049	0.125418
N	3.099023	0.587305	0.407326
C	4.456383	0.512113	-0.122046
H	5.112738	1.126346	0.494517
H	4.807283	-0.517135	-0.092795
H	4.518902	0.873543	-1.160937
H	2.755956	-1.664659	1.000749
C	2.600328	1.955452	0.333405
H	2.533715	2.320319	-0.704152
H	1.619104	2.017243	0.794356
H	3.289798	2.602038	0.877031
H	-0.000169	-1.814768	-1.574681
H	-0.237528	-2.411572	0.758144

TS4

M05-2X/BS1 SCF energy in gas phase: -923.029128 a.u.

M05-2X/BS2 SCF energy in THF solution: -923.251476 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -923.253617 a.u.

M05-2X/BS2 Free energy in THF solution: -923.040853 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -923.042994 a.u.

Si	-0.274931	1.648335	-0.196489
C	-1.863147	0.639289	-0.141087
C	-3.000743	1.113967	0.520113
C	-1.928212	-0.628136	-0.742008
C	-4.168338	0.356027	0.581507
H	-2.973272	2.087939	0.997269
C	-3.089930	-1.392508	-0.678955
H	-1.060489	-1.020408	-1.264091
C	-4.212428	-0.899096	-0.016568
H	-5.039089	0.741711	1.097608
H	-3.124149	-2.367283	-1.150648
H	-5.117859	-1.491813	0.031125
O	1.470885	-1.355007	-0.953642
C	2.133136	-0.240081	-0.875966
H	1.982027	0.490840	-1.664991
O	0.985033	0.797523	0.407862
N	3.309672	-0.169565	-0.244860
C	3.606337	-1.124063	0.812952
H	3.101471	-0.845067	1.741603
H	3.272739	-2.112583	0.508386
H	4.683940	-1.139085	0.971031
H	1.054588	-1.595080	0.032920
C	3.889990	1.152456	-0.082975
H	4.971334	1.061144	0.017535
H	3.665276	1.758612	-0.959850
H	3.465412	1.640447	0.796836
O	0.532385	-1.431465	1.267758
H	-0.417056	-1.599515	1.254569
H	0.650430	-0.384047	1.091261
H	0.012514	2.016321	-1.621938
H	-0.552901	2.912594	0.548332

$TS2_{N2}$

M05-2X/BS1 SCF energy in gas phase: -1665.697076 a.u.

M05-2X/BS2 SCF energy in THF solution: -1666.119262 a.u.

M05-2X/BS2 Free energy in THF solution: -1665.675333 a.u.

O	1.519917	-0.397144	0.479517
O	0.747390	1.704778	0.236577
C	1.687804	0.833583	0.318167
N	-0.584233	-2.091127	1.278971
H	0.124470	-1.355841	1.294135
N	0.156930	-2.436879	-0.858315
H	0.804527	-1.676462	-0.651475
N	-1.735023	-3.567020	-0.113005
C	-0.741644	-2.689661	0.095574
C	-1.640536	-2.109905	2.278572
H	-2.408142	-1.371099	2.031383
H	-1.196652	-1.843435	3.235972
C	-2.219325	-3.516253	2.307076
H	-1.443211	-4.220549	2.613299
H	-3.043862	-3.580895	3.017084
C	-2.730912	-3.863402	0.917531
H	-2.964813	-4.928350	0.845956
H	-3.633818	-3.291190	0.690733
C	-2.100311	-3.997845	-1.464182
H	-3.186856	-3.919990	-1.540104
H	-1.819272	-5.047668	-1.594361
C	-1.446664	-3.122339	-2.521998
H	-1.590165	-3.570541	-3.505170
H	-1.911513	-2.135508	-2.507193
C	0.032887	-2.979185	-2.199202
H	0.540206	-3.946529	-2.271302
H	0.521592	-2.287682	-2.883208
Si	-1.104310	1.201724	0.378345
H	-0.916917	0.299541	-0.802769
H	-0.819800	0.705163	1.764189
C	-1.639666	3.001971	0.124593
C	-2.942802	3.379658	0.474740
C	-0.801353	3.990041	-0.412100
C	-3.387989	4.689212	0.315161
H	-3.622210	2.633266	0.867456
C	-1.245076	5.297382	-0.589207
H	0.209416	3.728410	-0.693743
C	-2.539421	5.652434	-0.220282
H	-4.399274	4.953650	0.600242
H	-0.579167	6.040397	-1.012523
H	-2.884581	6.670917	-0.353105
N	2.962023	1.354152	0.211320
H	-2.640688	0.697546	0.530596
C	-3.874275	-0.130420	-0.503306
O	-3.418654	-1.223414	-0.554503
O	-4.625367	0.751841	-0.685679
C	4.108632	0.525328	0.133287
C	5.121390	0.842515	-0.775808
C	4.275376	-0.575599	0.980262
C	6.279554	0.073556	-0.838621
H	5.000839	1.684885	-1.444515
C	5.429815	-1.343190	0.901026
H	3.495857	-0.820102	1.684488
C	6.440112	-1.025590	-0.003792
H	7.053146	0.335980	-1.549712
H	5.545159	-2.191291	1.564903
H	7.340218	-1.625021	-0.053086
C	3.110607	2.783540	-0.039799
H	2.975787	3.033127	-1.096354
H	2.362787	3.319569	0.537135
H	4.105876	3.088220	0.277974

$TS3_{N2}$

M05-2X/BS1 SCF energy in gas phase: -1114.75514 a.u.

M05-2X/BS2 SCF energy in THF solution: -1115.026832 a.u.

M05-2X/BS2 Free energy in THF solution: -1114.766598 a.u.

Si	-1.187145	-1.825274	-0.370443
C	-2.554018	-0.559342	-0.195283
C	-2.302335	0.810376	-0.335629
C	-3.861638	-0.970836	0.089776
C	-3.330177	1.740271	-0.197303
H	-1.294569	1.145646	-0.551409
C	-4.891441	-0.046039	0.226168
H	-4.083845	-2.027081	0.210036
C	-4.624747	1.313372	0.082048
H	-3.120094	2.797260	-0.308699
H	-5.897495	-0.382010	0.445680
H	-5.424315	2.036516	0.188238
O	1.471909	-2.738853	-0.442364
C	1.409681	-1.469401	-0.828458
H	1.751791	-1.295326	-1.857980
O	0.167800	-0.866397	-0.641428
N	2.394780	-0.635086	0.077251

H	2.134546	-1.158259	1.091114
O	1.605947	-2.131389	1.857851
H	2.208309	-2.622120	2.422328
H	1.474447	-2.651356	0.783577
H	-1.444336	-2.712917	-1.535072
H	-1.115356	-2.644821	0.861457
C	3.778697	-1.019382	-0.255683
H	4.468885	-0.473822	0.384748
H	3.861942	-2.091011	-0.091036
H	4.001787	-0.808113	-1.301720
C	2.134702	0.786026	0.102378
C	2.649056	1.637878	-0.869007
C	1.318202	1.274997	1.118677
C	2.345859	2.995712	-0.814756
H	3.274418	1.256576	-1.665667
C	1.019358	2.631241	1.163631
H	0.919408	0.583516	1.850995
C	1.533642	3.494276	0.198323
H	2.743989	3.662047	-1.569298
H	0.381434	3.012026	1.950822
H	1.301315	4.550905	0.235561

$TS4_{N2}$

M05-2X/BS1 SCF energy in gas phase: -1114.756043 a.u.

M05-2X/BS2 SCF energy in THF solution: -1115.027245 a.u.

M05-2X/BS2 Free energy in THF solution: -1114.767391 a.u.

Si	0.072445	-1.495729	-1.676490
C	1.620539	-1.215968	-0.649526
C	2.216192	-2.270863	0.054595
C	2.185511	0.060398	-0.528620
C	3.333989	-2.060840	0.857012
H	1.802664	-3.270666	-0.029909
C	3.302072	0.278321	0.273847
H	1.744205	0.895535	-1.062941
C	3.877309	-0.783181	0.966996
H	3.782482	-2.889059	1.392190
H	3.721865	1.273902	0.356433
H	4.748267	-0.616508	1.589463
O	-2.010728	-1.588877	1.635142
C	-1.307014	-0.637566	1.107530
H	-0.226397	-0.674234	1.212978
O	-1.283991	-1.250148	-0.796828
N	-1.824029	0.594268	0.944538
H	-2.753672	-1.963504	0.929081
C	-3.261125	0.714514	0.715461
H	-3.532872	1.764762	0.789558
H	-3.536121	0.319735	-0.264760
H	-3.782296	0.145001	1.482181
O	-3.359422	-2.314282	-0.231164
H	-3.367533	-3.268509	-0.348595
H	-2.472783	-1.924084	-0.700955
H	0.148540	-0.566089	-2.844865
H	0.152966	-2.902190	-2.183875
C	-0.959903	1.595304	0.404871
C	0.016032	2.158056	1.222387
C	-1.092449	2.000930	-0.922154
C	0.864225	3.135538	0.711227
H	0.095591	1.829398	2.251101
C	-0.250071	2.988815	-1.422414
H	-1.832218	1.526174	-1.553166
C	0.727847	3.557372	-0.608459
H	1.623534	3.572453	1.347399
H	-0.350011	3.305265	-2.452838
H	1.381953	4.324437	-1.003096

$TS2_{N3}$

M05-2X/BS1 SCF energy in gas phase: -1857.425921 a.u.

M05-2X/BS2 SCF energy in THF solution: -1857.894872 a.u.

M05-2X/BS2 Free energy in THF solution: -1857.404668 a.u.

O	-0.111995	-1.400709	-0.577434
O	-1.042049	0.647463	-0.554907
C	-1.085046	-0.624492	-0.452490
N	2.585992	-1.164252	-1.309110
H	1.566411	-1.101436	-1.341935
N	2.237406	-1.956252	0.809976
H	1.248184	-1.861102	0.582895
N	4.407915	-1.507755	0.107348
C	3.085275	-1.521567	-0.124255
C	3.395950	-0.472434	-2.299047
H	3.457514	0.593005	-2.061409
H	2.906826	-0.583983	-3.265037
C	4.775047	-1.114050	-2.298468

H	4.690012	-2.158451	-2.605399
H	5.439133	-0.602224	-2.995006
C	5.355190	-1.022825	-0.896166
H	6.258209	-1.631966	-0.810584
H	5.608400	0.013044	-0.655668
C	4.948292	-1.603998	1.465476
H	5.687198	-0.806814	1.572274
H	5.459969	-2.564716	1.579113
C	3.858634	-1.440460	2.514056
H	4.253886	-1.708194	3.493986
H	3.529921	-0.400643	2.533604
C	2.678915	-2.325373	2.141921
H	2.962751	-3.382266	2.175658
H	1.842695	-2.176465	2.822614
Si	0.619784	1.648444	-0.479246
H	0.978888	0.830698	0.725257
H	0.962925	1.123219	-1.838352
C	-0.365338	3.260430	-0.300064
C	0.303945	4.426504	0.097876
C	-1.743305	3.355991	-0.547824
C	-0.373029	5.633116	0.258701
H	1.369669	4.391638	0.286873
C	-2.422448	4.561719	-0.396566
H	-2.290642	2.476990	-0.855967
C	-1.740133	5.704162	0.011256
H	0.169310	6.516502	0.574533
H	-3.487275	4.603467	-0.595076
H	-2.268851	6.642259	0.133096
N	-2.341212	-1.155433	-0.177277
H	2.041324	2.414255	-0.396933
C	3.555069	2.442743	0.619460
O	3.895916	1.312087	0.536724
O	3.574284	3.573508	0.930998
C	-2.547335	-2.562989	-0.101853
C	-3.321006	-3.074932	0.941005
C	-2.028549	-3.428498	-1.066390
C	-3.571878	-4.440058	1.019684
H	-3.727265	-2.394846	1.679148
C	-2.274061	-4.793447	-0.972231
H	-1.428337	-3.027496	-1.869557
C	-3.046792	-5.306693	0.065894
H	-4.175783	-4.824864	1.832023
H	-1.866930	-5.458240	-1.724111
H	-3.240727	-6.369943	0.128470
C	-3.467213	-0.303256	0.045090
C	-4.637346	-0.532278	-0.678064
C	-3.420639	0.723997	0.986259
C	-5.754330	0.266915	-0.463635
H	-4.660324	-1.338121	-1.401240
C	-4.535611	1.531743	1.181649
H	-2.504663	0.907092	1.530566
C	-5.706108	1.304988	0.462821
H	-6.659321	0.083547	-1.029193
H	-4.483631	2.341923	1.898102
H	-6.573298	1.933243	0.622536

$TS3_{N3}$

M05-2X/BS1 SCF energy in gas phase: -1306.482079 a.u.

M05-2X/BS2 SCF energy in THF solution: -1306.795357 a.u.

M05-2X/BS2 Free energy in THF solution: -1306.486694 a.u.

Si	-1.716707	-1.863659	0.127804
C	-3.261961	-0.861825	-0.178856
C	-4.524270	-1.464648	-0.153026
C	-3.185364	0.517395	-0.407224
C	-5.680970	-0.712719	-0.337655
H	-4.608673	-2.535435	0.004422
C	-4.338797	1.272891	-0.593698
H	-2.215951	0.999527	-0.449694
C	-5.587878	0.658811	-0.557155
H	-6.650656	-1.194851	-0.316813
H	-4.261827	2.339164	-0.770770
H	-6.486578	1.245594	-0.704264
O	0.982432	-2.547779	0.003308
C	0.784389	-1.398844	-0.624164
H	1.270505	-1.314043	-1.602129
O	-0.538834	-1.023517	-0.742519
N	1.516731	-0.206272	0.241265
H	1.540200	-0.762845	1.303581
O	1.430146	-1.715173	2.184333
H	2.284546	-1.987059	2.532441
H	1.183062	-2.318787	1.212529
H	-1.933294	-3.244374	-0.369725
H	-1.381294	-1.894669	1.573449
C	2.912552	-0.048057	-0.133935
C	3.545534	1.193693	-0.089962
C	3.643579	-1.193663	-0.460075

C	4.898211	1.288942	-0.402089
H	2.992781	2.079250	0.189311
C	4.993859	-1.080640	-0.774214
H	3.154372	-2.159129	-0.458796
C	5.627144	0.157375	-0.751074
H	5.380451	2.257636	-0.367277
H	5.550684	-1.972013	-1.034199
H	6.678301	0.239020	-0.995693
C	0.736267	1.006736	0.329317
C	0.561397	1.826068	-0.784228
C	0.130758	1.314811	1.541561
C	-0.208793	2.976453	-0.670100
H	1.026205	1.557821	-1.725016
C	-0.646766	2.466886	1.645757
H	0.262992	0.647934	2.385319
C	-0.811654	3.300924	0.545782
H	-0.346111	3.616697	-1.532215
H	-1.123106	2.706756	2.587425
H	-1.413199	4.197152	0.629257

$TS4_{N3}$

M05-2X/BS1 SCF energy in gas phase: -1306.482568 a.u.

M05-2X/BS2 SCF energy in THF solution: -1306.796567 a.u.

M05-2X/BS2 Free energy in THF solution: -1306.487886 a.u.

Si	1.883107	-1.758255	0.369702
C	3.506465	-0.841378	0.121737
C	4.579999	-1.027783	0.999389
C	3.667961	0.065024	-0.938763
C	5.777740	-0.336465	0.830174
H	4.478482	-1.719823	1.828656
C	4.860126	0.763567	-1.108345
H	2.850686	0.227698	-1.634786
C	5.917466	0.561406	-0.223074
H	6.597341	-0.495307	1.520297
H	4.968344	1.458561	-1.932303
H	6.846476	1.102210	-0.355511
O	0.357290	0.757042	-1.550610
C	-0.378961	-0.214481	-1.130593
H	-0.253239	-1.194400	-1.582722
O	0.620270	-0.722727	0.521046
N	-1.615418	0.018531	-0.631667
H	0.739553	1.373221	-0.655313
O	1.200033	1.630580	0.502790
H	2.161146	1.702350	0.447483
H	0.991998	0.601067	0.741154
H	1.638746	-2.648829	-0.811991
H	2.070369	-2.632549	1.565162
C	-1.935702	1.322854	-0.124505
C	-2.045622	1.498178	1.251540
C	-2.129915	2.383510	-1.002755
C	-2.367390	2.753662	1.752715
H	-1.864267	0.652980	1.903901
C	-2.442193	3.639079	-0.491217
H	-2.025292	2.216451	-2.066517
C	-2.565326	3.823439	0.882918
H	-2.452597	2.899807	2.821875
H	-2.592380	4.471305	-1.166987
H	-2.811774	4.801373	1.276609
C	-2.496724	-1.061260	-0.337168
C	-3.872767	-0.839030	-0.429331
C	-2.012138	-2.320892	0.012103
C	-4.756897	-1.880574	-0.185161
H	-4.236217	0.145425	-0.694394
C	-2.910433	-3.361048	0.236185
H	-0.950556	-2.467981	0.142960
C	-4.280527	-3.149004	0.140688
H	-5.822135	-1.701819	-0.259308
H	-2.529308	-4.337668	0.506480
H	-4.972669	-3.960202	0.326081

1b

M05-2X/BS1 SCF energy in gas phase: -248.470865 a.u.

M05-2X/BS2 SCF energy in THF solution: -248.553093 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -248.554519 a.u.

M05-2X/BS2 Free energy in THF solution: -248.47778 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -248.479206 a.u.

C	-0.855572	-0.652385	-0.000060
O	-1.939889	-0.102327	0.000117
C	1.593428	-0.745852	0.000118
H	2.184173	-0.501649	0.887340

H	1.393686	-1.817236	-0.000067
H	2.184909	-0.501416	-0.886520
H	-0.746998	-1.750243	-0.000033
N	0.344817	-0.020865	-0.000379
C	0.403557	1.425509	0.000037
H	-0.616856	1.799173	-0.000813
H	0.928148	1.786040	0.888919
H	0.929855	1.786372	-0.887678

[Si]H_2OH

M05-2X/BS1 SCF energy in gas phase: -598.151459 a.u.
M05-2X/BS2 SCF energy in THF solution: -598.27126 a.u.
M05-2X/BS2 SCF energy in Acetonitrile solution: -598.273074 a.u.
M05-2X/BS2 Free energy in THF solution: -598.180578 a.u.
M05-2X/BS2 Free energy in Acetonitrile solution: -598.182392 a.u.

Si	1.923188	0.473136	-0.250987
C	0.081358	0.192388	-0.109019
C	-0.801873	1.258347	0.095962
C	-0.445965	-1.101886	-0.207608
C	-2.174106	1.042666	0.185182
H	-0.414405	2.267208	0.193634
C	-1.816027	-1.323841	-0.114034
H	0.224083	-1.942735	-0.353512
C	-2.680868	-0.249524	0.079786
H	-2.845642	1.877538	0.343285
H	-2.209673	-2.329845	-0.191412
H	-3.747921	-0.420259	0.153184
O	2.747211	-0.782435	0.463235
H	2.504125	-1.005475	1.364243
H	2.393282	0.485582	-1.656570
H	2.218714	1.794660	0.373483

[TBD]H^+

M05-2X/BS1 SCF energy in gas phase: -439.202751 a.u.
M05-2X/BS2 SCF energy in THF solution: -439.389055 a.u.
M05-2X/BS2 SCF energy in Acetonitrile solution: -439.39772 a.u.
M05-2X/BS2 Free energy in THF solution: -439.199676 a.u.
M05-2X/BS2 Free energy in Acetonitrile solution: -439.208341 a.u.

N	1.146949	-1.362799	-0.118441
H	1.096470	-2.366835	-0.146502
N	-1.146940	-1.362811	0.118403
H	-1.096462	-2.366843	0.146416
N	-0.000006	0.652108	0.000009
C	0.000002	-0.679600	-0.000012
C	2.446954	-0.719515	-0.311258
H	2.642494	-0.577572	-1.376872
H	3.208496	-1.381739	0.095354
C	2.428389	0.612182	0.420869
H	2.347834	0.439285	1.495432
H	3.351302	1.158163	0.230093
C	1.245112	1.431436	-0.066174
H	1.102823	2.310143	0.564005
H	1.395517	1.770080	-1.094807
C	-1.245125	1.431440	0.066140
H	-1.102837	2.310105	-0.564099
H	-1.395523	1.770154	1.094750
C	-2.428410	0.612162	-0.420844
H	-3.351321	1.158138	-0.230044
H	-2.347896	0.439241	-1.495406
C	-2.446927	-0.719522	0.311309
H	-2.642382	-0.577555	1.376936
H	-3.208504	-1.381753	-0.095226

[N_1]CO_2^-

M05-2X/BS1 SCF energy in gas phase: -323.127987 a.u.
M05-2X/BS2 SCF energy in THF solution: -323.326049 a.u.
M05-2X/BS2 SCF energy in Acetonitrile solution: -323.338377 a.u.
M05-2X/BS2 Free energy in THF solution: -323.260032 a.u.
M05-2X/BS2 Free energy in Acetonitrile solution: -323.27236 a.u.

O	-1.410671	1.133125	0.038871
O	-1.410856	-1.133115	0.038422
C	-0.888840	-0.000013	-0.034171

C	1.270755	1.204943	0.052801
H	2.183953	1.293129	-0.552941
H	1.580841	1.249857	1.114670
H	0.605415	2.040745	-0.144750
N	0.559182	-0.000059	-0.269195
C	1.270902	-1.204927	0.053164
H	2.184085	-1.293288	-0.552604
H	1.581286	-1.249424	1.115002
H	0.605468	-2.040705	-0.144118

IM7$^-$

M05-2X/BS1 SCF energy in gas phase: -846.04775 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -846.316561 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -846.143328 a.u.

O	2.777794	-1.528801	0.126434
O	0.928568	-0.236878	-0.022795
C	2.202558	-0.453127	-0.036854
C	4.367660	0.665633	0.024909
H	4.571866	1.029752	1.044439
H	4.934822	1.290755	-0.673425
H	4.697333	-0.366477	-0.049365
N	2.964348	0.706460	-0.298231
C	2.341732	2.003406	-0.208041
H	2.284122	2.375669	0.827181
H	2.923724	2.724908	-0.791076
H	1.334832	1.943795	-0.610279
Si	-0.321792	-1.769849	0.111135
H	-1.331212	-2.966705	0.184713
H	0.291558	-2.048370	1.447114
H	0.277264	-2.225473	-1.185333
C	-1.754135	-0.475769	0.055960
C	-1.606148	0.887668	0.352818
C	-3.045659	-0.910885	-0.269902
C	-2.687253	1.766492	0.326766
H	-0.620246	1.251898	0.607211
C	-4.131602	-0.038532	-0.320749
H	-3.193422	-1.964219	-0.481152
C	-3.956396	1.308228	-0.017299
H	-2.538213	2.813197	0.571538
H	-5.114958	-0.411207	-0.588445
H	-4.798264	1.991901	-0.046147

TS5$^-$

M05-2X/BS1 SCF energy in gas phase: -1034.605182 a.u.

M05-2X/BS2 SCF energy in THF solution: -1034.924214 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1034.932922 a.u.

M05-2X/BS2 Free energy in THF solution: -1034.747399 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1034.756176 a.u.

O	-2.529219	-1.859975	-0.252380
O	-1.317748	0.034694	-0.029090
C	-2.416725	-0.663615	-0.003114
C	-4.839305	-0.478966	0.141501
H	-5.268495	-0.143000	-0.814492
H	-5.527985	-0.186615	0.941044
H	-4.735971	-1.559723	0.118779
N	-3.535897	0.087972	0.378523
C	-3.471226	1.528303	0.420329
H	-3.670293	1.986487	-0.560465
H	-4.222041	1.902300	1.123531
H	-2.483663	1.833294	0.752691
Si	0.355273	-0.803909	-0.355049
H	1.809284	-1.464865	-0.622750
H	-0.108984	-1.246156	-1.703933
H	0.172059	-1.641389	0.872235
C	1.195618	0.916496	-0.185953
C	0.531006	2.127250	-0.428349
C	2.550379	0.991762	0.164533
C	1.187334	3.352966	-0.334639
H	-0.517703	2.098050	-0.694274
C	3.208862	2.213628	0.286835
H	3.092930	0.069992	0.342502
C	2.529648	3.401517	0.030693
H	0.648772	4.271935	-0.541359
H	4.254892	2.237469	0.573580
H	3.041166	4.354499	0.113196
C	2.712277	-2.965190	0.134705
O	3.465994	-2.394101	0.836802
O	2.151759	-3.832900	-0.422646

IM8$^-$

M05-2X/BS1 SCF energy in gas phase:

-1034.670919 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1034.999074 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1034.812434 a.u.

O	-2.650444	-1.788414	0.120434
O	-1.335134	0.045149	0.119257
C	-2.485069	-0.572126	0.119666
C	-4.881033	-0.245628	-0.144191
H	-5.163255	-0.096653	-1.196719
H	-5.638134	0.239585	0.480297
H	-4.855491	-1.310731	0.066261
N	-3.577262	0.296374	0.145800
C	-3.406044	1.708737	-0.092924
H	-3.438093	1.959281	-1.163593
H	-4.211434	2.257430	0.404919
H	-2.450555	2.028341	0.311706
Si	0.240091	-0.970554	0.241699
H	1.917923	-2.349583	-1.566340
H	-0.079973	-1.625687	-1.059784
H	-0.160734	-1.436283	1.591863
C	1.277427	0.637171	0.121746
C	0.770647	1.808051	-0.461593
C	2.593522	0.686404	0.604759
C	1.535780	2.967260	-0.564179
H	-0.243020	1.801926	-0.840130
C	3.359812	1.847632	0.524351
H	3.021512	-0.205895	1.043746
C	2.834796	2.993572	-0.064503
H	1.115850	3.852201	-1.030360
H	4.371353	1.852849	0.915278
H	3.431705	3.896433	-0.135803
C	2.415436	-2.520418	-0.591100
O	1.756164	-2.043447	0.426296
O	3.475695	-3.115038	-0.533227

TS6$^-$

M05-2X/BS1 SCF energy in gas phase: -1169.786994 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1170.152505 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1169.880725 a.u.

C	-0.342113	1.623908	-0.927355
O	0.011807	2.772008	-1.194872
O	0.643583	0.659064	-0.786219
C	-0.306468	0.775152	1.969145
H	-0.624030	0.924756	3.010997
H	-0.514586	-0.256143	1.694236
H	0.767053	0.984946	1.908250
H	-1.974211	1.247793	0.858993
H	-1.307353	1.183124	-1.179699
N	-1.036567	1.631974	1.056856
C	-1.079830	3.023947	1.442640
H	-1.714889	3.566571	0.743507
H	-1.460329	3.162719	2.464047
H	-0.076596	3.454292	1.375616
C	3.244742	-0.180316	-0.309457
C	2.673161	-1.331795	0.246097
C	4.626178	-0.170245	-0.533448
C	3.460553	-2.433236	0.573360
H	1.602087	-1.360600	0.410375
C	5.419088	-1.266637	-0.206755
H	5.091733	0.704671	-0.978249
C	4.834201	-2.401469	0.349591
H	3.000326	-3.316373	1.000280
H	6.487200	-1.239758	-0.389640
H	5.446528	-3.259155	0.603394
O	-3.376588	0.600261	-0.088692
O	-2.627207	-1.140368	1.136224
C	-3.386437	-0.605063	0.300939
C	-5.052988	-0.979799	-1.472311
H	-6.073689	-1.377649	-1.526387
H	-4.520135	-1.310640	-2.379949
H	-5.077189	0.105449	-1.461960
N	-4.409216	-1.425763	-0.264467
C	-4.266742	-2.852764	-0.144839
H	-5.252741	-3.332976	-0.126552
H	-3.699758	-3.290640	-0.983845
H	-3.733712	-3.059835	0.778132
Si	2.182450	1.320128	-0.713866
H	2.689742	1.878675	-1.995118
H	2.357900	2.327691	0.363797

IM9$^-$

M05-2X/BS1 SCF energy in gas phase: -1169.814968 a.u.

M05-2X/BS2 SCF energy in Acetonitrile

solution: -1170.168722 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1169.891912 a.u.

C	0.056579	0.679673	-0.872967
O	0.286079	1.776564	-0.122964
O	1.294648	0.043859	-0.928097
C	-1.062120	-1.502514	-0.980432
H	-1.881731	-2.073100	-0.547860
H	-1.291777	-1.260912	-2.019032
H	-0.112085	-2.033316	-0.932178
H	-2.012862	0.213198	-0.264058
H	-0.358891	0.871431	-1.874982
N	-0.953190	-0.244475	-0.223635
C	-0.635127	-0.502295	1.191269
H	-0.497345	0.459875	1.677455
H	-1.481147	-1.041541	1.613615
H	0.284808	-1.085291	1.256386
C	3.763092	0.299520	0.084632
C	4.102097	-0.724808	-0.810399
C	4.719827	0.632340	1.051033
C	5.334169	-1.374074	-0.751942
H	3.375185	-1.019053	-1.558777
C	5.958737	-0.001833	1.119181
H	4.481989	1.407232	1.775944
C	6.270911	-1.011833	0.212998
H	5.564736	-2.165558	-1.457872
H	6.676546	0.283626	1.881454
H	7.230360	-1.515223	0.262337
O	-3.328882	0.583865	-0.359434
O	-3.704422	-1.352008	0.736705
C	-4.079322	-0.281226	0.220986
C	-5.958429	1.155898	-0.488485
H	-6.726029	1.684367	0.088012
H	-6.420116	0.819361	-1.429053
H	-5.142734	1.833466	-0.718740
N	-5.436220	0.054201	0.278186
C	-6.390824	-0.937470	0.698103
H	-7.161156	-0.479515	1.328801
H	-6.896627	-1.409181	-0.157902
H	-5.859964	-1.700586	1.259056
Si	2.099430	1.315377	0.005128
H	2.601937	2.495813	-0.774125
H	2.103831	1.625053	1.484334

TS7

M05-2X/BS1 SCF energy in gas phase: -1169.802734 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1170.162122 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1557.642756 a.u.

C	0.087730	1.640498	0.712117
O	-0.051052	0.429185	1.409683
O	1.455374	1.792926	0.662572
C	-0.696370	2.817827	-1.223668
H	-1.291117	2.718435	-2.134946
H	-1.197733	3.528476	-0.561847
H	0.290362	3.228465	-1.489381
H	-1.854304	0.112324	0.569311
H	-0.409760	2.466765	1.247656
N	-0.593874	1.527315	-0.572432
C	0.051182	0.564609	-1.456768
H	0.194446	-0.372201	-0.920124
H	-0.611574	0.367852	-2.299719
H	1.028437	0.917038	-1.810619
C	3.064294	-0.423522	0.479653
C	3.651389	0.365055	-0.520884
C	3.553226	-1.725710	0.633696
C	4.682138	-0.120676	-1.322014
H	3.269948	1.369153	-0.660396
C	4.585341	-2.224269	-0.160260
H	3.104692	-2.358671	1.392810
C	5.153898	-1.419736	-1.143283
H	5.117482	0.511234	-2.089389
H	4.941056	-3.239520	-0.017991
H	5.953722	-1.802063	-1.768601
O	-2.781707	-0.143389	0.772331
O	-2.904729	-0.694640	-1.422297
C	-3.413574	-0.547994	-0.324198
C	-5.315264	-0.801494	1.245057
H	-5.392036	-1.823325	1.638247
H	-6.321380	-0.372595	1.215206
H	-4.693447	-0.213906	1.911409
N	-4.750061	-0.785700	-0.085055
C	-5.528036	-1.422065	-1.119825
H	-5.701718	-2.482428	-0.895377
H	-6.500626	-0.929675	-1.213997
H	-4.981817	-1.340560	-2.054596

Si	1.691654	0.244191	1.657571
H	2.314585	0.941687	2.839375
H	1.466370	-1.124255	2.323338

$TS6_{by}^-$

M05-2X/BS1 SCF energy in gas phase: -1557.527988 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1557.937585 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1169.884228 a.u.

O	-4.831085	-1.452945	0.732925
O	-3.312766	0.166059	0.318078
C	-4.526911	-0.306029	0.420861
N	-5.510204	0.650212	0.163329
C	-5.173199	1.903771	-0.468285
H	-5.192234	1.833647	-1.565846
H	-5.898665	2.665886	-0.167070
H	-4.179572	2.208223	-0.154980
Si	-1.847112	-0.956724	0.590027
H	-0.494548	-1.909878	0.754351
H	-2.249272	-1.850948	-0.529314
H	-2.203810	-1.211190	2.019869
C	-0.674028	0.516689	0.293915
C	-0.932314	1.515101	-0.653333
C	0.514299	0.616221	1.028571
C	-0.031201	2.554780	-0.876075
H	-1.853999	1.469713	-1.221125
C	1.406201	1.669971	0.838632
H	0.752891	-0.164200	1.743431
C	1.140135	2.637143	-0.127428
H	-0.244456	3.303686	-1.631567
H	2.321834	1.717695	1.417138
H	1.844661	3.443937	-0.297540
C	0.547176	-2.724867	-0.296232
O	0.150844	-2.618077	-1.452813
O	1.709755	-2.068703	0.075777
H	0.374544	-3.601923	0.332974
C	3.816767	-0.296416	-0.338594
C	4.361730	-0.798280	0.848224
C	4.399939	0.845989	-0.898711
C	5.458188	-0.185341	1.450933
H	3.904124	-1.666063	1.308576
C	5.497879	1.461870	-0.305683
H	3.972512	1.275928	-1.799563
C	6.030402	0.944365	0.872924
H	5.862130	-0.584815	2.374104
H	5.931672	2.348432	-0.753616
H	6.881549	1.424286	1.341877
Si	2.332237	-1.110175	-1.165858
H	2.846551	-1.965783	-2.272550
H	1.480146	-0.036673	-1.719603
C	-6.863049	0.189852	-0.027917
H	-7.102327	0.048442	-1.091990
H	-6.971292	-0.761247	0.484712
H	-7.568826	0.918367	0.383518

$IM10^-$

M05-2X/BS1 SCF energy in gas phase: -1169.813014 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1170.169266 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1169.892434 a.u.

C	-0.094648	1.234619	0.617630
O	-0.321301	-0.012800	-0.079302
O	1.092314	0.940783	1.236866
C	-1.286495	2.570526	-0.950635
H	-1.506639	1.776133	-1.681428
H	-2.094345	2.575592	-0.218118
H	-1.268464	3.529613	-1.476719
H	-1.624563	-0.477035	-0.349789
H	-0.935288	1.408219	1.297544
N	-0.015519	2.361305	-0.279318
C	1.067297	2.239033	-1.239176
H	1.990398	2.016762	-0.708101
H	0.886230	1.443152	-1.977239
H	1.177791	3.186824	-1.773889
C	3.000768	-0.724689	0.237127
C	3.837384	0.308584	0.685835
C	3.597750	-1.757045	-0.494719
C	5.205533	0.304221	0.423909
H	3.386788	1.123145	1.240218
C	4.965663	-1.773772	-0.763549
H	2.967198	-2.560296	-0.862294
C	5.775034	-0.739635	-0.302394
H	5.829783	1.115659	0.783157
H	5.399042	-2.587464	-1.335782

H	6.839587	-0.743580	-0.510929
O	-2.580353	-0.865129	-0.593848
O	-3.369593	0.658980	0.876432
C	-3.528588	-0.275189	0.096585
C	-4.969360	-2.040079	-0.867154
H	-5.867814	-1.977911	-1.489304
H	-5.093804	-2.885274	-0.176507
H	-4.105884	-2.224716	-1.496758
N	-4.786300	-0.795954	-0.157621
C	-5.886212	-0.367724	0.670418
H	-6.784402	-0.233336	0.059260
H	-6.113792	-1.104032	1.453262
H	-5.612942	0.572938	1.138616
Si	1.120121	-0.792730	0.654635
H	0.911920	-1.433659	1.998330
H	0.876964	-2.027746	-0.224294

TS8^{-}

M05-2X/BS1 SCF energy in gas phase: -1169.797452 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1170.155896 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1169.881109 a.u.

C	0.017870	1.471263	-0.695977
O	0.225193	-0.121043	0.225098
O	-1.022962	1.096483	-1.347879
C	1.083598	2.559749	1.127431
H	1.068851	1.788967	1.908728
H	1.983447	2.405080	0.532620
H	1.102659	3.548458	1.593366
H	1.265106	-0.508726	0.417946
H	1.015057	1.431394	-1.138866
N	-0.087015	2.440698	0.275899
C	-1.344932	2.469394	0.996354
H	-2.164264	2.411777	0.285043
H	-1.421595	1.620280	1.687006
H	-1.408455	3.400928	1.563679
C	-2.784274	-0.814942	-0.274677
C	-3.653447	0.164489	-0.778615
C	-3.340863	-1.798780	0.552349
C	-5.011190	0.159250	-0.470344
H	-3.238553	0.938874	-1.410055
C	-4.696642	-1.806356	0.877459
H	-2.692543	-2.572966	0.947602
C	-5.537774	-0.825364	0.362995
H	-5.660928	0.926595	-0.877433
H	-5.094697	-2.577312	1.528323
H	-6.594313	-0.826484	0.608463
O	2.467233	-0.931333	0.637756
O	3.219044	0.790403	-0.619529
C	3.376873	-0.252542	0.036538
C	4.874169	-2.108463	0.663949
H	5.810493	-2.169184	1.229569
H	4.933536	-2.833517	-0.162025
H	4.039916	-2.376382	1.303823
N	4.677162	-0.761568	0.188653
C	5.718197	-0.243707	-0.661670
H	6.672897	-0.236670	-0.124472
H	5.848661	-0.849660	-1.571500
H	5.448444	0.767027	-0.951813
Si	-0.927863	-0.930103	-0.708883
H	-0.658820	-1.217485	-2.148460
H	-0.713425	-2.323490	-0.127377

IM11^{-}

M05-2X/BS1 SCF energy in gas phase: -921.336034 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -921.631971 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -921.455765 a.u.

O	0.112481	-1.335825	-0.451761
H	-0.839660	-1.567213	-0.498032
C	2.310305	0.143945	0.048701
C	3.035312	0.611037	-1.054098
C	3.059709	-0.348621	1.124822
C	4.428494	0.579724	-1.095959
H	2.489035	1.016110	-1.902170
C	4.452376	-0.389040	1.103823
H	2.533526	-0.704516	2.006957
C	5.143989	0.076570	-0.012441
H	4.957564	0.949486	-1.968822
H	5.000783	-0.778079	1.956134
H	6.228370	0.052102	-0.034902
O	-1.691491	0.505032	0.216459
O	-2.569609	-1.483317	-0.398986
C	-2.657444	-0.300191	-0.010775

C	-4.115092	1.642852	0.404128
H	-4.944923	1.829266	1.094608
H	-4.348658	2.147776	-0.545613
H	-3.200436	2.064014	0.807861
N	-3.934946	0.223393	0.231942
C	-5.082833	-0.497458	-0.255287
H	-5.918916	-0.388992	0.444366
H	-5.416352	-0.127390	-1.236890
H	-4.813319	-1.544786	-0.348866
Si	0.359029	0.214296	0.101487
H	0.252797	1.383664	-0.834610
H	0.278463	0.504620	1.572385

TSa

M05-2X/BS1 SCF energy in gas phase: -846.54597 a.u.

M05-2X/BS2 SCF energy in THF solution: -846.751691 a.u.

M05-2X/BS2 Free energy in THF solution: -846.566155 a.u.

C	3.080451	-1.355467	-0.000044
O	3.607473	-2.427037	-0.000299
O	3.300308	-0.149546	0.000176
H	1.721017	-1.555126	0.000040
Si	0.888953	-0.039992	0.000094
H	1.268552	0.068522	-1.428322
H	1.268433	0.068225	1.428572
C	-0.942308	-0.475534	-0.000042
C	-1.646393	-0.630244	1.201323
C	-1.646385	-0.629467	-1.201512
C	-3.008738	-0.916582	1.205608
H	-1.118757	-0.532421	2.144971
C	-3.008734	-0.915791	-1.205993
H	-1.118735	-0.531081	-2.145094
C	-3.690807	-1.057216	-0.000241
H	-3.536174	-1.035424	2.144074
H	-3.536167	-1.034016	-2.144539
H	-4.750174	-1.282743	-0.000316
C	0.082951	2.542330	-1.219081
H	0.091861	3.633851	-1.225715
H	0.610279	2.163616	-2.092008
H	-0.945816	2.184190	-1.241628
H	1.705645	2.293982	0.001043
N	0.724639	2.018363	0.000395
C	0.081485	2.541781	1.219337
H	0.607425	2.162211	2.092733
H	0.090895	3.633293	1.226751
H	-0.947465	2.184079	1.240209

TSb

M05-2X/BS1 SCF energy in gas phase: -1150.205741 a.u.

M05-2X/BS2 SCF energy in THF solution: -1150.489132 a.u.

M05-2X/BS2 Free energy in THF solution: -1150.199388 a.u.

C	-0.775876	-3.785919	-0.066893
O	-1.623702	-4.610729	-0.094168
O	0.382858	-3.471786	-0.053466
H	-1.609792	-2.413464	-0.016521
Si	-0.861895	-0.936687	0.092097
H	-0.241316	-1.236432	-1.221690
H	-0.427196	-1.345596	1.456373
C	-2.390711	0.145842	-0.008181
C	-2.587130	0.996866	-1.103046
C	-3.375807	0.105365	0.983907
C	-3.729307	1.786160	-1.203415
H	-1.834396	1.043826	-1.884330
C	-4.518166	0.895817	0.892412
H	-3.253446	-0.557939	1.833704
C	-4.695751	1.737495	-0.202051
H	-3.867772	2.435063	-2.059877
H	-5.270606	0.851762	1.670471
H	-5.586312	2.349620	-0.276711
N	0.487233	0.590428	0.226165
N	2.191156	-0.921820	-0.198257
H	1.522010	-1.677410	-0.157641
N	2.716287	1.322554	0.086003
C	1.768028	0.342409	0.031950
C	0.165367	1.920106	0.729557
H	0.473682	2.018547	1.778598
H	-0.912669	2.050289	0.683397
C	0.883742	2.961188	-0.116586
H	0.588259	2.825029	-1.158759
H	0.626349	3.977445	0.184158
C	2.378135	2.744113	0.052107
H	2.938626	3.208796	-0.765885
H	2.722812	3.199515	0.986860

C	4.150335	1.064988	0.013900
H	4.641101	1.730722	0.729925
H	4.515878	1.332124	-0.985399
C	4.480636	-0.386298	0.315202
H	5.528908	-0.577423	0.084399
H	4.310291	-0.602761	1.371316
C	3.562882	-1.255698	-0.527593
H	3.765460	-1.097065	-1.592908
H	3.702445	-2.313661	-0.312759

TSc

M05-2X/BS1 SCF energy in gas phase: -1285.36572 a.u.

M05-2X/BS2 SCF energy in THF solution: -1285.684126 a.u.

M05-2X/BS2 Free energy in THF solution: -1285.306679 a.u.

C	-0.975307	3.352180	-0.033461
O	-1.720693	4.275681	-0.009822
O	0.151454	2.932966	-0.067464
H	-1.886464	2.141188	-0.008886
Si	-1.570884	0.517284	-0.019598
H	-0.863596	0.668778	1.280845
H	-0.916893	0.678260	-1.345856
C	-3.378590	0.005149	0.016327
C	-4.102140	-0.164700	-1.171179
C	-4.047053	-0.201426	1.230010
C	-5.442593	-0.539681	-1.148924
H	-3.616258	0.004196	-2.126791
C	-5.387532	-0.576292	1.258187
H	-3.517731	-0.061384	2.167016
C	-6.086809	-0.748786	0.067107
H	-5.984594	-0.663653	-2.078478
H	-5.886416	-0.728916	2.207436
H	-7.130379	-1.038107	0.086602
C	-1.166022	-2.175638	1.173525
H	-0.646340	-3.137613	1.168892
H	-0.841753	-1.602107	2.041364
H	-2.241127	-2.348179	1.239470
N	1.924131	-1.182193	-0.198643
H	0.175841	-1.249089	-0.078948
N	2.345737	1.050007	0.131324
H	1.364471	1.228922	-0.008024
N	4.150378	-0.407232	-0.016064
C	2.788853	-0.221207	-0.029568
C	2.471770	-2.498808	-0.460951
H	2.776067	-2.604150	-1.512678
H	1.689281	-3.241720	-0.283462
C	3.674487	-2.772625	0.435646
H	3.360413	-2.680040	1.477707
H	4.082071	-3.773566	0.284592
C	4.736724	-1.734046	0.116416
H	5.492704	-1.697543	0.908767
H	5.253456	-1.994145	-0.815273
C	5.117095	0.681084	0.030164
H	5.946275	0.418667	-0.634807
H	5.528031	0.766065	1.045095
C	4.493796	2.003435	-0.384331
H	5.194964	2.815178	-0.186462
H	4.263775	1.992721	-1.451538
C	3.205532	2.181031	0.403186
H	3.434796	2.260782	1.473431
H	2.662984	3.076922	0.109360
N	-0.866072	-1.414346	-0.044468
C	-1.239376	-2.161690	-1.251594
H	-0.955229	-1.583050	-2.130005
H	-0.730116	-3.128471	-1.283990
H	-2.318178	-2.322630	-1.261136

TSIV

M05-2X/BS1 SCF energy in gas phase: -954.223935 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -954.513689 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -954.194548 a.u.

C	-1.737165	0.063014	0.185262
C	-1.566351	2.074351	-1.137534
C	-2.700376	1.506426	-1.978666
C	-3.700144	0.844528	-1.044904
H	-1.933845	2.927158	-0.553993
H	-0.766735	2.449923	-1.779980
H	-3.190623	2.292450	-2.554702
H	-2.308024	0.760600	-2.673899
H	-4.189803	1.600072	-0.417026
H	-4.478488	0.329794	-1.612046
N	-3.025198	-0.149246	-0.222639
N	-1.002243	1.064638	-0.259288

C	-3.041520	-2.338597	0.849426
C	-1.872968	-1.878756	1.704219
C	-3.865735	-1.119748	0.465917
H	-2.236321	-1.539859	2.681136
H	-1.171611	-2.694633	1.879315
H	-2.671232	-2.822315	-0.056645
H	-3.657962	-3.051374	1.398115
H	-4.325078	-0.674696	1.357885
H	-4.670218	-1.397716	-0.217626
N	-1.161781	-0.812091	1.026057
H	-0.267019	-0.489475	1.449638
N	1.537458	1.132116	0.184819
H	0.279781	1.085372	-0.011605
C	1.684446	1.124494	1.740330
O	2.412708	1.994796	2.183910
O	1.019602	0.203508	2.244074
C	2.073739	2.367657	-0.414653
H	1.517122	3.214984	-0.018012
H	3.121803	2.487953	-0.146268
H	1.961999	2.310592	-1.498189
C	2.167500	-0.043582	-0.381527
C	3.417444	-0.448500	0.082792
C	1.540068	-0.731861	-1.414485
C	4.033905	-1.555831	-0.487117
H	3.884527	0.103346	0.890549
C	2.166185	-1.838193	-1.982998
H	0.567451	-0.402236	-1.758551
C	3.411499	-2.251603	-1.521496
H	5.001753	-1.876334	-0.122869
H	1.678266	-2.377115	-2.785738
H	3.894964	-3.113631	-1.963390

IMIII

M05-2X/BS1 SCF energy in gas phase: -954.237778 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -954.528099 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -954.204067 a.u.

C	1.222733	-0.605436	0.746576
C	0.998740	-2.672551	-0.607441
C	2.140522	-2.090696	-1.424912
C	3.157191	-1.485060	-0.468929
H	1.335785	-3.567634	-0.075297
H	0.167526	-2.962217	-1.250449
H	2.609143	-2.867768	-2.029321
H	1.759842	-1.307063	-2.083347
H	3.609395	-2.265927	0.153950
H	3.958678	-0.994394	-1.022480
N	2.512832	-0.472173	0.356189
N	0.512174	-1.679610	0.336892
C	2.403233	1.865859	1.021381
C	1.256327	1.503092	1.950371
C	3.300901	0.646613	0.861571
H	1.615879	1.398711	2.978956
H	0.490490	2.279957	1.943352
H	2.004354	2.149616	0.044674
H	2.975213	2.701742	1.425629
H	3.771799	0.386180	1.816242
H	4.093416	0.840313	0.137633
N	0.622494	0.268506	1.521232
H	-0.502092	0.161075	1.732600
N	-2.310057	-0.542469	-0.104677
H	-0.490446	-1.581605	0.453084
C	-2.672471	-0.479666	1.306442
O	-3.698035	-1.039395	1.657937
O	-1.815245	0.121629	2.044672
C	-1.598870	0.489567	-0.743921
C	-0.964240	0.226734	-1.967051
C	-1.519595	1.792180	-0.224773
C	-0.246936	1.217696	-2.631145
H	-1.032349	-0.763385	-2.401070
C	-0.798440	2.772305	-0.893879
H	-2.011976	2.015366	0.710167
C	-0.149285	2.497835	-2.097552
H	0.229772	0.983961	-3.576048
H	-0.759018	3.771336	-0.475072
H	0.401631	3.272114	-2.616275
C	-3.114084	-1.414721	-0.955252
H	-3.888623	-1.840785	-0.325007
H	-3.570201	-0.845953	-1.768425
H	-2.518444	-2.223784	-1.390729

TSV

M05-2X/BS1 SCF energy in gas phase: -954.237578 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -954.528583 a.u.

M05-2X/BS2 Free energy in Acetonitrile

solution: -954.204165 a.u

C	-1.218245	-0.640206	-0.753924
C	-0.765843	-2.661753	0.622180
C	-1.932630	-2.162091	1.459006
C	-3.022967	-1.655523	0.524994
H	-1.018503	-3.618580	0.155666
H	0.117450	-2.814583	1.243724
H	-2.314002	-2.966644	2.088046
H	-1.604827	-1.337551	2.095385
H	-3.404942	-2.470992	-0.100533
H	-3.859736	-1.249893	1.094562
N	-2.488159	-0.576971	-0.293417
N	-0.436169	-1.682268	-0.402124
C	-2.546608	1.760596	-0.971369
C	-1.432087	1.454276	-1.960768
C	-3.365456	0.496892	-0.745331
H	-1.840980	1.313028	-2.966210
H	-0.718644	2.277879	-2.004081
H	-2.109903	2.079116	-0.022304
H	-3.188234	2.556706	-1.350468
H	-3.887278	0.205210	-1.663887
H	-4.114793	0.656047	0.031238
N	-0.701883	0.268715	-1.550022
H	0.411214	0.195363	-1.751892
N	2.397916	-0.408132	0.118394
H	0.535383	-1.572392	-0.660122
C	2.679379	-0.417875	-1.306415
O	3.720548	-0.937055	-1.678438
O	1.750060	0.074835	-2.039092
C	1.592743	0.565577	0.725108
C	0.991462	0.293975	1.963221
C	1.396774	1.838286	0.161284
C	0.200049	1.245594	2.601191
H	1.147493	-0.670780	2.430634
C	0.604766	2.778945	0.805182
H	1.864590	2.068191	-0.784912
C	-0.008002	2.494132	2.026061
H	-0.246848	1.006715	3.559450
H	0.480096	3.756967	0.354186
H	-0.614077	3.238824	2.526225
C	3.274050	-1.190189	0.980435
H	4.087141	-1.550800	0.357798
H	3.670485	-0.569571	1.786870
H	2.757820	-2.047721	1.425909

IMIV

M05-2X/BS1 SCF energy in gas phase: -954.249217 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -954.534565 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -954.207568 a.u

C	-1.727815	0.411865	-0.479369
C	0.029252	2.132877	-0.337805
C	-1.100116	3.082218	0.025542
C	-2.081209	2.361000	0.937514
H	0.661473	1.919889	0.529728
H	0.669511	2.557036	-1.110116
H	-0.706372	3.964338	0.530385
H	-1.619467	3.404229	-0.879372
H	-1.608298	2.124578	1.898501
H	-2.952761	2.986552	1.138519
N	-2.562927	1.138919	0.300364
N	-0.542436	0.899785	-0.855472
C	-4.291404	-0.586036	0.015766
C	-3.172221	-1.545725	-0.352629
C	-3.734926	0.512832	0.909499
H	-2.799163	-2.097913	0.513831
H	-3.507140	-2.273186	-1.090151
H	-4.707014	-0.142947	-0.891347
H	-5.090351	-1.109798	0.541038
H	-3.466060	0.104540	1.891025
H	-4.478426	1.296714	1.065505
N	-2.083546	-0.784568	-0.944324
H	-1.281119	-1.312376	-1.354139
N	1.688998	-1.799462	0.403421
H	0.078954	0.181303	-1.257887
C	0.525620	-2.133578	-0.354747
O	-0.280245	-2.917842	0.159457
O	0.392545	-1.553021	-1.487975
C	2.424811	-0.628028	0.172305
C	2.874709	0.147158	1.254282
C	2.762497	-0.202715	-1.126332
C	3.607620	1.313238	1.046442
H	2.644647	-0.154615	2.266768
C	3.481690	0.969726	-1.318613
H	2.448034	-0.802969	-1.964799
C	3.908720	1.743603	-0.239940

H	3.940121	1.886230	1.904230
H	3.729703	1.270005	-2.330066
H	4.478534	2.649842	-0.401027
C	1.784189	-2.424996	1.711098
H	1.397401	-3.434393	1.623315
H	2.828444	-2.447324	2.023944
H	1.191832	-1.906198	2.474267

TSVI

M05-2X/BS1 SCF energy in gas phase: -954.246401 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -954.529123 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -954.205143 a.u

O	-0.710653	0.370294	-0.466552
O	-0.032942	-1.450974	0.658426
C	-0.913513	-0.659846	0.275939
N	1.648953	1.247007	-0.192363
H	0.577557	0.956437	-0.302092
N	2.003962	-0.781670	-1.176497
H	0.988980	-0.760563	-1.196564
N	3.773223	0.260972	-0.076121
C	2.478197	0.252015	-0.453797
C	2.069149	2.386557	0.598740
H	1.894010	2.201802	1.664597
H	1.464566	3.245396	0.307965
C	3.547413	2.657031	0.352839
H	3.694172	2.943835	-0.690548
H	3.902568	3.469454	0.987242
C	4.340304	1.392231	0.648840
H	5.377535	1.506373	0.326661
H	4.342086	1.182876	1.724786
C	4.569424	-0.955262	-0.204845
H	5.333022	-0.926173	0.574258
H	5.075145	-0.981949	-1.176188
C	3.664055	-2.167032	-0.032413
H	4.240149	-3.088600	-0.117768
H	3.202568	-2.130023	0.956876
C	2.575775	-2.124516	-1.093418
H	2.983594	-2.408639	-2.067021
H	1.764236	-2.802492	-0.832518
N	-2.241817	-0.911855	0.655988
C	-2.488612	-2.152501	1.373184
H	-2.694552	-2.990818	0.698694
H	-1.597597	-2.387921	1.944436
H	-3.340724	-2.018399	2.039847
C	-3.352617	-0.176820	0.193922
C	-3.308151	1.213448	0.009756
C	-4.567371	-0.836632	-0.033279
C	-4.439892	1.901648	-0.403453
H	-2.380394	1.733102	0.180712
C	-5.698029	-0.133919	-0.439083
H	-4.630698	-1.908827	0.092046
C	-5.645009	1.240272	-0.630972
H	-4.379413	2.975043	-0.539640
H	-6.621734	-0.673371	-0.610752
H	-6.523318	1.787659	-0.948835

IM12

M05-2X/BS1 SCF energy in gas phase: -954.257283 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -954.539389 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -954.218668 a.u

O	-0.841490	0.404967	0.148317
O	-0.292034	-1.774627	0.168476
C	-1.126883	-0.824682	0.168970
N	1.646677	1.046381	0.139845
H	0.602064	0.739827	0.146714
N	2.201343	-1.160400	-0.059498
H	1.145862	-1.388718	0.043642
N	3.892779	0.449891	-0.091118
C	2.579297	0.112344	-0.003888
C	1.983769	2.447993	0.267097
H	2.201247	2.709812	1.309575
H	1.114433	3.025240	-0.045548
C	3.193362	2.751120	-0.605443
H	2.936174	2.565403	-1.650133
H	3.503633	3.791571	-0.504199
C	4.333438	1.837691	-0.182020
H	5.148567	1.878935	-0.910020
H	4.737428	2.157223	0.785788
C	4.954045	-0.550753	-0.106303
H	5.771592	-0.176335	0.516247
H	5.338585	-0.659697	-1.127172
C	4.456818	-1.889675	0.416168

H	5.213376	-2.654228	0.236984
H	4.275887	-1.825309	1.490990
C	3.150800	-2.227740	-0.288858
H	3.332324	-2.374572	-1.360473
H	2.715838	-3.146706	0.102223
N	-2.476210	-1.191052	0.192363
C	-2.788967	-2.608947	0.098691
H	-2.847563	-2.956063	-0.938198
H	-2.001217	-3.162506	0.597786
H	-3.744055	-2.793992	0.589573
C	-3.531321	-0.263110	0.064446
C	-3.499120	0.990820	0.690903
C	-4.677391	-0.619215	-0.656721
C	-4.579151	1.855234	0.578652
H	-2.622078	1.274373	1.249168
C	-5.757840	0.252688	-0.754102
H	-4.723197	-1.576517	-1.157933
C	-5.717884	1.497646	-0.140192
H	-4.532669	2.818688	1.072314
H	-6.630791	-0.048531	-1.320751
H	-6.557191	2.177150	-0.216472

$[N_2]CO_2^-$

M05-2X/BS1 SCF energy in gas phase: -514.874367 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -515.118256 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -515.004713 a.u

O	-1.813920	-1.744596	0.000114
O	-3.280070	-0.034444	0.000528
C	-2.150409	-0.550354	0.000160
N	-1.028886	0.450629	-0.000264
C	-1.419932	1.841391	-0.000485
H	-1.045808	2.369403	0.886553
H	-1.045149	2.369220	-0.887331
H	-2.504076	1.848146	-0.000797
C	0.323439	0.170364	-0.000155
C	0.858932	-1.143444	-0.000407
C	1.267194	1.226679	0.000177
C	2.227562	-1.356160	-0.000208
H	0.160425	-1.962370	-0.000736
C	2.638283	0.987664	0.000374
H	0.933443	2.253042	0.000304
C	3.145389	-0.304154	0.000216
H	2.586383	-2.380770	-0.000412
H	3.313057	1.838188	0.000677
H	4.213085	-0.488859	0.000425

IMV^-

M05-2X/BS1 SCF energy in gas phase: -1037.784151 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1038.093603 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1037.871725 a.u

O	1.154845	-1.882081	0.222155
O	-0.547066	-0.418803	0.069351
C	0.688680	-0.761126	0.044465
N	1.560585	0.347328	-0.230002
C	0.953992	1.651746	-0.423589
H	0.903518	2.235391	0.504247
H	1.530895	2.216504	-1.159043
H	-0.055975	1.500155	-0.786460
Si	-1.988319	-1.848989	0.206165
H	-3.110100	-2.927910	0.277393
H	-1.408430	-2.143433	1.549483
H	-1.385466	-2.368912	-1.059806
C	-3.251517	-0.401756	0.088628
C	-2.974588	0.930423	0.430519
C	-4.557779	-0.686993	-0.330166
C	-3.950527	1.922238	0.360424
H	-1.973461	1.181277	0.754251
C	-5.536048	0.300585	-0.428175
H	-4.807804	-1.713268	-0.576210
C	-5.235826	1.613071	-0.077071
H	-3.705841	2.940845	0.643142
H	-6.533633	0.043761	-0.768584
H	-5.994580	2.385692	-0.140647
C	2.951144	0.283061	-0.110317
C	3.680746	-0.912944	-0.269663
C	3.683591	1.459268	0.136560
C	5.064958	-0.909216	-0.181256
H	3.138523	-1.825674	-0.445964
C	5.072669	1.444242	0.216274
H	3.167267	2.395851	0.288809
C	5.782568	0.261735	0.058316
H	5.592818	-1.847468	-0.311421

H	5.596123	2.373655	0.411726
H	6.863910	0.249140	0.121043

TSVII$^-$

M05-2X/BS1 SCF energy in gas phase: -1226.339585 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1226.709079 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1226.481615 a.u

C	-1.134409	0.360119	0.113799
O	-1.354475	1.539709	0.349655
O	0.020178	-0.227379	0.133931
C	3.744891	3.161083	-0.088308
O	3.086285	3.967312	0.458204
O	4.580445	2.698672	-0.781259
H	3.006789	1.612453	0.587030
Si	1.625965	0.793931	0.386764
H	1.291150	1.589638	-0.832606
H	1.164013	1.194674	1.746801
C	2.626874	-0.827941	0.179073
C	2.109747	-2.100234	0.460968
C	3.958403	-0.758585	-0.252863
C	2.885160	-3.249658	0.323555
H	1.082460	-2.183146	0.791387
C	4.733362	-1.904634	-0.417632
H	4.390103	0.214194	-0.460806
C	4.200032	-3.156227	-0.123709
H	2.461107	-4.219589	0.560918
H	5.756481	-1.818807	-0.766990
H	4.803064	-4.050241	-0.240041
N	-2.186795	-0.533456	-0.226757
C	-1.857147	-1.929924	-0.458048
H	-1.921608	-2.533243	0.455415
H	-2.542633	-2.342631	-1.199966
H	-0.840752	-1.983009	-0.830796
C	-3.540555	-0.180649	-0.137897
C	-3.996604	1.137395	-0.328270
C	-4.501634	-1.176562	0.104858
C	-5.352816	1.424234	-0.269831
H	-3.274032	1.915976	-0.503291
C	-5.858421	-0.872028	0.154223
H	-4.190759	-2.197023	0.277431
C	-6.300787	0.430799	-0.031685
H	-5.672114	2.449016	-0.421771
H	-6.568669	-1.667922	0.348142
H	-7.356580	0.669193	0.008086

IM13$^-$

M05-2X/BS1 SCF energy in gas phase: -1226.404474 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1226.775067 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1226.538411 a.u

C	1.163942	0.417658	0.123010
O	1.395543	1.618487	0.091742
O	-0.011657	-0.131664	0.099252
C	-3.649611	2.588043	-0.699515
O	-4.682273	3.227858	-0.655825
O	-3.003694	2.120097	0.333387
H	-3.165786	2.361318	-1.670046
Si	-1.552495	0.977681	0.183014
H	-1.107936	1.458226	1.513181
H	-1.179242	1.566114	-1.134588
C	-2.651707	-0.588293	0.111864
C	-2.208162	-1.791780	-0.456219
C	-3.959222	-0.567191	0.618712
C	-3.027269	-2.916296	-0.521763
H	-1.202214	-1.841112	-0.852358
C	-4.778437	-1.693658	0.576389
H	-4.338810	0.352530	1.045570
C	-4.316390	-2.873197	0.001504
H	-2.657426	-3.828069	-0.978345
H	-5.781669	-1.644941	0.984929
H	-4.954741	-3.748877	-0.041660
N	2.206320	-0.539559	0.194607
C	1.850273	-1.949204	0.201927
H	1.836648	-2.382319	-0.805119
H	2.570235	-2.498454	0.810553
H	0.859732	-2.048094	0.630495
C	3.561689	-0.201217	0.062095
C	4.073338	1.055164	0.436753
C	4.468102	-1.159789	-0.420908
C	5.430581	1.320295	0.322466
H	3.392467	1.807162	0.797048
C	5.826934	-0.878845	-0.522752
H	4.112606	-2.129021	-0.739680

C	6.324864	0.363308	-0.153030
H	5.793535	2.297243	0.620484
H	6.494211	-1.643930	-0.903037
H	7.382182	0.583402	-0.233517

TS9$^-$

M05-2X/BS1 SCF energy in gas phase: -1749.260739 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1749.713536 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1749.371967 a.u

O	-2.681110	-0.024727	-1.119693
O	-2.059127	1.339186	0.558762
C	-2.909015	0.591926	-0.091251
N	-4.175601	0.550668	0.537037
C	-4.417639	1.409312	1.685856
H	-4.844265	2.376951	1.399357
H	-5.105923	0.908894	2.368859
H	-3.471370	1.587934	2.181800
Si	-0.303745	1.584522	-0.062514
H	1.228727	1.916662	-0.573452
H	-0.140403	2.659713	0.958794
H	-0.782789	1.963011	-1.427053
C	0.256562	-0.184203	0.395936
C	-0.438816	-0.983529	1.312609
C	1.440733	-0.706655	-0.140954
C	0.028791	-2.242376	1.681539
H	-1.357979	-0.610472	1.747704
C	1.914992	-1.967706	0.215625
H	2.007766	-0.106606	-0.844257
C	1.207695	-2.739521	1.132586
H	-0.528339	-2.835535	2.398534
H	2.841324	-2.334983	-0.212566
H	1.574004	-3.718533	1.420848
C	-5.272336	-0.119070	-0.030121
C	-5.124144	-1.272119	-0.821399
C	-6.573772	0.332163	0.238392
C	-6.241764	-1.926724	-1.318659
H	-4.132575	-1.627439	-1.045288
C	-7.684580	-0.339535	-0.263578
H	-6.726791	1.224626	0.828453
C	-7.531987	-1.474642	-1.047793
H	-6.096313	-2.813809	-1.924398
H	-8.674619	0.040388	-0.038761
H	-8.395735	-1.996785	-1.440382
C	2.415027	2.933350	-0.923471
O	2.540366	3.753749	-0.020208
O	3.386877	1.937602	-1.078397
H	1.945175	3.150841	-1.889067
C	5.018803	-0.057984	-0.024844
C	5.044773	-0.568222	-1.327918
C	5.597991	-0.823095	0.993637
C	5.632891	-1.800444	-1.604931
H	4.579648	0.002530	-2.123134
C	6.188025	-2.054357	0.725050
H	5.574047	-0.462085	2.017523
C	6.205289	-2.545848	-0.578020
H	5.636394	-2.182275	-2.619137
H	6.623830	-2.634814	1.529851
H	6.657675	-3.507584	-0.790001
Si	4.180511	1.583793	0.357544
H	5.231877	2.579818	0.701454
H	3.269976	1.397659	1.511169

IM14

M05-2X/BS1 SCF energy in gas phase: -1037.184395 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1037.418326 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1037.200691 a.u

O	0.212893	0.162133	-1.022617
O	-0.411902	-1.764701	-0.067812
C	0.475573	-0.774448	-0.285891
N	1.645219	-0.951886	0.391616
C	1.865476	-2.160667	1.183510
H	2.214556	-2.993123	0.568125
H	2.611108	-1.936076	1.943204
H	0.936861	-2.448496	1.664852
Si	-1.910445	-1.595125	-0.888506
H	-2.592699	-2.859532	-0.519945
H	-1.656908	-1.551604	-2.345281
C	-2.951282	-0.185815	-0.262216
C	-4.054401	-0.478974	0.550560
C	-2.709373	1.152101	-0.606594
C	-4.891122	0.532011	1.014672
H	-4.263995	-1.507623	0.823693

C	-3.546497	2.162469	-0.146873
H	-1.853166	1.395156	-1.222319
C	-4.636556	1.853714	0.664012
H	-5.738305	0.288768	1.643863
H	-3.349328	3.191862	-0.419794
H	-5.286612	2.643267	1.020889
C	2.731010	-0.049752	0.206998
C	2.523158	1.330166	0.143197
C	4.029468	-0.556211	0.134651
C	3.610010	2.182978	-0.000148
H	1.518869	1.721068	0.194265
C	5.111102	0.308871	0.002161
H	4.197610	-1.624652	0.167376
C	4.907400	1.681717	-0.067940
H	3.438548	3.250929	-0.050072
H	6.112916	-0.097970	-0.053968
H	5.748522	2.354571	-0.174281

IM15$^-$

M05-2X/BS1 SCF energy in gas phase: -712.1004 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -712.331403 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -712.220627 a.u

H	3.797628	0.990066	-0.342463
C	2.730145	0.789822	-0.547945
O	2.524129	-0.583231	-0.812271
O	1.925690	1.002819	0.555383
H	2.429150	1.396623	-1.423092
C	-0.512196	-0.269814	0.170905
C	-0.949924	1.062325	0.190562
C	-1.482334	-1.254048	-0.055260
C	-2.290398	1.394667	0.003377
H	-0.201808	1.828834	0.353628
C	-2.827353	-0.936886	-0.237568
H	-1.163118	-2.290864	-0.093645
C	-3.236248	0.393946	-0.208909
H	-2.600764	2.434894	0.022371
H	-3.555357	-1.723625	-0.409183
H	-4.280730	0.649163	-0.355535
Si	1.333683	-0.748932	0.455600
H	1.118239	-2.239520	0.105450
H	1.596488	-0.997297	1.928199

IM15

M05-2X/BS1 SCF energy in gas phase: -1145.985479 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1146.315939 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1145.945784 a.u

O	0.006088	-1.122741	0.038536
O	0.005643	1.124486	-0.040154
C	-0.562618	0.000996	-0.000633
N	2.587096	-1.141492	0.000414
H	1.505349	-1.099613	0.019478
N	2.590028	1.144277	-0.001622
H	1.510011	1.103770	-0.020952
N	4.624401	-0.001066	0.000101
C	3.266024	0.000350	-0.000330
C	3.251876	-2.426113	-0.060364
H	3.458805	-2.715781	-1.097607
H	2.575199	-3.167544	0.362592
C	4.552916	-2.349338	0.725143
H	4.326555	-2.140397	1.772549
H	5.103662	-3.288755	0.669959
C	5.400397	-1.228112	0.144701
H	6.247145	-1.007960	0.800733
H	5.804826	-1.522201	-0.830946
C	5.403314	1.224250	-0.143300
H	6.250203	1.002401	-0.798571
H	5.807476	1.517080	0.832849
C	4.559040	2.347672	-0.724168
H	5.111987	3.285747	-0.668201
H	4.333084	2.139586	-1.771828
C	3.257520	2.427391	0.060219
H	3.464222	2.716296	1.097718
H	2.582979	3.170499	-0.363185
N	-1.970608	0.000378	-0.000142
C	-2.707712	1.217089	-0.000331
C	-3.785075	1.354573	-0.878123
C	-2.405560	2.256131	0.881746
C	-4.551203	2.514312	-0.873136
H	-4.016797	0.542702	-1.556112
C	-3.168287	3.418164	0.871406
H	-1.565785	2.149054	1.551888
C	-4.245453	3.554112	-0.000354

H	-5.384350	2.605805	-1.559123
H	-2.923506	4.219415	1.558111
H	-4.839637	4.459320	0.001408
C	-2.706962	-1.216756	0.000290
C	-3.783334	-1.355220	0.879115
C	-2.405199	-2.255259	-0.882595
C	-4.548871	-2.515372	0.874405
H	-4.014804	-0.543768	1.557695
C	-3.167268	-3.417695	-0.871968
H	-1.566201	-2.147391	-1.553588
C	-4.243458	-3.554617	0.000875
H	-5.381267	-2.607578	1.561208
H	-2.922809	-4.218524	-1.559280
H	-4.837134	-4.460158	-0.000696

$[N_3]CO_2^-$

M05-2X/BS1 SCF energy in gas phase: -706.606618 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -706.89584 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -706.732817 a.u

O	1.125012	2.755019	0.114574
O	-1.125003	2.755047	-0.114513
C	-0.000001	2.257039	0.000009
N	-0.000018	0.732397	0.000016
C	-1.203607	0.014296	-0.052181
C	-1.297600	-1.157748	-0.821119
C	-2.345152	0.427467	0.653977
C	-2.473562	-1.896598	-0.868298
H	-0.429190	-1.483451	-1.379956
C	-3.519972	-0.310629	0.588828
H	-2.292905	1.343908	1.219209
C	-3.599796	-1.480231	-0.164593
H	-2.509569	-2.797582	-1.471280
H	-4.386205	0.033246	1.143806
H	-4.519992	-2.051273	-0.204723
C	1.203601	0.014319	0.052192
C	1.297696	-1.157582	0.821322
C	2.345041	0.427379	-0.654189
C	2.473671	-1.896416	0.868481
H	0.429347	-1.483186	1.380316
C	3.519881	-0.310690	-0.589065
H	2.292711	1.343726	-1.219571
C	3.599806	-1.480158	0.164556
H	2.509765	-2.797297	1.471613
H	4.386042	0.033093	-1.144209
H	4.520013	-2.051185	0.204670

TS10

M05-2X/BS1 SCF energy in gas phase: -1151.449864 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1151.73005 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1151.414784 a.u

C	1.692858	-3.240568	0.113730
O	2.005727	-1.541292	-1.009794
O	0.986202	-2.942666	1.080165
H	2.776373	-3.360677	0.225213
C	1.987765	0.911385	0.537947
C	1.021163	0.563488	1.492905
C	2.136920	2.263915	0.213495
C	0.221238	1.535517	2.088060
H	0.897628	-0.481254	1.764190
C	1.342713	3.243677	0.809423
H	2.879354	2.556445	-0.522348
C	0.377170	2.877664	1.742316
H	-0.512695	1.254575	2.835422
H	1.475088	4.286201	0.545288
H	-0.241711	3.634890	2.209025
Si	2.988632	-0.434858	-0.330456
H	3.904647	-1.075077	0.664799
H	3.845641	0.298179	-1.317528
H	1.266801	-3.669116	-0.800816
N	-1.305287	-1.576384	0.385902
H	-0.471529	-2.165769	0.516834
N	-0.293501	-0.689631	-1.472874
H	0.726694	-1.163592	-1.226331
N	-2.270058	0.266426	-0.665281
C	-1.271769	-0.649261	-0.587423
C	-2.218417	-1.483513	1.506451
H	-1.851295	-0.780928	2.264423
H	-2.280060	-2.469142	1.965561
C	-3.569131	-1.026615	0.980894
H	-3.949328	-1.768014	0.275707
H	-4.290299	-0.914424	1.790904
C	-3.377642	0.309358	0.282905
H	-4.277462	0.588888	-0.271500

H	-3.183558	1.096502	1.022093
C	-2.183149	1.427045	-1.550000
H	-2.504150	2.300250	-0.975223
H	-2.883575	1.297269	-2.382415
C	-0.766600	1.625738	-2.060291
H	-0.768310	2.366710	-2.860923
H	-0.128715	1.984665	-1.250716
C	-0.242367	0.283516	-2.548860
H	-0.828154	-0.061586	-3.408587
H	0.799733	0.353729	-2.863186

IM16

M05-2X/BS1 SCF energy in gas phase: -114.476814 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -114.522018 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -114.516142 a.u

C	-0.000007	0.528279	0.000000
H	0.935544	1.113488	0.000000
H	-0.935445	1.113695	0.000000
O	-0.000007	-0.674607	0.000000

IM16$^-$

M05-2X/BS1 SCF energy in gas phase: -1418.134515 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1418.551821 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1418.267521 a.u

C	0.780424	-1.100108	-0.105871
O	0.922183	-2.307079	-0.223163
O	-0.330897	-0.449129	-0.018349
C	-4.223401	-2.852530	0.602201
O	-5.317666	-3.374770	0.518251
O	-3.543916	-2.356667	-0.395960
H	-3.707473	-2.770784	1.578720
Si	-1.990802	-1.377617	-0.188281
H	-1.568095	-1.841217	-1.531195
H	-1.689989	-2.064300	1.101650
C	-2.910496	0.298487	-0.093126
C	-2.306969	1.462798	0.406501
C	-4.234269	0.410523	-0.545517
C	-2.985876	2.678197	0.449530
H	-1.285662	1.415906	0.757759
C	-4.916640	1.625154	-0.514850
H	-4.733124	-0.471398	-0.926538
C	-4.294820	2.765396	-0.015703
H	-2.485580	3.556685	0.842627
H	-5.936713	1.678085	-0.878960
H	-4.825117	3.711101	0.011797
N	1.923695	-0.246426	-0.050591
C	3.231802	-0.786255	-0.085104
C	3.563338	-1.967231	0.588810
C	4.231015	-0.108339	-0.793244
C	4.866167	-2.449325	0.544240
H	2.791820	-2.505067	1.116812
C	5.533193	-0.592506	-0.819256
H	3.975740	0.801834	-1.320480
C	5.861083	-1.769094	-0.152649
H	5.103701	-3.367488	1.068316
H	6.290099	-0.050491	-1.374018
H	6.874163	-2.151350	-0.177789
C	1.784871	1.164282	0.048373
C	0.950245	1.880192	-0.813134
C	2.516289	1.855241	1.018496
C	0.835684	3.259774	-0.684729
H	0.367627	1.344100	-1.548065
C	2.415649	3.237259	1.125358
H	3.161878	1.294716	1.683266
C	1.569886	3.947506	0.277851
H	0.163435	3.796056	-1.343485
H	2.988291	3.756772	1.884495
H	1.479688	5.023080	0.369858

TS11

M05-2X/BS1 SCF energy in gas phase: -880.160266 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -880.415865 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -880.075758 a.u

N	-1.527031	0.021879	1.089433
H	-0.591714	-0.307212	0.607892
C	-1.662907	-0.648902	2.380429
H	-0.665971	-0.740155	2.810178
H	-2.288559	-0.059073	3.054967

H	-2.097409	-1.642092	2.262754
C	-2.631240	-0.064447	0.189500
C	-3.925842	-0.343019	0.625081
C	-2.383835	0.205127	-1.158245
C	-4.970109	-0.369667	-0.295296
H	-4.127770	-0.538228	1.670084
C	-3.435633	0.179255	-2.065076
H	-1.375045	0.443045	-1.463708
C	-4.730201	-0.111044	-1.640221
H	-5.973726	-0.592203	0.045069
H	-3.242295	0.388972	-3.109619
H	-5.545555	-0.133551	-2.352029
C	-1.102252	1.675171	1.340786
H	-0.341247	1.488081	2.125805
H	-2.052530	2.018718	1.789498
O	-0.720967	2.213373	0.244781
C	1.858152	-0.039078	-0.076114
C	2.743452	2.256106	-0.302779
C	4.112432	1.667129	-0.011854
C	4.207607	0.328992	-0.725939
H	2.694970	2.553084	-1.359050
H	2.567107	3.154351	0.291093
H	4.902485	2.335799	-0.356922
H	4.230224	1.510140	1.062418
H	4.185077	0.480784	-1.814393
H	5.148039	-0.171772	-0.484685
N	3.126221	-0.541799	-0.294257
N	1.707850	1.297270	0.016976
C	2.304974	-2.754615	0.284296
C	0.912647	-2.238662	-0.050436
C	3.304627	-1.962421	-0.540994
H	0.657686	-2.534435	-1.077265
H	0.168458	-2.712527	0.597498
H	2.512362	-2.597227	1.345341
H	2.396249	-3.820258	0.066370
H	3.182024	-2.196942	-1.607649
H	4.329627	-2.221271	-0.264149
N	0.804575	-0.800982	0.105506
H	0.702735	1.672862	0.059823

IM17

M05-2X/BS1 SCF energy in gas phase: -441.385975 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -441.517617 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -441.369376 a.u

N	-1.250832	0.499905	-0.063580
H	-2.598116	-1.158263	-1.216123
C	-1.659866	1.890935	-0.056385
H	-2.744744	1.940177	-0.134589
H	-1.349961	2.424925	0.850849
H	-1.240733	2.410774	-0.919336
C	0.120590	0.212785	-0.038316
C	1.084527	1.230777	-0.063220
C	0.557847	-1.122610	0.006516
C	2.440263	0.918028	-0.034727
H	0.789796	2.269920	-0.092390
C	1.913797	-1.414887	0.046375
H	-0.171418	-1.920156	-0.025910
C	2.869192	-0.401712	0.026548
H	3.164080	1.723892	-0.052230
H	2.225235	-2.451986	0.081417
H	3.924927	-0.637886	0.052029
C	-2.148554	-0.465302	0.522099
H	-3.063385	0.062755	0.806933
H	-1.713305	-0.924025	1.413767
O	-2.441666	-1.540944	-0.346588

TS12

M05-2X/BS1 SCF energy in gas phase: -1478.535263 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1478.912377 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1478.523983 a.u

N	-3.373596	1.079075	-0.612335
H	-2.759319	-2.750713	-2.531281
C	-4.226349	0.660790	0.509655
H	-4.809198	1.516286	0.843857
H	-4.873207	-0.148856	0.186070
H	-3.569922	0.313809	1.307352
C	-2.463553	2.174892	-0.342140
C	-2.992446	3.426441	-0.037317
C	-1.100973	1.926372	-0.358880
C	-2.111662	4.462466	0.246199
H	-4.062376	3.594682	-0.042196
C	-0.232659	2.973750	-0.060127

H	-0.689290	0.946900	-0.568160
C	-0.734671	4.235320	0.238981
H	-2.500367	5.446531	0.473610
H	0.828376	2.760655	-0.051933
H	-0.057281	5.046569	0.473406
C	-3.348170	0.439028	-1.719738
H	-2.653561	0.742320	-2.491314
H	-3.985730	-0.415244	-1.877198
O	-2.434027	-1.868842	-2.336836
Si	-0.879394	-1.904589	-1.435397
H	-0.505228	-0.611108	-2.085979
H	-0.563768	-3.288704	-1.901315
C	-1.686138	-1.802068	0.303039
C	-1.108323	-1.140958	1.396951
C	-2.905686	-2.457954	0.528080
C	-1.723891	-1.130232	2.649129
H	-0.169532	-0.617349	1.262278
C	-3.510647	-2.486897	1.783371
H	-3.387884	-2.962680	-0.301397
C	-2.921349	-1.814366	2.851117
H	-1.256792	-0.602666	3.472676
H	-4.437454	-3.030493	1.928509
H	-3.385889	-1.827210	3.830013
O	1.267850	0.226083	-0.369820
O	0.880327	-1.966264	-0.712031
C	1.648826	-0.941024	-0.506564
N	3.000741	-1.269900	-0.428212
C	3.389406	-2.673805	-0.465933
H	4.421612	-2.740031	-0.807543
H	3.302369	-3.155761	0.512554
H	2.738409	-3.195217	-1.159381
C	3.970515	-0.311288	-0.059726
C	3.948871	0.989071	-0.581505
C	5.011835	-0.673427	0.800528
C	4.939551	1.896370	-0.232109
H	3.153460	1.269767	-1.253591
C	6.004914	0.241944	1.136815
H	5.040497	-1.669816	1.221059
C	5.975032	1.533894	0.627098
H	4.908881	2.895992	-0.649076
H	6.800075	-0.061707	1.806825
H	6.746804	2.246345	0.889486

IM18^{+}

M05-2X/BS1 SCF energy in gas phase: -365.322549 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -365.497078 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -365.363223 a.u

N	1.621761	-0.090003	-0.074576
C	2.358397	0.941417	0.683823
H	1.980293	0.941754	1.703380
H	3.420589	0.715075	0.660470
H	2.175576	1.909703	0.224092
C	0.175036	-0.032330	-0.038189
C	-0.467596	1.166918	-0.331159
C	-0.523436	-1.187978	0.300235
C	-1.856642	1.193101	-0.302309
H	0.087348	2.052966	-0.609477
C	-1.912428	-1.140210	0.328587
H	0.004348	-2.093522	0.574241
C	-2.575981	0.045674	0.026242
H	-2.376135	2.111003	-0.541509
H	-2.471450	-2.025542	0.599668
H	-3.657063	0.078683	0.052780
C	2.225343	-1.025113	-0.702139
H	3.305379	-1.090436	-0.661250
H	1.642621	-1.738545	-1.270899

TS13

M05-2X/BS1 SCF energy in gas phase: -1207.260233 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1207.60831 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1207.199616 a.u

N	0.643976	-0.964151	0.072536
C	-0.287781	-1.020511	-1.067891
H	-0.934513	-0.147692	-1.006956
H	0.312421	-1.018696	-1.975766
H	-0.879679	-1.932163	-0.993649
C	1.758781	-1.874865	0.068329
C	3.046466	-1.352736	0.077014
C	1.506223	-3.242054	0.038302
C	4.116945	-2.242576	0.069721
H	3.199800	-0.279086	0.060540
C	2.588108	-4.114426	0.032349

H	0.485782	-3.606028	0.046943
C	3.889533	-3.615468	0.047007
H	5.127741	-1.856384	0.069597
H	2.414872	-5.182436	0.020389
H	4.727605	-4.300326	0.037457
C	0.492313	-0.096387	0.999619
H	-0.353163	0.592282	0.934461
H	1.213475	-0.086578	1.808058
N	0.752582	2.888395	1.044057
H	-0.204328	2.794647	0.705679
O	-1.635494	1.623558	0.208565
O	-3.221906	3.016320	-0.564724
C	-2.806530	1.919804	-0.209901
N	-3.727735	0.807307	-0.305898
C	-4.915377	1.021679	-1.114306
H	-4.744162	0.819549	-2.178343
H	-5.722055	0.379399	-0.758250
H	-5.190303	2.065825	-1.008278
C	-3.390515	-0.492368	0.054199
C	-2.679021	-0.759961	1.240448
C	-3.787775	-1.588918	-0.729689
C	-2.328492	-2.058258	1.582655
H	-2.426495	0.071810	1.881683
C	-3.442902	-2.889478	-0.370213
H	-4.353961	-1.419958	-1.635794
C	-2.694280	-3.139229	0.776153
H	-1.790673	-2.234402	2.507980
H	-3.762766	-3.712287	-0.998806
H	-2.438163	-4.152409	1.060313
C	1.753443	2.538964	0.180795
C	1.419592	2.024589	-1.092914
C	3.115852	2.638067	0.521619
C	2.412123	1.628738	-1.974906
H	0.369921	1.977068	-1.361467
C	4.097491	2.241763	-0.384471
H	3.406514	3.040028	1.483184
C	3.764154	1.729384	-1.634174
H	2.128542	1.253769	-2.951915
H	5.139447	2.343212	-0.103292
H	4.534108	1.430372	-2.332962
C	0.998365	3.642039	2.246973
H	1.543679	4.571448	2.046971
H	0.039520	3.895266	2.694307
H	1.573972	3.067157	2.982019

TS14

M05-2X/BS1 SCF energy in gas phase: -1478.521374 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1478.908317 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1478.521292 a.u

N	4.009700	1.311082	0.542113
C	4.317410	2.629322	-0.042194
H	4.904093	2.471979	-0.942625
H	3.363214	3.096216	-0.292710
H	4.877074	3.227368	0.674769
C	4.916322	0.216722	0.307276
C	6.286729	0.442573	0.390885
C	4.394545	-1.035181	0.000582
C	7.153368	-0.623035	0.177584
H	6.671338	1.424459	0.634881
C	5.276276	-2.089110	-0.210504
H	3.327146	-1.178059	-0.117155
C	6.650433	-1.887190	-0.121054
H	8.221273	-0.463849	0.247538
H	4.878012	-3.063381	-0.461973
H	7.330810	-2.711166	-0.292103
C	2.907406	1.136629	1.176231
H	2.689638	0.161235	1.588990
H	2.219823	1.960285	1.313228
C	-2.731160	0.963154	0.088984
O	-2.994216	1.286527	-1.071850
O	-1.612438	1.224309	0.706720
C	-3.254937	-0.168421	2.203732
H	-2.761950	-1.146476	2.183793
H	-2.567516	0.558124	2.623158
H	-4.144108	-0.234392	2.829785
N	-3.650560	0.277536	0.875914
H	1.476045	2.287325	-0.509677
Si	0.026848	1.793462	-0.056172
H	0.286630	2.294863	1.352343
C	0.541467	-0.034574	-0.316340
C	1.160637	-0.393475	-1.522529
C	0.318857	-1.051757	0.623813
C	1.506110	-1.714950	-1.801267
H	1.348430	0.381365	-2.259360
C	0.716838	-2.366405	0.381401
H	-0.193167	-0.807040	1.548247

C	1.296599	-2.704142	-0.840930
H	1.946595	-1.972368	-2.757526
H	0.544854	-3.133341	1.127865
H	1.571504	-3.732050	-1.047255
C	-4.884877	-0.178844	0.357611
C	-5.634446	0.581402	-0.549897
C	-5.403097	-1.400508	0.800891
C	-6.863675	0.115796	-0.996241
H	-5.238832	1.518889	-0.905191
C	-6.640601	-1.851819	0.352094
H	-4.834261	-2.011846	1.488403
C	-7.379922	-1.098889	-0.550751
H	-7.428153	0.718080	-1.697730
H	-7.018514	-2.802196	0.709199
H	-8.341691	-1.449883	-0.902500
O	-0.681751	2.626928	-1.299499
H	-1.612596	2.351165	-1.415407

2c

M05-2X/BS1 SCF energy in gas phase: -366.171989 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -366.2712 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -366.127789 a.u

C	2.253693	-1.127756	0.508945
H	3.260466	-1.272143	0.114247
H	1.731914	-2.079011	0.454635
N	1.572530	-0.113962	-0.285012
C	0.175389	-0.036802	-0.131079
C	-0.604067	-1.196858	-0.275535
C	-0.486505	1.171682	0.121501
C	-1.983954	-1.147576	-0.156687
H	-0.123636	-2.136099	-0.515667
C	-1.875422	1.212478	0.226309
H	0.073359	2.087091	0.248604
C	-2.635666	0.058775	0.096107
H	-2.557191	-2.058786	-0.277626
H	-2.359321	2.161754	0.422137
H	-3.713764	0.095073	0.182988
C	2.297613	1.139500	-0.278548
H	2.292531	1.637145	0.703575
H	3.334307	0.940050	-0.551792
H	1.875957	1.819077	-1.018726
H	2.331189	-0.837080	1.566634

2d

M05-2X/BS1 SCF energy in gas phase: -691.850228 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -692.034702 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -691.772447 a.u

N	-0.219957	-1.873852	0.494017
C	0.247041	-2.006465	1.861802
H	0.935186	-2.851542	1.907411
H	0.778013	-1.121583	2.229397
H	-0.604057	-2.211709	2.511973
C	-1.295430	-0.999021	0.248528
C	-1.707664	-0.048837	1.189665
C	-2.006866	-1.094184	-0.957553
C	-2.774103	0.801118	0.913011
H	-1.172079	0.057340	2.122817
C	-3.056585	-0.229356	-1.231648
H	-1.743625	-1.866073	-1.669945
C	-3.449192	0.729303	-0.299766
H	-3.065540	1.537441	1.652362
H	-3.586460	-0.320867	-2.172243
H	-4.273718	1.397544	-0.511837
C	0.833497	-1.970056	-0.489722
H	1.260211	-2.978316	-0.460428
H	0.398835	-1.827428	-1.486196
N	1.942595	-1.054802	-0.219611
C	1.568359	0.330849	-0.173769
C	2.041788	1.097378	0.889926
C	0.766274	0.931997	-1.145415
C	1.704930	2.443186	0.995652
H	2.666108	0.612054	1.630776
C	0.414619	2.272467	-1.029892
H	0.389126	0.349508	-1.976782
C	0.882112	3.031330	0.039407
H	2.074337	3.027977	1.829095
H	-0.230790	2.722098	-1.774118
H	0.604217	4.074089	0.127866
C	3.065857	-1.293897	-1.118101
H	3.889686	-0.635521	-0.844368
H	3.398815	-2.328939	-1.015170
H	2.815454	-1.110366	-2.174204

IM18

M05-2X/BS1 SCF energy in gas phase: -1112.465265 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1112.730005 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1112.506899 a.u

C	0.492784	-0.919161	0.188775
O	0.329247	-0.805499	-1.017868
O	-0.472815	-1.402629	0.996259
C	1.678082	-0.691439	2.321419
H	1.224504	0.177162	2.804927
H	1.149638	-1.584178	2.639703
H	2.721787	-0.764558	2.618399
N	1.628696	-0.591121	0.863728
Si	-2.013196	-1.647024	0.286397
H	-2.708291	-2.490379	1.277898
C	-2.771078	0.032298	0.062276
C	-3.662527	0.264127	-0.991513
C	-2.490444	1.079191	0.948477
C	-4.263384	1.508733	-1.152923
H	-3.877453	-0.533437	-1.693933
C	-3.088742	2.324635	0.790160
H	-1.792772	0.921047	1.764187
C	-3.976914	2.538255	-0.260949
H	-4.949078	1.677609	-1.973893
H	-2.861904	3.128011	1.480048
H	-4.442583	3.508074	-0.386474
C	2.720999	0.020172	0.183505
C	3.157995	-0.453462	-1.055058
C	3.387896	1.083907	0.791850
C	4.249726	0.143452	-1.672599
H	2.637817	-1.272641	-1.527291
C	4.486694	1.667098	0.168943
H	3.043970	1.466018	1.744280
C	4.921396	1.201800	-1.066404
H	4.581500	-0.229417	-2.633377
H	4.994748	2.492844	0.650849
H	5.774244	1.657648	-1.552387
O	-1.920996	-2.496445	-1.116250
H	-1.250632	-2.118665	-1.701478

$TS9_{by}^-$

M05-2X/BS1 SCF energy in gas phase: -1553.261084 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1553.713696 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1553.339525 a.u

C	1.080740	-1.245115	0.689200
O	0.972464	-2.407753	0.234891
O	2.399127	-0.741329	0.680299
H	-0.761505	-0.310130	-0.299349
H	0.559725	-0.915090	1.598743
N	0.264752	-0.074620	-0.405623
C	0.652497	-0.393036	-1.783883
H	0.560186	-1.473883	-1.880421
H	-0.030281	0.116060	-2.461227
H	1.688173	-0.110658	-1.965425
C	5.067046	-1.009151	0.071226
C	5.181953	0.293433	0.572736
C	6.223649	-1.622027	-0.426297
C	6.407791	0.956738	0.577423
H	4.296351	0.785008	0.959052
C	7.452129	-0.968429	-0.422312
H	6.165319	-2.629961	-0.828513
C	7.545213	0.327197	0.081078
H	6.474733	1.965253	0.969228
H	8.333755	-1.464006	-0.812434
H	8.498878	0.842290	0.084480
O	-2.402465	-0.467266	-0.097842
O	-2.298012	0.662917	-2.033813
C	-2.908003	0.113755	-1.102503
N	-4.348753	0.153322	-1.164948
C	-4.922530	0.936606	-2.240865
H	-5.792747	0.422870	-2.657625
H	-5.235180	1.935032	-1.910184
H	-4.152122	1.049075	-2.994838
Si	3.407870	-1.924552	0.040020
H	3.574777	-3.136119	0.883204
H	3.215722	-2.313844	-1.381282
C	0.459971	1.269275	0.033529
C	1.625515	1.981183	-0.257078
C	-0.515917	1.840995	0.851940
C	1.802013	3.259010	0.260606
H	2.400284	1.533289	-0.862889
C	-0.326784	3.119530	1.365977
H	-1.420639	1.277184	1.045449

C	0.829588	3.835862	1.073710
H	2.710420	3.803144	0.030065
H	-1.094598	3.558070	1.992097
H	0.972475	4.832750	1.473080
C	-5.210416	-0.343560	-0.185797
C	-4.854285	-1.383912	0.698106
C	-6.521623	0.160454	-0.091102
C	-5.766807	-1.866144	1.623706
H	-3.855999	-1.783337	0.646792
C	-7.425524	-0.338994	0.842282
H	-6.841651	0.962619	-0.739816
C	-7.061872	-1.356511	1.713101
H	-5.455417	-2.666842	2.285315
H	-8.423513	0.083741	0.882952
H	-7.764313	-1.745223	2.440311

$IM9_{by}^-$

M05-2X/BS1 SCF energy in gas phase: -1553.279769 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1553.72094 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1553.34278 a.u

C	-0.933426	0.374908	-1.345280
O	-0.266205	-0.841966	-1.203849
O	-2.240039	-0.004887	-1.477390
H	0.879197	1.193136	-0.095275
H	-0.551148	0.955597	-2.198765
N	-0.649327	1.225835	-0.152538
C	-1.129240	0.605429	1.096171
H	-0.734135	-0.408148	1.137449
H	-0.739790	1.172894	1.938824
H	-2.219634	0.569825	1.116762
C	-3.055617	-2.262774	-0.113987
C	-4.102237	-1.393636	0.228224
C	-3.039535	-3.517835	0.504918
C	-5.087660	-1.762584	1.140432
H	-4.120413	-0.413166	-0.232035
C	-4.020684	-3.899943	1.418662
H	-2.233875	-4.203576	0.263998
C	-5.049844	-3.020002	1.739448
H	-5.884888	-1.069710	1.387877
H	-3.978906	-4.878918	1.884229
H	-5.813699	-3.308865	2.453266
O	1.918029	1.016830	-0.091975
O	1.877725	1.559505	2.092653
C	2.369288	0.965975	1.136702
N	3.504624	0.180451	1.280633
C	4.199182	0.250733	2.554486
H	4.567410	-0.740603	2.820124
H	5.044602	0.946148	2.525700
H	3.487672	0.599091	3.296634
Si	-1.719238	-1.819486	-1.420059
H	-2.206706	-2.098888	-2.814578
H	-0.913481	-3.107997	-1.210044
C	-1.080631	2.586230	-0.280266
C	-2.103614	2.967679	-1.150862
C	-0.432509	3.548964	0.500198
C	-2.456234	4.312302	-1.247900
H	-2.617098	2.204924	-1.722206
C	-0.806867	4.883451	0.406654
H	0.365265	3.228648	1.162769
C	-1.816422	5.272955	-0.472148
H	-3.246943	4.605210	-1.928881
H	-0.298791	5.624186	1.012966
H	-2.100598	6.315762	-0.550037
C	4.019732	-0.664311	0.268150
C	3.185655	-1.357727	-0.622235
C	5.401392	-0.870234	0.203690
C	3.745912	-2.214599	-1.559384
H	2.113129	-1.219458	-0.598985
C	5.947006	-1.741341	-0.735611
H	6.055803	-0.337230	0.881205
C	5.123771	-2.417217	-1.626403
H	3.082614	-2.738018	-2.237115
H	7.021251	-1.882128	-0.767572
H	5.544801	-3.094311	-2.359627

$TS10_{by}^-$

M05-2X/BS1 SCF energy in gas phase: -1553.268192 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1553.711771 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1553.334462 a.u

C	-1.451190	0.090829	-1.185518
O	-0.123830	-0.355621	-1.198613
O	-2.149328	-1.088139	-1.126136

H	0.400954	1.821425	-0.852577
H	-1.684444	0.675129	-2.092189
N	-1.575295	1.037827	-0.079522
C	-1.332496	0.426172	1.228789
H	-0.409424	-0.147870	1.167387
H	-1.210977	1.210674	1.973635
H	-2.148751	-0.245769	1.514124
C	-0.913962	-3.357707	-0.131051
C	-2.136554	-3.412071	0.553933
C	0.035382	-4.340495	0.172699
C	-2.401299	-4.409793	1.489332
H	-2.872109	-2.647167	0.339139
C	-0.219596	-5.346524	1.102915
H	0.996291	-4.305738	-0.330458
C	-1.443239	-5.382709	1.765319
H	-3.354598	-4.428846	2.006795
H	0.536064	-6.095040	1.316744
H	-1.646647	-6.158963	2.495203
O	1.343838	2.052575	-0.761022
O	0.818210	2.930560	1.258401
C	1.595631	2.362755	0.510281
N	2.872756	2.009543	0.887453
C	3.348075	2.507673	2.168444
H	3.948933	1.736443	2.649769
H	3.954283	3.411842	2.055827
H	2.480725	2.741868	2.778562
Si	-0.528630	-2.034147	-1.465587
H	-0.950922	-2.461298	-2.842986
H	0.962713	-2.413797	-1.573041
C	-2.721019	1.867870	-0.111241
C	-3.901204	1.485245	-0.756768
C	-2.653924	3.116448	0.519558
C	-4.989906	2.354790	-0.782519
H	-3.950646	0.502609	-1.210379
C	-3.753023	3.964489	0.507321
H	-1.714642	3.402830	0.979806
C	-4.926583	3.591038	-0.148464
H	-5.899035	2.052892	-1.290239
H	-3.688481	4.931002	0.994180
H	-5.779425	4.259340	-0.166493
C	3.702446	1.123352	0.149509
C	3.180228	0.000230	-0.504255
C	5.081896	1.340233	0.148361
C	4.039707	-0.871992	-1.158058
H	2.114086	-0.186837	-0.523504
C	5.933815	0.450690	-0.501327
H	5.489030	2.211285	0.646396
C	5.417586	-0.658255	-1.160260
H	3.609534	-1.732503	-1.655505
H	7.001786	0.634909	-0.493163
H	6.078556	-1.350573	-1.667382

$IM10_{by}^{-}$

M05-2X/BS1 SCF energy in gas phase: -1553.279768 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1553.720933 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1553.342774 a.u

C	0.933929	-0.374888	-1.345838
O	0.266457	0.841851	-1.204794
O	2.240495	0.005184	-1.477790
H	-0.878453	-1.193375	-0.095965
H	0.552018	-0.955832	-2.199320
N	0.649762	-1.225727	-0.153065
C	1.129063	-0.604943	1.095743
H	0.733247	0.408352	1.136963
H	0.739976	-1.172759	1.938318
H	2.219426	-0.568602	1.116455
C	3.054420	2.263584	-0.113762
C	4.101165	1.394960	0.229364
C	3.037217	3.518682	0.505032
C	5.085608	1.764424	1.142410
H	4.120237	0.414479	-0.230863
C	4.017398	3.901311	1.419599
H	2.231440	4.204017	0.263365
C	5.046681	3.021861	1.741322
H	5.882964	1.071962	1.390584
H	3.974768	4.880288	1.885086
H	5.809780	3.311112	2.455788
O	-1.917432	-1.017429	-0.092656
O	-1.877802	-1.561524	2.091593
C	-2.369181	-0.967523	1.135822
N	-3.504928	-0.182516	1.279829
C	-4.200131	-0.254075	2.553250
H	-4.567737	0.737146	2.820211
H	-5.046076	-0.948782	2.523020
H	-3.489212	-0.604058	3.295181
Si	1.719322	1.819600	-1.420899

H	2.207989	2.098884	-2.815041
H	0.913013	3.107990	-1.212225
C	1.081727	-2.586001	-0.280392
C	2.105014	-2.967123	-1.150781
C	0.433881	-3.548841	0.500155
C	2.458249	-4.311601	-1.247497
H	2.618202	-2.204216	-1.722189
C	0.808871	-4.883177	0.406918
H	-0.364165	-3.228749	1.162506
C	1.818736	-5.272385	-0.471648
H	3.249176	-4.604320	-1.928297
H	0.301033	-5.624035	1.013275
H	2.103405	-6.315080	-0.549293
C	-4.019673	0.663179	0.267958
C	-3.185390	1.357196	-0.621795
C	-5.401285	0.869528	0.203551
C	-3.745389	2.214994	-1.558232
H	-2.112889	1.218765	-0.598654
C	-5.946642	1.741536	-0.735072
H	-6.055916	0.336169	0.880566
C	-5.123199	2.417981	-1.625235
H	-3.081890	2.738863	-2.235422
H	-7.020854	1.882569	-0.766966
H	-5.543980	3.095808	-2.357916

$TS11_{by}^{-}$

M05-2X/BS1 SCF energy in gas phase: -1553.262688 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1553.712 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1553.335493 a.u

C	-1.652305	0.957489	-1.052463
O	-0.778861	-0.224391	0.064687
O	-2.425742	0.077933	-1.566701
H	0.304309	-0.232724	0.190841
H	-0.741499	1.271807	-1.561560
N	-2.203294	1.938340	-0.242920
C	-3.508521	1.685340	0.340519
H	-3.801336	0.676862	0.066771
H	-3.456149	1.774411	1.427683
H	-4.258959	2.384608	-0.039627
C	-3.182120	-2.223855	-0.136691
C	-4.376270	-1.855579	-0.774392
C	-3.270546	-3.161526	0.900067
C	-5.600113	-2.398281	-0.391727
H	-4.330402	-1.123011	-1.569857
C	-4.492308	-3.700161	1.299621
H	-2.360615	-3.472739	1.400848
C	-5.662511	-3.320465	0.650523
H	-6.507697	-2.099775	-0.904814
H	-4.529624	-4.416425	2.112904
H	-6.615891	-3.739198	0.953178
O	1.656811	-0.325817	0.257289
O	1.654209	0.912327	-1.615910
C	2.198890	0.171699	-0.782163
N	3.572960	-0.143502	-0.985524
C	4.240341	0.549091	-2.071911
H	4.781511	1.439657	-1.730131
H	4.949326	-0.124365	-2.557807
H	3.474553	0.860681	-2.773154
Si	-1.456747	-1.607989	-0.657027
H	-1.080385	-1.958551	-2.053780
H	-0.655900	-2.638201	0.121098
C	4.350355	-0.930708	-0.126254
C	3.812037	-1.976736	0.647336
C	5.739035	-0.725359	-0.069627
C	4.637956	-2.758675	1.440697
H	2.749240	-2.150422	0.622495
C	6.554487	-1.522523	0.728635
H	6.190272	0.073463	-0.640959
C	6.015152	-2.546947	1.494099
H	4.191431	-3.556801	2.022746
H	7.621164	-1.328758	0.748656
H	6.648191	-3.167736	2.116321
C	-1.441080	3.012502	0.232652
C	-0.041584	3.029988	0.124798
C	-2.083661	4.102263	0.838718
C	0.672183	4.125963	0.591396
H	0.497382	2.197807	-0.309070
C	-1.349899	5.185429	1.309730
H	-3.160762	4.109919	0.933429
C	0.034278	5.211696	1.186815
H	1.751490	4.113203	0.496730
H	-1.872473	6.014762	1.772904
H	0.605508	6.055213	1.554453

TS18

M05-2X/BS1 SCF energy in gas phase:

-1114.754328 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1115.027506 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1114.768123 a.u

C	1.408915	0.737324	0.151868
O	0.894693	1.142774	1.178318
O	1.464623	-0.549718	-0.203919
C	2.817181	0.961886	-1.847758
H	3.787236	0.655202	-1.448978
H	2.329826	0.084892	-2.262639
H	2.959713	1.704815	-2.629635
N	1.962744	1.549309	-0.813972
Si	1.731643	-1.891693	0.850014
H	0.943338	-3.043730	0.364989
C	3.475083	-2.342865	0.278017
C	3.649169	-3.155017	-0.847621
C	4.621539	-1.832168	0.900391
C	4.916796	-3.443147	-1.347548
H	2.777894	-3.578228	-1.340166
C	5.893370	-2.115839	0.409777
H	4.507779	-1.217660	1.786129
C	6.042507	-2.920040	-0.717727
H	5.028113	-4.076883	-2.219693
H	6.768763	-1.715980	0.907970
H	7.031743	-3.143559	-1.099205
C	1.987925	2.955866	-0.618720
C	0.818725	3.640401	-0.277664
C	3.170633	3.668711	-0.813045
C	0.844409	5.019620	-0.122472
H	-0.097258	3.085701	-0.131034
C	3.183554	5.053263	-0.668018
H	4.083307	3.142559	-1.061381
C	2.023887	5.734907	-0.318905
H	-0.066881	5.541258	0.144142
H	4.108860	5.594635	-0.819934
H	2.036718	6.810851	-0.201141
Si	-1.307062	-0.598584	2.581172
H	-2.293553	-1.466809	3.310084
H	-0.415020	0.027715	3.602757
C	-2.398734	0.763361	1.846363
C	-3.700897	0.460897	1.425354
C	-1.963531	2.089393	1.717465
C	-4.530869	1.431552	0.867142
H	-4.079966	-0.549876	1.551131
C	-2.791488	3.069840	1.171374
H	-0.961645	2.349513	2.036053
C	-4.073504	2.741639	0.736195
H	-5.538290	1.175049	0.558034
H	-2.436829	4.091113	1.090235
H	-4.718151	3.503768	0.314992
O	-0.477988	-1.484816	1.491044
H	-1.435147	-2.219177	0.696545
C	-2.445950	-1.473753	-0.890712
C	-1.652560	0.697566	-1.709369
C	-2.539259	0.456670	-2.920397
C	-3.830506	-0.202311	-2.458262
H	-2.110414	1.431679	-1.037519
H	-0.668846	1.064615	-2.003584
H	-2.769646	1.398457	-3.418493
H	-2.025298	-0.195932	-3.628774
H	-4.414872	0.500505	-1.853492
H	-4.436549	-0.505610	-3.314005
N	-3.546079	-1.404384	-1.677978
N	-1.464975	-0.569839	-1.023811
C	-4.152369	-3.654683	-0.959544
C	-3.251166	-3.474617	0.252994
C	-4.668324	-2.292922	-1.401672
H	-3.847869	-3.202846	1.130886
H	-2.728194	-4.401839	0.487586
H	-3.585625	-4.103671	-1.777676
H	-4.989044	-4.310878	-0.718602
H	-5.318542	-1.857324	-0.632156
H	-5.250292	-2.380049	-2.320741
N	-2.259388	-2.448752	-0.012762
H	-0.750357	-0.638819	-0.299906
O	2.038859	-1.481049	2.413730
H	1.296066	-1.044650	2.841862

IM19

M05-2X/BS1 SCF energy in gas phase: -1145.985479 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1146.315939 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1145.945784 a.u

O	0.006088	-1.122741	0.038536
O	0.005643	1.124486	-0.040154

C	-0.562618	0.000996	-0.000633
N	2.587096	-1.141492	0.000414
H	1.505349	-1.099613	0.019478
N	2.590028	1.144277	-0.001622
H	1.510011	1.103770	-0.020952
N	4.624401	-0.001066	0.000101
C	3.266024	0.000350	-0.000330
C	3.251876	-2.426113	-0.060364
H	3.458805	-2.715781	-1.097607
H	2.575199	-3.167544	0.362592
C	4.552916	-2.349338	0.725143
H	4.326555	-2.140397	1.772549
H	5.103662	-3.288755	0.669959
C	5.400397	-1.228112	0.144701
H	6.247145	-1.007960	0.800733
H	5.804826	-1.522201	-0.830946
C	5.403314	1.224250	-0.143300
H	6.250203	1.002401	-0.798571
H	5.807476	1.517080	0.832849
C	4.559040	2.347672	-0.724168
H	5.111987	3.285747	-0.668201
H	4.333084	2.139586	-1.771828
C	3.257520	2.427391	0.060219
H	3.464222	2.716296	1.097718
H	2.582979	3.170499	-0.363185
N	-1.970608	0.000378	-0.000142
C	-2.707712	1.217089	-0.000331
C	-3.785075	1.354573	-0.878123
C	-2.405560	2.256131	0.881746
C	-4.551203	2.514312	-0.873136
H	-4.016797	0.542702	-1.556112
C	-3.168287	3.418164	0.871406
H	-1.565785	2.149054	1.551888
C	-4.245453	3.554112	-0.000354
H	-5.384350	2.605805	-1.559123
H	-2.923506	4.219415	1.558111
H	-4.839637	4.459320	0.001408
C	-2.706962	-1.216756	0.000290
C	-3.783334	-1.355220	0.879115
C	-2.405199	-2.255259	-0.882595
C	-4.548871	-2.515372	0.874405
H	-4.014804	-0.543768	1.557695
C	-3.167268	-3.417695	-0.871968
H	-1.566201	-2.147391	-1.553588
C	-4.243458	-3.554617	0.000875
H	-5.381267	-2.607578	1.561208
H	-2.922809	-4.218524	-1.559280
H	-4.837134	-4.460158	-0.000696

TS15^{-}

M05-2X/BS1 SCF energy in gas phase: -1418.070007 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1418.486113 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1418.21107 a.u

C	-0.738510	-1.083506	0.120631
O	-0.832462	-2.300213	0.118648
O	0.332624	-0.374005	0.224751
C	4.498093	-3.231707	-0.262391
O	3.904714	-4.151369	0.168949
O	5.322823	-2.627403	-0.852433
H	3.546131	-1.847863	0.447157
Si	2.073272	-1.197201	0.333850
H	1.687326	-1.798429	1.644263
H	1.809245	-1.906910	-0.953000
C	2.849665	0.553059	0.253072
C	2.150433	1.732256	0.549478
C	4.194115	0.681985	-0.123261
C	2.763317	2.981111	0.472896
H	1.109522	1.667858	0.834798
C	4.809995	1.928266	-0.217079
H	4.763132	-0.213550	-0.346946
C	4.095950	3.084676	0.084208
H	2.192327	3.872549	0.710248
H	5.848751	1.995081	-0.521895
H	4.573712	4.056201	0.017267
N	-1.915934	-0.276274	-0.001473
C	-3.202340	-0.857706	-0.068025
C	-3.540467	-2.002572	0.665021
C	-4.181777	-0.258732	-0.870446
C	-4.826717	-2.522798	0.586511
H	-2.784302	-2.482500	1.265320
C	-5.467873	-0.781195	-0.930155
H	-3.924464	0.621621	-1.445069
C	-5.801726	-1.919714	-0.203528
H	-5.067640	-3.411091	1.158687
H	-6.207415	-0.298563	-1.558457
H	-6.802279	-2.331451	-0.253993

C	-1.820395	1.140927	-0.047644
C	-2.592161	1.906954	0.829828
C	-0.985018	1.785628	-0.961961
C	-2.531725	3.295089	0.792441
H	-3.236541	1.398530	1.536352
C	-0.913211	3.174118	-0.980887
H	-0.368142	1.189615	-1.619229
C	-1.687989	3.936537	-0.110357
H	-3.134427	3.874948	1.481416
H	-0.240584	3.658486	-1.678301
H	-1.630169	5.018050	-0.131640

TS16$^-$

M05-2X/BS1 SCF energy in gas phase: -1940.989416 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1941.489825 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1941.097614 a.u

O	-1.714694	-0.578172	-1.787177
O	-1.567681	1.291729	-0.535286
C	-2.164153	0.231481	-0.995749
N	-3.468219	0.055783	-0.459548
Si	0.277302	1.514083	-0.787300
H	1.894704	1.790693	-1.005455
H	0.164409	2.862826	-0.162854
H	0.173792	1.425241	-2.275775
C	0.714538	0.018600	0.317198
C	-0.129449	-0.436487	1.339364
C	1.943167	-0.634090	0.155641
C	0.241373	-1.494801	2.166409
H	-1.086954	0.048358	1.493470
C	2.319019	-1.699756	0.970656
H	2.620033	-0.294980	-0.620317
C	1.466006	-2.131292	1.982545
H	-0.426246	-1.820867	2.956467
H	3.280213	-2.178797	0.819078
H	1.755442	-2.954127	2.626683
C	-4.183644	-1.136366	-0.742291
C	-3.558821	-2.386073	-0.707118
C	-5.549799	-1.060932	-1.024870
C	-4.298875	-3.535179	-0.958682
H	-2.499641	-2.437798	-0.500689
C	-6.284410	-2.217285	-1.260534
H	-6.026627	-0.089015	-1.051021
C	-5.662614	-3.461798	-1.232442
H	-3.802520	-4.497785	-0.932047
H	-7.343465	-2.141183	-1.476781
H	-6.232001	-4.363447	-1.422487
C	3.055330	2.489062	-1.785971
O	3.278182	3.594819	-1.298546
O	3.990228	1.460102	-1.575579
H	2.541015	2.332143	-2.742201
C	5.572908	-0.048603	0.150866
C	5.563772	-1.019294	-0.857509
C	6.117971	-0.394531	1.392406
C	6.085339	-2.291666	-0.634115
H	5.122183	-0.774569	-1.816514
C	6.642204	-1.662817	1.623186
H	6.119090	0.331292	2.200229
C	6.626515	-2.615060	0.607022
H	6.061444	-3.032033	-1.425201
H	7.052468	-1.912387	2.594756
H	7.027324	-3.606219	0.784637
Si	4.829532	1.657738	-0.137950
H	5.938641	2.645148	-0.234000
H	3.961739	1.990403	1.017276
C	-4.053750	0.987238	0.437183
C	-4.060608	2.357956	0.165807
C	-4.666701	0.519840	1.603213
C	-4.665785	3.238679	1.053937
H	-3.571658	2.719088	-0.726855
C	-5.284302	1.406133	2.477942
H	-4.656386	-0.542891	1.810457
C	-5.286010	2.771587	2.209992
H	-4.654975	4.299661	0.835370
H	-5.753984	1.026174	3.377340
H	-5.759808	3.463990	2.894952

TS16w

M05-2X/BS1 SCF energy in gas phase: -1306.482079 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1306.798983 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1306.49032 a.u

Si	-1.716707	-1.863659	0.127804
C	-3.261961	-0.861825	-0.178856

C	-4.524270	-1.464648	-0.153026
C	-3.185364	0.517395	-0.407224
C	-5.680970	-0.712719	-0.337655
H	-4.608673	-2.535435	0.004422
C	-4.338797	1.272891	-0.593698
H	-2.215951	0.999527	-0.449694
C	-5.587878	0.658811	-0.557155
H	-6.650656	-1.194851	-0.316813
H	-4.261827	2.339164	-0.770770
H	-6.486578	1.245594	-0.704264
O	0.982432	-2.547779	0.003308
C	0.784389	-1.398844	-0.624164
H	1.270505	-1.314043	-1.602129
O	-0.538834	-1.023517	-0.742519
N	1.516731	-0.206272	0.241265
H	1.540200	-0.762845	1.303581
O	1.430146	-1.715173	2.184333
H	2.284546	-1.987059	2.532441
H	1.183062	-2.318787	1.212529
H	-1.933294	-3.244374	-0.369725
H	-1.381294	-1.894669	1.573449
C	2.912552	-0.048057	-0.133935
C	3.545534	1.193693	-0.089962
C	3.643579	-1.193663	-0.460075
C	4.898211	1.288942	-0.402089
H	2.992781	2.079250	0.189311
C	4.993859	-1.080640	-0.774214
H	3.154372	-2.159129	-0.458796
C	5.627144	0.157375	-0.751074
H	5.380451	2.257636	-0.367277
H	5.550684	-1.972013	-1.034199
H	6.678301	0.239020	-0.995693
C	0.736267	1.006736	0.329317
C	0.561397	1.826068	-0.784228
C	0.130758	1.314811	1.541561
C	-0.208793	2.976453	-0.670100
H	1.026205	1.557821	-1.725016
C	-0.646766	2.466886	1.645757
H	0.262992	0.647934	2.385319
C	-0.811654	3.300924	0.545782
H	-0.346111	3.616697	-1.532215
H	-1.123106	2.706756	2.587425
H	-1.413199	4.197152	0.629257

TS16$_{by}^{-}$

M05-2X/BS1 SCF energy in gas phase: -1936.722572 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1937.264157 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1936.793952 a.u

C	2.578301	0.559888	-1.266144
O	1.557893	1.408170	-0.940985
O	3.706669	1.028358	-0.904378
H	1.097123	-1.066800	-0.567423
H	2.444962	0.041104	-2.220345
N	2.146823	-0.932009	-0.273429
C	0.931891	3.818016	0.160723
C	-0.029775	3.499274	1.129837
C	0.736885	4.991272	-0.576485
C	-1.143265	4.306063	1.343875
H	0.094633	2.598658	1.722851
C	-0.371129	5.811519	-0.367686
H	1.464778	5.266319	-1.333853
C	-1.316429	5.467139	0.593470
H	-1.879084	4.028379	2.089769
H	-0.498747	6.713783	-0.955523
H	-2.184219	6.096053	0.755841
O	-0.280138	-1.134356	-1.082826
O	-0.863735	-2.815544	0.292647
C	-1.098274	-1.811950	-0.391131
N	-2.447723	-1.307737	-0.413177
Si	2.429061	2.682933	-0.174451
H	3.001616	2.451952	1.174511
H	3.254132	3.554483	-1.055016
C	2.889167	-2.091319	-0.703173
C	4.195926	-1.978649	-1.177308
C	2.242614	-3.327842	-0.670005
C	4.864133	-3.123333	-1.606483
H	4.661132	-1.000940	-1.210397
C	2.923772	-4.459648	-1.105015
H	1.218811	-3.376440	-0.307086
C	4.233639	-4.362803	-1.570777
H	5.879948	-3.040608	-1.974499
H	2.425889	-5.421511	-1.080360
H	4.758082	-5.249225	-1.907955
C	-2.771481	-0.099184	-1.089308
C	-1.980677	1.049761	-0.986523
C	-3.941036	-0.048363	-1.855402

C	-2.362962	2.221016	-1.631064
H	-1.050110	1.020572	-0.441459
C	-4.324109	1.129341	-2.486632
H	-4.548979	-0.940859	-1.940536
C	-3.537674	2.272599	-2.377489
H	-1.731565	3.096798	-1.534686
H	-5.236219	1.147304	-3.072252
H	-3.832959	3.190589	-2.871342
C	-3.472325	-1.957578	0.310135
C	-4.414883	-1.195584	1.012238
C	-3.586639	-3.353108	0.333873
C	-5.448945	-1.809238	1.708628
H	-4.328135	-0.116614	1.001134
C	-4.617086	-3.957283	1.043799
H	-2.846405	-3.943199	-0.183111
C	-5.558764	-3.196265	1.731946
H	-6.165090	-1.196381	2.243754
H	-4.685650	-5.039110	1.052328
H	-6.361522	-3.676218	2.278652
C	2.258940	-0.578276	1.103168
C	1.115022	-0.141916	1.772880
C	3.493368	-0.571685	1.750588
C	1.209449	0.287541	3.092012
H	0.166503	-0.153804	1.253996
C	3.576094	-0.138942	3.069533
H	4.375991	-0.899490	1.220262
C	2.438920	0.294039	3.744961
H	0.315277	0.612938	3.610157
H	4.538119	-0.132621	3.567651
H	2.509616	0.632013	4.771580

IM17$_{by}^{-}$

M05-2X/BS1 SCF energy in gas phase: -1936.731848 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1937.270005 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1936.795177 a.u

C	2.304397	0.669569	-1.078891
O	1.206139	1.445290	-0.722236
O	3.366380	1.448060	-0.753607
H	0.752855	-1.084055	-0.838033
H	2.264532	0.357179	-2.133487
N	2.230292	-0.641327	-0.319070
C	0.553471	3.814339	0.228772
C	-0.302935	3.451780	1.279257
C	0.163533	4.910984	-0.548387
C	-1.488958	4.135079	1.535877
H	-0.029398	2.610586	1.911219
C	-1.019575	5.610566	-0.303812
H	0.803890	5.224047	-1.368500
C	-1.853215	5.220608	0.740471
H	-2.132112	3.823641	2.352112
H	-1.292417	6.455820	-0.927384
H	-2.776459	5.755137	0.934033
O	-0.202690	-1.147433	-1.209076
O	-0.566559	-2.752961	0.327293
C	-0.962387	-1.865079	-0.409430
N	-2.306013	-1.493585	-0.491044
Si	2.175976	2.795780	-0.153847
H	2.745904	2.827287	1.234760
H	2.771740	3.829309	-1.071722
C	3.130805	-1.648020	-0.798514
C	4.298136	-1.335765	-1.497983
C	2.789949	-2.982788	-0.560560
C	5.112284	-2.366665	-1.964093
H	4.559900	-0.294701	-1.641388
C	3.618729	-3.999111	-1.017448
H	1.864252	-3.195080	-0.035849
C	4.781658	-3.696084	-1.724888
H	6.017483	-2.123014	-2.507883
H	3.348641	-5.032086	-0.832518
H	5.422722	-4.491219	-2.086526
C	-2.712637	-0.284123	-1.144389
C	-2.055459	0.925613	-0.918204
C	-3.822598	-0.326411	-1.988730
C	-2.510976	2.085032	-1.536993
H	-1.162984	0.971787	-0.310566
C	-4.281132	0.838894	-2.592795
H	-4.321576	-1.273036	-2.156934
C	-3.627078	2.047781	-2.368967
H	-1.981367	3.012412	-1.352403
H	-5.145536	0.797650	-3.245070
H	-3.981919	2.954807	-2.843154
C	-3.281444	-2.225902	0.235103
C	-4.290623	-1.542038	0.918244
C	-3.264218	-3.622956	0.259199
C	-5.269587	-2.246243	1.609335
H	-4.299893	-0.460019	0.899684

C	-4.241283	-4.316469	0.962568
H	-2.473195	-4.149845	-0.253105
C	-5.251789	-3.637224	1.637852
H	-6.044062	-1.700143	2.134480
H	-4.212747	-5.399466	0.976721
H	-6.012710	-4.184513	2.180470
C	2.290367	-0.436304	1.105769
C	1.117238	-0.162314	1.805227
C	3.510870	-0.445826	1.779296
C	1.164500	0.084506	3.173562
H	0.178352	-0.134875	1.272722
C	3.552108	-0.205840	3.147863
H	4.418396	-0.629348	1.220216
C	2.379995	0.060219	3.850009
H	0.246007	0.292788	3.708749
H	4.505009	-0.211901	3.663350
H	2.414046	0.251820	4.915769

TS17$_{by}^{-}$

M05-2X/BS1 SCF energy in gas phase: -1936.72452 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1937.262946 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1936.788355 a.u

C	2.363338	0.542399	-1.151318
O	1.207893	1.125775	-0.623567
O	3.260700	1.572980	-1.134376
H	0.322449	-0.823598	-0.777953
H	2.182701	0.133468	-2.158620
N	2.708237	-0.635773	-0.323464
C	0.280367	3.458779	0.240675
C	-0.348703	2.879696	1.354419
C	-0.307317	4.616599	-0.281285
C	-1.503696	3.422530	1.913117
H	0.076452	1.976541	1.785021
C	-1.459855	5.178592	0.271421
H	0.149376	5.089738	-1.146458
C	-2.065362	4.578400	1.371636
H	-1.968632	2.946683	2.770084
H	-1.888424	6.078107	-0.158921
H	-2.964312	5.004248	1.803129
O	-0.576866	-0.956179	-1.131807
O	-0.883774	-2.420412	0.558691
C	-1.317016	-1.654617	-0.279982
N	-2.671618	-1.418009	-0.482122
Si	1.935872	2.729363	-0.496086
H	2.817650	3.223402	0.619746
H	1.982125	3.647074	-1.687805
C	3.750390	-1.449998	-0.813217
C	4.530860	-1.084141	-1.918467
C	4.001266	-2.681551	-0.189438
C	5.507277	-1.953188	-2.399464
H	4.403763	-0.103801	-2.356613
C	4.990250	-3.528095	-0.666932
H	3.401974	-2.959548	0.668587
C	5.746848	-3.176572	-1.784436
H	6.101563	-1.652452	-3.254871
H	5.164604	-4.474930	-0.168855
H	6.514726	-3.841670	-2.160281
C	-3.116291	-0.252670	-1.187624
C	-2.582127	1.001754	-0.897819
C	-4.127017	-0.383585	-2.138174
C	-3.056466	2.123523	-1.567942
H	-1.781123	1.107358	-0.178881
C	-4.608654	0.745038	-2.792612
H	-4.530193	-1.366427	-2.349701
C	-4.074432	1.999705	-2.510637
H	-2.621332	3.087749	-1.335320
H	-5.395585	0.639949	-3.529892
H	-4.446384	2.876493	-3.026511
C	-3.630257	-2.196554	0.219780
C	-4.757288	-1.580893	0.768826
C	-3.473984	-3.579452	0.344109
C	-5.716177	-2.341664	1.428324
H	-4.874616	-0.509318	0.674788
C	-4.432265	-4.327350	1.016116
H	-2.595275	-4.052697	-0.067929
C	-5.560621	-3.717695	1.558341
H	-6.584196	-1.849460	1.849830
H	-4.295320	-5.397911	1.110086
H	-6.306469	-4.307165	2.076909
C	2.768424	-0.358586	1.086530
C	1.776431	-0.851235	1.930918
C	3.810226	0.413096	1.603793
C	1.827621	-0.571293	3.294657
H	0.979761	-1.457753	1.516835
C	3.851968	0.693369	2.965559
H	4.548221	0.805176	0.916969

C	2.862451	0.201711	3.813539
H	1.054231	-0.956721	3.948264
H	4.652831	1.305425	3.362881
H	2.896136	0.423822	4.873782

IM21

M05-2X/BS1 SCF energy in gas phase: -1195.185593 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1195.418847 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1195.232571 a.u

Si	-1.996184	-1.203481	0.806032
H	-2.052461	-1.395428	2.275191
C	-1.704128	0.579263	0.378380
C	-1.028548	1.420792	1.268975
C	-2.078676	1.086787	-0.872859
C	-0.721354	2.732119	0.918631
H	-0.731540	1.047893	2.243714
C	-1.770949	2.396573	-1.229331
H	-2.619234	0.451369	-1.565359
C	-1.088719	3.217813	-0.333459
H	-0.194717	3.371334	1.616318
H	-2.065436	2.778443	-2.199047
H	-0.850006	4.237803	-0.609554
Si	0.417762	-1.996736	-0.917088
H	0.997536	-3.346559	-1.129136
H	-0.198947	-1.492443	-2.174540
C	1.780667	-0.831294	-0.407508
C	2.937826	-1.316210	0.215380
C	1.676977	0.546173	-0.643617
C	3.958840	-0.452757	0.600421
H	3.045077	-2.380193	0.398861
C	2.693869	1.413383	-0.257374
H	0.791602	0.949600	-1.124056
C	3.835110	0.913817	0.364399
H	4.847892	-0.843067	1.080048
H	2.593141	2.476042	-0.441368
H	4.628723	1.587952	0.662978
O	-0.764263	-2.158461	0.246397
O	-3.413746	-1.630562	0.067271
H	-3.615145	-2.566268	-0.000845

IM3$_{OH}$

M05-2X/BS1 SCF energy in gas phase: -1360.690348 a.u.

M05-2X/BS2 SCF energy in THF solution: -1361.029956 a.u.

M05-2X/BS2 Free energy in THF solution: -1360.637159 a.u

O	-0.426060	2.316064	-0.729732
O	1.033554	0.906539	0.263683
C	0.722928	2.028502	-0.297280
N	-2.315797	0.340267	-1.353746
H	-1.562208	1.025626	-1.456650
N	-2.483354	1.233921	0.743211
H	-1.726691	1.836489	0.400390
N	-3.521005	-0.802687	0.291186
C	-2.754210	0.231624	-0.093237
C	-2.375831	-0.778335	-2.281286
H	-1.526645	-1.453025	-2.130676
H	-2.317611	-0.376140	-3.291696
C	-3.691736	-1.505543	-2.057246
H	-4.524883	-0.840540	-2.293932
H	-3.757182	-2.385792	-2.696776
C	-3.772236	-1.931750	-0.600332
H	-4.764759	-2.321246	-0.364795
H	-3.040011	-2.722247	-0.396941
C	-3.840571	-1.007767	1.705782
H	-3.814152	-2.084175	1.887415
H	-4.858388	-0.657482	1.906209
C	-2.832042	-0.298106	2.596687
H	-3.143844	-0.376558	3.638548
H	-1.850080	-0.752638	2.466174
C	-2.749017	1.159175	2.171515
H	-3.679490	1.684790	2.408076
H	-1.932753	1.664730	2.685024
Si	0.805256	-0.822417	-0.547932
H	0.559465	-0.067265	-1.827792
C	2.583028	-1.286046	-0.069110
C	3.272894	-2.218319	-0.852856
C	3.231936	-0.793799	1.071322
C	4.570198	-2.616376	-0.540697
H	2.777978	-2.644435	-1.719380
C	4.518077	-1.208198	1.409476
H	2.716198	-0.075533	1.697120
C	5.195118	-2.113834	0.597121
H	5.088099	-3.326397	-1.174954

H	4.993704	-0.822208	2.303746
H	6.199503	-2.430179	0.852697
N	1.716146	2.953741	-0.396989
C	1.438363	4.296234	-0.858674
H	1.640437	5.023684	-0.065362
H	2.073859	4.539485	-1.714811
H	0.395885	4.355231	-1.152314
C	3.066029	2.695684	0.058707
H	3.257095	3.175985	1.024771
H	3.223198	1.626499	0.152477
H	3.771586	3.101057	-0.670509
H	0.510933	-2.206299	-1.227139
O	-0.432412	-1.091385	0.611391
H	-0.652965	-2.022892	0.524413

$TS2_{OH}$

M05-2X/BS1 SCF energy in gas phase: -1549.249321 a.u.

M05-2X/BS2 SCF energy in THF solution: -1549.654362 a.u.

M05-2X/BS2 Free energy in THF solution: -1549.253458 a.u

O	-0.011761	2.528889	-0.599410
O	1.826768	1.326139	-0.062755
C	1.214728	2.429178	-0.350899
N	-2.012442	0.704175	-1.354943
H	-1.175944	1.292905	-1.377045
N	-2.317334	1.619922	0.718790
H	-1.409504	2.048369	0.522718
N	-3.618725	-0.202351	0.069542
C	-2.645181	0.687499	-0.178550
C	-2.163818	-0.376973	-2.314260
H	-1.513411	-1.217119	-2.050489
H	-1.853993	-0.003247	-3.288522
C	-3.628313	-0.787903	-2.324231
H	-4.235671	0.053731	-2.663169
H	-3.790211	-1.625489	-3.002586
C	-4.041897	-1.194134	-0.917742
H	-5.128690	-1.283116	-0.848048
H	-3.604979	-2.160291	-0.649041
C	-4.180310	-0.350000	1.410938
H	-4.367920	-1.414678	1.561293
H	-5.136975	0.179550	1.470711
C	-3.206162	0.161017	2.460048
H	-3.682525	0.147671	3.440503
H	-2.334639	-0.491947	2.487791
C	-2.771040	1.573115	2.101068
H	-3.596624	2.275788	2.247136
H	-1.937246	1.886307	2.727093
Si	1.036974	-0.347008	-0.247948
H	0.668426	0.018183	-1.658090
C	2.693410	-1.230335	0.005511
C	2.840252	-2.553801	-0.429010
C	3.793303	-0.628873	0.633317
C	4.039426	-3.243360	-0.269294
H	1.997515	-3.053800	-0.894173
C	4.988540	-1.318488	0.817370
H	3.702789	0.389801	0.987206
C	5.117189	-2.626698	0.358873
H	4.129143	-4.263036	-0.624956
H	5.821117	-0.834977	1.315249
H	6.049005	-3.162723	0.495168
N	2.007502	3.537046	-0.387013
C	1.428050	4.852134	-0.547695
H	1.509620	5.430910	0.378780
H	1.950011	5.396426	-1.339020
H	0.382161	4.740092	-0.813271
C	3.417212	3.477889	-0.058930
H	3.597997	3.739451	0.989417
H	3.792644	2.477035	-0.245978
H	3.955951	4.188713	-0.689199
H	0.244266	-1.755046	-0.434382
C	-0.954703	-3.146001	0.187214
O	-0.579659	-4.015541	-0.496541
O	-1.565361	-2.511321	0.974970
O	0.059099	0.007824	1.094956
H	-0.439763	-0.786411	1.309421

$IM4_{OH}$

M05-2X/BS1 SCF energy in gas phase: -786.750027 a.u.

M05-2X/BS2 SCF energy in THF solution: -786.934257 a.u.

M05-2X/BS2 Free energy in THF solution: -786.831289 a.u

O	3.803500	0.217893	-0.287573
O	1.738106	0.895223	0.302809
C	3.068856	1.037645	0.190765

Si	0.976106	-0.498341	-0.328308
H	1.445286	-0.710547	-1.707401
C	-0.827130	-0.095217	-0.149174
C	-1.760585	-1.140370	-0.142094
C	-1.292932	1.220185	-0.033572
C	-3.122490	-0.880267	-0.029189
H	-1.419210	-2.167458	-0.221105
C	-2.654353	1.483783	0.080067
H	-0.584059	2.039513	-0.021307
C	-3.568851	0.433891	0.080816
H	-3.832758	-1.697643	-0.025077
H	-3.002247	2.505220	0.171293
H	-4.628436	0.639560	0.169966
O	1.330355	-1.866058	0.518029
H	0.926431	-1.967780	1.383081
H	3.398737	2.001555	0.595032

$TS3_{OH}$

M05-2X/BS1 SCF energy in gas phase: -998.32169 a.u.

M05-2X/BS2 SCF energy in THF solution: -998.578684 a.u.

M05-2X/BS2 Free energy in THF solution: -998.357466 a.u

Si	0.389302	1.327141	0.019533
C	1.954816	0.310998	0.055788
C	3.043684	0.836898	0.761709
C	2.119520	-0.919507	-0.596410
C	4.259742	0.160809	0.823255
H	2.943265	1.790911	1.268867
C	3.332711	-1.596821	-0.538967
H	1.284388	-1.350293	-1.132916
C	4.404293	-1.058291	0.170314
H	5.089867	0.585368	1.374685
H	3.444363	-2.547035	-1.047282
H	5.348444	-1.588036	0.212290
O	-1.028975	-1.138830	-0.621432
C	-1.420787	-0.629013	0.550683
H	-1.311390	-1.335228	1.384171
O	-0.867655	0.592754	0.897761
N	-2.958385	-0.351883	0.449904
H	-2.993753	0.144855	-0.513007
C	-3.676758	-1.633637	0.315572
H	-4.721803	-1.438963	0.081299
H	-3.203873	-2.199611	-0.482034
H	-3.607031	-2.184879	1.253981
O	-2.341821	0.388139	-1.895830
H	-2.717047	0.171404	-2.751396
H	-1.571993	-0.486856	-1.415819
C	-3.482753	0.470955	1.553451
H	-3.280043	-0.032369	2.499753
H	-2.984715	1.433817	1.540474
H	-4.557468	0.591758	1.424309
O	-0.111228	1.752487	-1.473559
H	-0.970444	1.386704	-1.792490
H	0.658337	2.530915	0.844435

$TS3_{byOH}$

M05-2X/BS1 SCF energy in gas phase: -2147.458473 a.u.

M05-2X/BS2 SCF energy in THF solution: -2147.969624 a.u.

M05-2X/BS2 Free energy in THF solution: -2147.448142 a.u

O	-2.875902	2.253133	-0.466813
O	-0.795446	2.663185	0.310367
C	-1.844885	2.959013	-0.405114
N	-1.765419	4.129457	-1.090700
C	-0.566828	4.943673	-1.117264
H	-0.106701	4.919146	-2.110497
H	-0.823233	5.980295	-0.884014
H	0.140321	4.572791	-0.383198
Si	-0.478681	0.955439	0.980625
H	-0.277719	-0.596421	1.528210
H	-0.968531	0.324975	-0.278954
C	1.361681	1.309105	1.174541
C	2.082622	2.033768	0.217220
C	2.066695	0.781813	2.262231
C	3.458433	2.215941	0.334531
H	1.560636	2.449494	-0.637271
C	3.436089	0.981626	2.401408
H	1.533403	0.191590	2.999779
C	4.136759	1.692513	1.430529
H	4.002604	2.755247	-0.431688
H	3.961339	0.565218	3.252747
H	5.208808	1.821260	1.517675
C	0.071734	-2.016138	0.958523
O	-0.703433	-2.276333	0.015254

O	1.399969	-1.806497	0.714118
H	-0.074698	-2.432177	1.960506
C	3.698615	-1.254882	-0.805158
C	4.463722	-1.721751	0.269031
C	4.330495	-0.497048	-1.796756
C	5.827552	-1.454565	0.340324
H	3.980850	-2.282007	1.060978
C	5.693537	-0.226421	-1.731187
H	3.748992	-0.102894	-2.624273
C	6.442845	-0.708003	-0.661059
H	6.408841	-1.821067	1.177852
H	6.169692	0.360402	-2.507398
H	7.504269	-0.497511	-0.605306
Si	1.872154	-1.563967	-0.888393
H	1.205359	-0.398490	-1.511909
C	-2.857316	4.559896	-1.937214
H	-2.572246	4.510468	-2.993058
H	-3.711367	3.914050	-1.762247
H	-3.123428	5.593511	-1.701545
N	-3.328736	-0.435838	-1.389869
H	-3.131677	0.561762	-1.385919
N	-3.835059	-0.081353	0.817850
H	-3.522744	0.874494	0.651118
N	-3.653741	-2.259642	0.030888
C	-3.579488	-0.939146	-0.171155
C	-2.718988	-1.279709	-2.407846
H	-1.663352	-1.449190	-2.177178
H	-2.805727	-0.766091	-3.363917
C	-3.488430	-2.592200	-2.416146
H	-4.531208	-2.394387	-2.672108
H	-3.075959	-3.280557	-3.154060
C	-3.383573	-3.224549	-1.036760
H	-4.101062	-4.041870	-0.928052
H	-2.374703	-3.607824	-0.873511
C	-3.565377	-2.828620	1.379786
H	-2.775323	-3.581726	1.347463
H	-4.512801	-3.324043	1.613085
C	-3.229580	-1.773314	2.421396
H	-3.404305	-2.178801	3.418355
H	-2.184299	-1.474700	2.335378
C	-4.076642	-0.536483	2.177291
H	-5.140658	-0.750354	2.319197
H	-3.773799	0.267733	2.841739
O	1.529403	-2.940369	-1.747905
H	0.627243	-3.215711	-1.540152
O	-1.510565	1.217556	2.299173
H	-1.734998	2.151905	2.353295

IM5$_{OH}$

M05-2X/BS1 SCF energy in gas phase: -921.911739 a.u.

M05-2X/BS2 SCF energy in THF solution: -922.126211 a.u.

M05-2X/BS2 Free energy in THF solution: -921.926864 a.u

Si	0.046121	-1.009559	-0.054345
C	1.777247	-0.356064	-0.056765
C	2.875286	-1.207556	0.106410
C	2.003946	1.016564	-0.220795
C	4.171268	-0.701584	0.118370
H	2.719922	-2.275492	0.221297
C	3.298689	1.525028	-0.209602
H	1.159568	1.683106	-0.358956
C	4.381258	0.665652	-0.039270
H	5.014203	-1.369314	0.246150
H	3.464965	2.587486	-0.337581
H	5.389596	1.061178	-0.033405
O	-1.406166	1.677419	0.413243
C	-1.911361	0.769538	-0.512573
H	-2.319606	1.364480	-1.338530
O	-0.915727	-0.057904	-1.045195
N	-2.945353	-0.062217	0.108768
C	-4.020380	0.773085	0.645921
H	-4.752548	0.132004	1.136532
H	-3.620054	1.477946	1.368924
H	-4.530459	1.337566	-0.148804
H	-1.076015	1.161460	1.165161
C	-3.499817	-1.010190	-0.859317
H	-3.965804	-0.494187	-1.711637
H	-2.718558	-1.665281	-1.237218
H	-4.260548	-1.612840	-0.363462
O	-0.605273	-0.911687	1.472900
H	-1.578481	-0.932181	1.414490
H	0.006099	-2.396052	-0.585374

TS4$_{OH}$

M05-2X/BS1 SCF energy in gas phase: -998.308624 a.u.

M05-2X/BS2 SCF energy in THF solution:

-998.562483 a.u.

M05-2X/BS2 Free energy in THF solution: -998.345812 a.u

Si	-0.266280	1.405267	-0.418774
C	-1.832563	0.394370	-0.244898
C	-2.948844	0.890834	0.436759
C	-1.895467	-0.906669	-0.767495
C	-4.093246	0.113049	0.597617
H	-2.911603	1.894984	0.842492
C	-3.035185	-1.689583	-0.604551
H	-1.042949	-1.312704	-1.304758
C	-4.136088	-1.177984	0.079606
H	-4.950080	0.512290	1.126786
H	-3.069423	-2.691702	-1.014866
H	-5.025367	-1.783887	0.204951
O	1.527897	-1.572793	-0.890019
C	2.193741	-0.456852	-0.869707
H	2.072682	0.215080	-1.713868
O	1.002750	0.672754	0.296075
N	3.349192	-0.346484	-0.206573
C	3.609899	-1.226902	0.922568
H	3.081333	-0.882513	1.815346
H	3.278539	-2.232586	0.677795
H	4.682658	-1.236058	1.111072
H	1.090111	-1.746466	0.092479
C	3.935934	0.979113	-0.122127
H	5.013703	0.889047	0.011709
H	3.737342	1.525410	-1.043404
H	3.495408	1.528840	0.712585
O	0.532362	-1.499842	1.314709
H	-0.416627	-1.671419	1.287511
H	0.647549	-0.476451	1.073923
O	-0.605337	2.882876	0.270863
H	0.107017	3.246683	0.800543
H	0.042825	1.592877	-1.871090

[Si]H(OH)$_2$

M05-2X/BS1 SCF energy in gas phase: -673.432232 a.u.

M05-2X/BS2 SCF energy in THF solution: -673.58322 a.u.

M05-2X/BS2 Free energy in THF solution: -673.486665 a.u

Si	-0.266280	1.405267	-0.418774
C	-1.832563	0.394370	-0.244898
C	-2.948844	0.890834	0.436759
C	-1.895467	-0.906669	-0.767495
C	-4.093246	0.113049	0.597617
H	-2.911603	1.894984	0.842492
C	-3.035185	-1.689583	-0.604551
H	-1.042949	-1.312704	-1.304758
C	-4.136088	-1.177984	0.079606
H	-4.950080	0.512290	1.126786
H	-3.069423	-2.691702	-1.014866
H	-5.025367	-1.783887	0.204951
O	1.527897	-1.572793	-0.890019
C	2.193741	-0.456852	-0.869707
H	2.072682	0.215080	-1.713868
O	1.002750	0.672754	0.296075
N	3.349192	-0.346484	-0.206573
C	3.609899	-1.226902	0.922568
H	3.081333	-0.882513	1.815346
H	3.278539	-2.232586	0.677795
H	4.682658	-1.236058	1.111072
H	1.090111	-1.746466	0.092479
C	3.935934	0.979113	-0.122127
H	5.013703	0.889047	0.011709
H	3.737342	1.525410	-1.043404
H	3.495408	1.528840	0.712585
O	0.532362	-1.499842	1.314709
H	-0.416627	-1.671419	1.287511
H	0.647549	-0.476451	1.073923
O	-0.605337	2.882876	0.270863
H	0.107017	3.246683	0.800543
H	0.042825	1.592877	-1.871090

TS4$_{OH}^-$

M05-2X/BS1 SCF energy in gas phase: -1109.892112 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1110.247472 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1110.063337 a.u

C	2.102277	-0.838919	-0.327527
O	1.870258	-1.264514	-1.467210
O	1.241704	-0.724109	0.636928
C	-3.514541	-1.898265	0.112435

O	-3.371443	-2.851808	0.795411
O	-4.044948	-1.221107	-0.702371
H	-2.276384	-0.854979	0.667912
Si	-0.676543	-0.778788	0.563086
H	-0.565158	-1.242193	1.982315
C	-0.775924	1.107396	0.241552
C	0.293257	1.999912	0.402926
C	-2.000355	1.646884	-0.180149
C	0.147936	3.365629	0.168154
H	1.256549	1.614721	0.712273
C	-2.152099	3.009097	-0.429873
H	-2.842811	0.978853	-0.322166
C	-1.077645	3.875498	-0.250256
H	0.993007	4.031386	0.307954
H	-3.109717	3.393360	-0.763931
H	-1.192823	4.937511	-0.438525
N	3.384812	-0.425703	0.005377
C	3.764636	-0.157816	1.371684
H	4.292807	-1.012180	1.817410
H	4.433613	0.708143	1.408090
H	2.872259	0.045443	1.954537
O	-0.696144	-1.821038	-0.739033
H	0.167099	-1.831838	-1.190008
C	4.465539	-0.697382	-0.909625
H	5.039185	-1.584342	-0.606533
H	4.044795	-0.867580	-1.895539
H	5.151594	0.155058	-0.940350

$IM8_{OH}$

M05-2X/BS1 SCF energy in gas phase: -786.745168 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -786.934089 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -786.831142 a.u

O	-1.240787	2.208910	-0.422964
H	-2.017754	2.763040	-0.325422
C	0.681749	0.293611	0.271518
C	1.610643	1.042388	-0.460806
C	1.055224	-0.972227	0.743492
C	2.882970	0.538570	-0.713642
H	1.327835	2.016660	-0.841230
C	2.326400	-1.476751	0.492489
H	0.347187	-1.573060	1.305662
C	3.240275	-0.719109	-0.235886
H	3.593312	1.123723	-1.284151
H	2.603441	-2.456750	0.859899
H	4.230303	-1.111330	-0.433375
Si	-1.003533	0.966249	0.635137
H	-1.236278	1.390416	2.031657
O	-2.145354	-0.260085	0.425263
C	-2.157695	-1.146787	-0.595888
H	-1.284184	-1.064302	-1.259432
O	-3.032834	-1.945581	-0.746449

$TS5_{OH}^-$

M05-2X/BS1 SCF energy in gas phase: -1245.074903 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1245.467377 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1245.187018 a.u

C	-0.284989	1.084273	-0.906274
O	-0.058071	2.251500	-1.212466
O	0.764394	0.269871	-0.557828
H	-2.241231	1.151665	0.872437
H	-1.196075	0.517002	-1.100030
Si	2.205575	1.078182	-0.271344
N	-1.255193	1.203512	1.164087
C	-0.964768	2.458088	1.818559
H	-1.061563	3.267677	1.092427
H	-1.623282	2.664484	2.676361
H	0.067545	2.455199	2.180299
C	3.464635	-0.275339	-0.021222
C	4.812412	-0.078060	-0.342131
C	3.079089	-1.511462	0.510914
C	5.753063	-1.081632	-0.127449
H	5.121167	0.864955	-0.779823
C	4.016369	-2.517704	0.728318
H	2.033444	-1.688357	0.737742
C	5.355133	-2.301896	0.412186
H	6.792628	-0.915394	-0.385083
H	3.701748	-3.470745	1.136824
H	6.085374	-3.085338	0.579089
C	-3.848269	-0.355494	-0.195057
O	-3.992763	0.642963	0.558822
O	-2.777134	-0.815774	-0.663643
C	-0.971204	0.030245	1.962287

H	-1.478386	0.040960	2.939890
H	-1.307413	-0.837926	1.395301
H	0.107818	-0.048588	2.139439
N	-5.047636	-1.027770	-0.579637
C	-4.938854	-2.347452	-1.141862
H	-4.979933	-3.137322	-0.372196
H	-5.760749	-2.530662	-1.844741
H	-3.985619	-2.414721	-1.657297
C	-6.243534	-0.785704	0.182368
H	-6.189748	0.222668	0.581195
H	-7.129478	-0.890641	-0.456000
H	-6.356652	-1.491904	1.022905
O	2.718564	1.987459	-1.554495
H	1.956737	2.505198	-1.854327
H	2.070995	1.901723	0.956321

$TS5_{byOH^-}$

M05-2X/BS1 SCF energy in gas phase: -1708.089636 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1708.557967 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1708.254351 a.u

O	-4.271257	-1.565173	-0.558387
O	-3.034254	0.250864	-0.012934
C	-4.080820	-0.358321	-0.525342
N	-5.013166	0.534099	-1.046910
C	-4.703326	1.932337	-1.222072
H	-4.248505	2.138537	-2.202122
H	-5.626195	2.516185	-1.150852
H	-4.016852	2.249762	-0.443452
Si	-1.713698	-0.660857	0.843297
H	-0.499639	-1.481574	1.654463
H	-1.496985	-1.619741	-0.276737
C	-0.639405	0.929807	0.910812
C	-0.784898	1.985465	-0.002536
C	0.310858	1.098113	1.926325
C	-0.031254	3.153673	0.100285
H	-1.514330	1.888142	-0.796845
C	1.057033	2.268397	2.052551
H	0.473763	0.284378	2.623716
C	0.885837	3.304415	1.138391
H	-0.165587	3.949532	-0.624372
H	1.780396	2.365943	2.854147
H	1.467355	4.215595	1.227585
C	0.769932	-2.582495	1.357793
O	0.399849	-3.389797	0.505128
O	1.726754	-1.643924	1.056713
H	0.749728	-2.790795	2.430475
C	3.428207	-0.253102	-0.744891
C	4.743681	-0.665593	-0.980562
C	3.166529	1.114578	-0.604735
C	5.776594	0.264514	-1.063421
H	4.950996	-1.722624	-1.102980
C	4.197185	2.047027	-0.678636
H	2.150822	1.454769	-0.431583
C	5.503303	1.621605	-0.908190
H	6.792335	-0.066180	-1.247801
H	3.976969	3.101195	-0.556608
H	6.307555	2.346143	-0.969170
Si	2.023797	-1.465992	-0.597438
H	0.831235	-0.914516	-1.270610
C	-6.069779	0.005368	-1.872538
H	-5.839773	0.101527	-2.943358
H	-6.190570	-1.046426	-1.631299
H	-7.003609	0.542106	-1.677304
O	2.545824	-2.900474	-1.240439
H	1.916285	-3.581085	-0.960179
O	-2.734783	-0.948481	2.161530
H	-2.279760	-1.512515	2.788928

$IM9_{OH^-}$

M05-2X/BS1 SCF energy in gas phase: -1245.096106 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1245.481935 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1245.198645 a.u

C	0.272518	-0.195508	-0.163406
O	0.019701	-1.231009	0.668845
O	-0.995970	0.315167	-0.460164
H	2.198321	0.496658	0.667461
H	0.854327	-0.432440	-1.061807
Si	-1.844253	-0.865657	0.513506
N	1.100620	0.877548	0.520576
C	0.559486	1.233685	1.837745
H	0.419189	0.315354	2.400647
H	1.277288	1.884983	2.337398

H	-0.398345	1.742898	1.723381
C	-3.590608	-0.209776	0.002463
C	-4.691098	-1.065200	-0.142031
C	-3.829746	1.160706	-0.171304
C	-5.965226	-0.582317	-0.436798
H	-4.532592	-2.132090	-0.033815
C	-5.097706	1.657889	-0.464727
H	-2.995579	1.850574	-0.092231
C	-6.174633	0.784643	-0.596788
H	-6.795416	-1.272779	-0.546031
H	-5.246784	2.724698	-0.597252
H	-7.163879	1.165112	-0.827488
C	4.020191	0.027599	-0.312713
O	3.510166	0.272427	0.844671
O	3.423425	0.099663	-1.400034
C	1.225981	2.051836	-0.357100
H	1.854031	2.790653	0.142235
H	1.721252	1.727203	-1.270230
H	0.235704	2.457924	-0.561813
N	5.361202	-0.365428	-0.296540
C	6.084074	-0.454686	-1.537617
H	6.725944	0.423989	-1.702204
H	6.726279	-1.342482	-1.541406
H	5.358922	-0.520181	-2.343186
C	6.153461	-0.257950	0.900358
H	5.485921	-0.237004	1.755588
H	6.829658	-1.116373	0.982043
H	6.770019	0.653671	0.905164
O	-2.119549	-2.459485	0.031069
H	-1.273918	-2.913140	0.090154
H	-1.965909	-0.612506	1.992461

$TS6_{OH}^-$

M05-2X/BS1 SCF energy in gas phase: -1245.082773 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1245.474964 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1245.189957 a.u

C	-0.039690	-1.619228	0.545817
O	0.080489	-1.087862	-0.750679
O	-1.411337	-1.687796	0.699070
C	0.782218	-1.398807	2.785210
H	1.404638	-0.781232	3.437149
H	1.257795	-2.377058	2.681829
H	-0.198907	-1.539629	3.264247
H	1.914411	-0.380504	-0.312838
H	0.438168	-2.609980	0.611472
N	0.671117	-0.765687	1.486169
C	0.065243	0.553648	1.614681
H	-0.092604	0.973343	0.622513
H	0.759496	1.203868	2.147733
H	-0.900511	0.517791	2.134669
C	-2.892891	0.278360	-0.492536
C	-3.490890	0.325701	0.775499
C	-3.264151	1.266349	-1.409743
C	-4.420312	1.308042	1.106682
H	-3.199588	-0.424336	1.500955
C	-4.186000	2.262430	-1.088869
H	-2.811958	1.248639	-2.396566
C	-4.770042	2.283015	0.173752
H	-4.870217	1.320175	2.094091
H	-4.447937	3.020206	-1.820212
H	-5.488586	3.053898	0.431622
O	2.836104	-0.338523	-0.650983
O	3.046669	1.454744	0.717717
C	3.512584	0.641650	-0.061747
C	5.343794	-0.180107	-1.511174
H	5.361784	0.370402	-2.460609
H	6.366081	-0.492636	-1.279631
H	4.717514	-1.058075	-1.626315
N	4.841618	0.636969	-0.429072
C	5.654184	1.767771	-0.050545
H	5.779315	2.471237	-0.884101
H	6.645695	1.425841	0.259974
H	5.164769	2.277655	0.773581
Si	-1.663279	-1.108138	-1.007988
H	-1.481775	-0.540455	-2.436816
O	-2.410878	-2.551620	-1.502347
H	-2.513477	-2.508675	-2.454968

$IM10_{OH}^-$

M05-2X/BS1 SCF energy in gas phase: -1245.092334 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1245.479572 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1245.197438 a.u

C	0.090138	1.437935	-0.618969
O	0.371373	0.155962	-0.018101
O	-1.128425	1.165555	-1.176342
C	1.362855	2.688178	0.956192
H	1.633467	1.854960	1.624262
H	2.127486	2.744938	0.180682
H	1.369117	3.614158	1.538514
H	1.648012	-0.331809	0.226326
H	0.885625	1.666691	-1.337675
N	0.056024	2.503804	0.350592
C	-0.965850	2.299390	1.363251
H	-1.909777	2.071841	0.872319
H	-0.717872	1.474026	2.046978
H	-1.074386	3.215217	1.951194
C	-2.964413	-0.603520	-0.267967
C	-3.809156	0.443154	-0.666726
C	-3.551956	-1.667884	0.430775
C	-5.174917	0.427237	-0.389460
H	-3.370392	1.283378	-1.190372
C	-4.915621	-1.690533	0.717093
H	-2.911690	-2.478996	0.752238
C	-5.733840	-0.642183	0.304783
H	-5.802631	1.251751	-0.710975
H	-5.341162	-2.526174	1.263253
H	-6.796025	-0.656504	0.525624
O	2.567076	-0.821707	0.452153
O	3.465910	0.762821	-0.881647
C	3.561291	-0.246166	-0.190552
C	4.940055	-1.994873	0.899009
H	5.450375	-1.671544	1.816134
H	5.547758	-2.777966	0.433726
H	3.968555	-2.400583	1.159215
N	4.766687	-0.899211	-0.023178
C	5.967070	-0.294854	-0.542741
H	6.585704	0.124142	0.262053
H	6.565480	-1.039899	-1.077319
H	5.676947	0.500675	-1.222388
Si	-1.098375	-0.611660	-0.724845
H	-0.867303	-1.114068	-2.116575
O	-0.780612	-2.047770	0.186859
H	0.154472	-2.127318	0.387214

$TS7_{OH}^-$

M05-2X/BS1 SCF energy in gas phase: -1245.079474 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1245.467228 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1245.184493 a.u

C	0.004393	1.775967	0.675748
O	-0.205602	0.309405	-0.350875
O	1.096600	1.378618	1.227818
C	-1.201484	3.014308	-0.951369
H	-1.193052	2.357723	-1.831035
H	-2.056921	2.725569	-0.341377
H	-1.302658	4.052358	-1.278577
H	-1.174336	-0.144810	-0.538537
H	-0.957688	1.672637	1.184721
N	0.021915	2.853503	-0.185250
C	1.230018	2.986467	-0.977671
H	2.093363	2.875149	-0.327213
H	1.275204	2.214811	-1.756532
H	1.241436	3.972888	-1.447086
C	2.675171	-0.743411	0.265262
C	3.614825	0.221130	0.654754
C	3.151979	-1.867615	-0.424569
C	4.969482	0.071836	0.366438
H	3.264363	1.097975	1.181677
C	4.505008	-2.020898	-0.720518
H	2.435585	-2.621395	-0.725487
C	5.419698	-1.049861	-0.324722
H	5.674848	0.834034	0.679999
H	4.844796	-2.898986	-1.259320
H	6.473975	-1.165566	-0.552347
O	-2.312859	-0.876108	-0.662474
O	-3.187851	0.796465	0.573215
C	-3.256162	-0.305669	0.005410
C	-4.663551	-2.206278	-0.725153
H	-5.295195	-1.988269	-1.599500
H	-5.166021	-2.983968	-0.138411
H	-3.701909	-2.573346	-1.067705
N	-4.447153	-1.035058	0.082883
C	-5.621888	-0.414807	0.634391
H	-6.322250	-0.094424	-0.151696
H	-6.153229	-1.116032	1.288230
H	-5.305909	0.453676	1.204181
Si	0.818512	-0.633704	0.648808
H	0.416186	-0.791958	2.073591
O	0.363420	-2.153071	0.013243

H	-0.567669	-2.144815	-0.239729

IM11$_{OH}^-$

M05-2X/BS1 SCF energy in gas phase: -996.619263 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -996.945999 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -996.766023 a.u

O	-0.297076	-2.275307	-0.394839
H	0.560803	-1.825731	-0.604657
C	-2.273554	-0.251106	0.179514
C	-2.946026	-0.497155	-1.022869
C	-2.583291	0.920109	0.879974
C	-3.913180	0.383489	-1.500428
H	-2.689497	-1.383345	-1.593283
C	-3.549095	1.806570	0.410041
H	-2.043978	1.138423	1.795301
C	-4.219337	1.535894	-0.780431
H	-4.421855	0.178523	-2.435741
H	-3.774217	2.710796	0.964501
H	-4.970425	2.224843	-1.150396
O	1.685733	-0.546485	-0.196380
O	3.619939	-1.009232	-1.255269
C	2.910517	-0.328461	-0.509370
C	2.630867	1.870506	0.598561
H	2.392541	2.609128	-0.184202
H	3.130386	2.403870	1.414968
H	1.699898	1.450844	0.965431
N	3.485147	0.816340	0.108722
C	4.753103	1.270708	-0.402337
H	4.637675	1.987117	-1.232401
H	5.320790	1.769469	0.391338
H	5.299462	0.406456	-0.767440
Si	-1.007585	-1.475506	0.853128
H	-1.747915	-2.468535	1.687614
O	0.064907	-0.671000	1.807773
H	0.868438	-0.506265	1.237899

TS8$_{OH}^-$

M05-2X/BS1 SCF energy in gas phase: -1301.622251 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1302.021902 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1301.786376 a.u

C	-1.173317	-0.387947	-0.085119
O	-1.348693	-1.504746	0.412621
O	-0.063209	0.079135	-0.547440
C	4.030646	-2.644235	-0.303724
O	3.757271	-3.419741	-1.159450
O	4.622946	-2.311753	0.673300
H	3.205161	-1.316933	-0.710853
Si	1.700230	-0.726463	-0.602615
H	1.482824	-0.955988	-2.061176
C	2.430421	0.952738	-0.092819
C	1.960565	2.179235	-0.578380
C	3.532508	0.973314	0.771932
C	2.560359	3.382833	-0.214511
H	1.115678	2.185763	-1.257133
C	4.120075	2.174415	1.163279
H	3.937004	0.031405	1.127686
C	3.636944	3.383031	0.668501
H	2.186256	4.319289	-0.614347
H	4.963609	2.166337	1.844577
H	4.100538	4.318100	0.962951
N	-2.240319	0.520703	-0.194362
C	-1.967441	1.831765	-0.763053
H	-1.974773	1.826044	-1.858279
H	-2.720131	2.532640	-0.402879
H	-0.986633	2.153082	-0.429079
C	-3.579525	0.145368	0.018057
C	-3.954391	-0.783027	1.002524
C	-4.590490	0.747163	-0.745250
C	-5.294264	-1.088501	1.198497
H	-3.186524	-1.260960	1.587268
C	-5.929812	0.437695	-0.531176
H	-4.329092	1.446867	-1.527406
C	-6.295556	-0.483503	0.441730
H	-5.557120	-1.807938	1.965339
H	-6.686447	0.917686	-1.141022
H	-7.337464	-0.727816	0.607800
O	1.329011	-1.876388	0.537101
H	0.367186	-1.956133	0.671718

TS9$_{OH}^-$

M05-2X/BS1 SCF energy in gas phase: -1899.834194 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1900.338185 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1899.979441 a.u

O	3.028936	-0.857096	-1.351694
O	2.075956	-1.147959	0.671719
C	3.000604	-0.715007	-0.126843
N	4.024206	-0.038305	0.546335
C	3.965163	0.045512	2.000232
H	4.386512	-0.840654	2.485117
H	4.518735	0.927688	2.320904
H	2.926727	0.135858	2.301138
Si	0.346698	-1.828583	0.341121
H	-1.169233	-2.440941	0.117585
H	0.663047	-2.984903	1.230074
C	-0.448901	-0.334220	1.205115
C	0.117783	0.946427	1.245279
C	-1.686781	-0.511518	1.835958
C	-0.525322	2.005258	1.884927
H	1.076693	1.120992	0.770797
C	-2.330008	0.534077	2.492384
H	-2.171069	-1.480347	1.791019
C	-1.749435	1.798957	2.516339
H	-0.070508	2.989844	1.890685
H	-3.297986	0.362433	2.947171
H	-2.256204	2.622939	3.005418
C	5.213972	0.351880	-0.101399
C	5.220487	0.833350	-1.419414
C	6.426371	0.309465	0.599182
C	6.409538	1.245813	-2.004331
H	4.295200	0.861945	-1.970489
C	7.609774	0.734226	0.003033
H	6.451520	-0.074784	1.609626
C	7.613253	1.204689	-1.303781
H	6.389299	1.613597	-3.023410
H	8.532976	0.685850	0.568507
H	8.534066	1.532777	-1.769736
C	-2.280116	-2.730850	-0.842442
O	-3.094223	-3.506841	-0.300744
O	-2.681409	-1.414163	-1.097163
H	-1.564920	-3.050238	-1.604041
C	-4.379526	0.814998	-0.803144
C	-3.249497	1.618536	-0.610708
C	-5.599830	1.437999	-1.087175
C	-3.343857	3.005594	-0.684698
H	-2.293772	1.153162	-0.398230
C	-5.700149	2.824220	-1.162411
H	-6.484216	0.831029	-1.257204
C	-4.567950	3.609352	-0.959393
H	-2.459228	3.610440	-0.523695
H	-6.653606	3.290768	-1.381956
H	-4.639878	4.689619	-1.018684
Si	-4.261319	-1.043810	-0.699256
H	-5.200684	-1.609587	-1.709399
O	0.553041	-1.944358	-1.303724
H	1.428875	-1.631293	-1.594332
O	-4.668958	-1.571045	0.816894
H	-4.307269	-2.475404	0.860114

$TS9_{byOH}^-$

M05-2X/BS1 SCF energy in gas phase: -1628.541925 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1629.020366 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1628.638839 a.u

C	1.191766	-1.271595	-1.197634
O	0.317485	-0.218533	-0.125681
O	1.976198	-0.396705	-1.705597
C	0.634529	-3.062797	0.273738
H	0.264078	-2.540128	1.162995
H	-0.205907	-3.158904	-0.412085
H	1.003676	-4.049890	0.556194
H	-0.741722	-0.335766	0.064874
H	0.314180	-1.622737	-1.750020
N	1.690157	-2.312814	-0.387178
C	2.224949	2.224028	-0.516036
C	3.533130	1.860996	-0.861333
C	2.047229	3.421392	0.192920
C	4.619102	2.660069	-0.513500
H	3.688728	0.932873	-1.390921
C	3.130197	4.224652	0.542860
H	1.041735	3.710480	0.470192
C	4.421423	3.845270	0.189200
H	5.622510	2.351619	-0.785677
H	2.965323	5.144516	1.093023
H	5.267866	4.466165	0.462233
O	-2.097557	-0.276813	0.232031

O	-2.111040	-1.957392	-1.257514
C	-2.673678	-1.126849	-0.534439
N	-4.094045	-1.097924	-0.538438
C	-4.749962	-1.951769	-1.512174
H	-5.682429	-2.335407	-1.094201
H	-4.972587	-1.424666	-2.446902
H	-4.071063	-2.767280	-1.734847
Si	0.685696	1.231718	-0.977591
H	0.281373	1.237348	-2.406138
O	-0.489804	2.213597	-0.250954
H	-1.303609	1.732249	-0.059371
C	-4.878910	-0.175728	0.169560
C	-6.133388	0.198209	-0.337858
C	-4.493821	0.349951	1.416489
C	-6.963792	1.067624	0.363230
H	-6.460334	-0.175792	-1.297675
C	-5.329229	1.221060	2.099850
H	-3.535480	0.075907	1.824188
C	-6.571731	1.590669	1.587845
H	-7.922335	1.338527	-0.064670
H	-5.001324	1.610965	3.056545
H	-7.215223	2.270486	2.132404
C	2.916766	-2.166356	0.287464
C	3.050556	-2.512025	1.636707
C	4.061284	-1.747494	-0.411096
C	4.287214	-2.426076	2.272407
H	2.188234	-2.834709	2.202432
C	5.282561	-1.649151	0.237389
H	3.961521	-1.499451	-1.456155
C	5.410286	-1.988519	1.584149
H	4.361356	-2.695386	3.319807
H	6.148964	-1.312370	-0.320380
H	6.368795	-1.914139	2.083030

IM11$_{OH}$

M05-2X/BS1 SCF energy in gas phase: -1112.465376 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1112.72987 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1112.507055 a.u

C	0.844181	0.263775	-0.198030
O	1.104867	1.390154	-0.602897
O	-0.420203	-0.192410	-0.144141
Si	-1.627268	0.863725	-0.758642
H	-1.460099	0.848155	-2.229663
C	-3.252264	0.149197	-0.242019
C	-3.800197	-0.952584	-0.909258
C	-3.955707	0.704840	0.833256
C	-5.014836	-1.496614	-0.505644
H	-3.278846	-1.388622	-1.755535
C	-5.172795	0.164928	1.237461
H	-3.547011	1.567583	1.346007
C	-5.699987	-0.937004	0.569965
H	-5.429016	-2.349706	-1.028524
H	-5.710011	0.603220	2.069424
H	-6.647678	-1.357148	0.884175
N	1.756970	-0.645245	0.241835
C	1.331747	-1.989687	0.629451
H	1.242273	-2.652106	-0.234639
H	2.071598	-2.391909	1.317880
H	0.368820	-1.931976	1.125894
C	3.151893	-0.364703	0.172942
C	3.658891	0.885660	0.533523
C	4.027653	-1.377406	-0.220233
C	5.028724	1.110917	0.488938
H	2.981705	1.670413	0.832760
C	5.398723	-1.143278	-0.250844
H	3.641517	-2.344206	-0.515493
C	5.906189	0.101704	0.101225
H	5.411943	2.084009	0.769138
H	6.066423	-1.937580	-0.559803
H	6.972461	0.285362	0.073993
O	-1.477853	2.344179	-0.063466
H	-0.568899	2.665234	-0.127849

IM12$_{OH}^{-}$

M05-2X/BS1 SCF energy in gas phase: -787.381264 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -787.644319 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -787.527163 a.u

H	-3.530942	-1.427951	-0.364885
C	-2.460350	-1.258193	-0.575285
O	-2.277840	-0.034789	-1.258325
O	-1.714149	-1.063381	0.576985
H	-2.087479	-2.103556	-1.182205

C	0.654571	0.189086	-0.022530
C	1.175797	-1.019565	0.462156
C	1.572550	1.124045	-0.514552
C	2.545315	-1.276243	0.464731
H	0.470356	-1.753225	0.833115
C	2.945344	0.881221	-0.519961
H	1.189894	2.061587	-0.906348
C	3.436780	-0.324189	-0.026335
H	2.921329	-2.219880	0.847639
H	3.630916	1.627329	-0.909511
H	4.503777	-0.522020	-0.027483
Si	-1.232839	0.585180	-0.011583
H	-1.044010	1.926491	-0.779309
O	-1.793068	1.351476	1.405745
H	-1.733684	2.295287	1.246569

TS10$_{OH}$

M05-2X/BS1 SCF energy in gas phase: -1226.715195 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1227.033267 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1226.705953 a.u

C	2.509601	1.879872	-1.788936
O	1.065402	2.003938	-0.778842
O	3.462804	1.468665	-1.078112
H	2.481565	2.927177	-2.128106
C	1.670585	-0.340807	0.883492
C	2.625402	-1.099270	0.188459
C	0.751541	-1.024094	1.693272
C	2.660296	-2.487828	0.309603
H	3.327273	-0.569877	-0.447483
C	0.775844	-2.413826	1.807644
H	0.014561	-0.452275	2.245781
C	1.736012	-3.149327	1.115663
H	3.411568	-3.055176	-0.227249
H	0.061949	-2.920018	2.448221
H	1.767770	-4.228556	1.209962
Si	1.543431	1.540441	0.726034
H	2.667492	2.268443	1.358576
H	2.056817	1.202880	-2.545485
N	-1.627629	1.616867	-0.556439
H	-0.725320	2.092283	-0.710305
N	-0.549608	-0.131734	-1.557500
H	0.238279	0.525485	-1.556859
N	-2.526779	-0.528687	-0.375190
C	-1.569722	0.308238	-0.809927
C	-2.563728	2.196682	0.394952
H	-3.414678	2.633804	-0.135857
H	-2.029575	2.981880	0.924705
C	-3.026998	1.123899	1.366355
H	-2.172830	0.832326	1.979492
H	-3.818385	1.504672	2.012419
C	-3.537267	-0.073977	0.580292
H	-3.743009	-0.911345	1.249851
H	-4.463839	0.171001	0.051196
C	-2.453935	-1.967923	-0.626799
H	-3.477275	-2.332027	-0.737438
H	-2.000889	-2.460650	0.240605
C	-1.638542	-2.256030	-1.877346
H	-1.495129	-3.331949	-1.976410
H	-2.169875	-1.893248	-2.759724
C	-0.297659	-1.551471	-1.753837
H	0.275379	-1.959720	-0.917853
H	0.291950	-1.661599	-2.663105
O	0.211207	1.923967	1.719797
H	0.472383	2.337813	2.544416

TS11$_{OH}$

M05-2X/BS1 SCF energy in gas phase: -880.160266 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -880.415865 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -880.075758 a.u

N	-1.527031	0.021879	1.089433
H	-0.591714	-0.307212	0.607892
C	-1.662907	-0.648902	2.380429
H	-0.665971	-0.740155	2.810178
H	-2.288559	-0.059073	3.054967
H	-2.097409	-1.642092	2.262754
C	-2.631240	-0.064447	0.189500
C	-3.925842	-0.343019	0.625081
C	-2.383835	0.205127	-1.158245
C	-4.970109	-0.369667	-0.295296
H	-4.127770	-0.538228	1.670084
C	-3.435633	0.179255	-2.065076
H	-1.375045	0.443045	-1.463708

C	-4.730201	-0.111044	-1.640221
H	-5.973726	-0.592203	0.045069
H	-3.242295	0.388972	-3.109619
H	-5.545555	-0.133551	-2.352029
C	-1.102252	1.675171	1.340786
H	-0.341247	1.488081	2.125805
H	-2.052530	2.018718	1.789498
O	-0.720967	2.213373	0.244781
C	1.858152	-0.039078	-0.076114
C	2.743452	2.256106	-0.302779
C	4.112432	1.667129	-0.011854
C	4.207607	0.328992	-0.725939
H	2.694970	2.553084	-1.359050
H	2.567107	3.154351	0.291093
H	4.902485	2.335799	-0.356922
H	4.230224	1.510140	1.062418
H	4.185077	0.480784	-1.814393
H	5.148039	-0.171772	-0.484685
N	3.126221	-0.541799	-0.294257
N	1.707850	1.297270	0.016976
C	2.304974	-2.754615	0.284296
C	0.912647	-2.238662	-0.050436
C	3.304627	-1.962421	-0.540994
H	0.657686	-2.534435	-1.077265
H	0.168458	-2.712527	0.597498
H	2.512362	-2.597227	1.345341
H	2.396249	-3.820258	0.066370
H	3.182024	-2.196942	-1.607649
H	4.329627	-2.221271	-0.264149
N	0.804575	-0.800982	0.105506
H	0.702735	1.672862	0.059823

IM13$_{OH}$

M05-2X/BS1 SCF energy in gas phase: -441.385975 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -441.517617 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -441.369376 a.u

N	-1.250832	0.499905	-0.063580
H	-2.598116	-1.158263	-1.216123
C	-1.659866	1.890935	-0.056385
H	-2.744744	1.940177	-0.134589
H	-1.349961	2.424925	0.850849
H	-1.240733	2.410774	-0.919336
C	0.120590	0.212785	-0.038316
C	1.084527	1.230777	-0.063220
C	0.557847	-1.122610	0.006516
C	2.440263	0.918028	-0.034727
H	0.789796	2.269920	-0.092390
C	1.913797	-1.414887	0.046375
H	-0.171418	-1.920156	-0.025910
C	2.869192	-0.401712	0.026548
H	3.164080	1.723892	-0.052230
H	2.225235	-2.451986	0.081417
H	3.924927	-0.637886	0.052029
C	-2.148554	-0.465302	0.522099
H	-3.063385	0.062755	0.806933
H	-1.713305	-0.924025	1.413767
O	-2.441666	-1.540944	-0.346588

TS12$_{OH}$

M05-2X/BS1 SCF energy in gas phase: -1553.820166 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1554.226177 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1553.832584 a.u

N	-3.317206	1.199763	-0.672552
H	-2.530791	-2.706259	-2.598247
C	-4.172342	0.842648	0.469740
H	-4.775897	1.706874	0.738355
H	-4.799173	-0.000312	0.195775
H	-3.516328	0.564459	1.294242
C	-2.405192	2.306684	-0.469524
C	-2.923085	3.567286	-0.184835
C	-1.043190	2.057603	-0.531595
C	-2.032870	4.612178	0.028206
H	-3.992221	3.736294	-0.152470
C	-0.165345	3.113650	-0.300080
H	-0.641486	1.068150	-0.715125
C	-0.657074	4.384831	-0.024948
H	-2.413507	5.603261	0.237998
H	0.895774	2.901958	-0.319423
H	0.027994	5.203025	0.157150
C	-3.286275	0.495602	-1.739534
H	-2.592966	0.767391	-2.524327
H	-3.900840	-0.386118	-1.837468

O	-2.527868	-1.977688	-1.971115
Si	-0.938251	-1.895709	-1.195716
H	-0.504006	-0.710909	-1.997275
C	-1.686528	-1.590696	0.534277
C	-1.100628	-0.783878	1.520661
C	-2.877763	-2.253487	0.868197
C	-1.685978	-0.635287	2.778687
H	-0.180146	-0.257749	1.298226
C	-3.450923	-2.139246	2.133707
H	-3.351327	-2.865889	0.110608
C	-2.857807	-1.321673	3.093107
H	-1.216465	0.001891	3.519139
H	-4.357029	-2.685053	2.371031
H	-3.300043	-1.223887	4.077741
O	1.287654	0.297125	-0.402389
O	0.854473	-1.912387	-0.462768
C	1.643646	-0.885028	-0.387556
N	2.989381	-1.225760	-0.259121
C	3.352826	-2.629639	-0.126931
H	4.411591	-2.736798	-0.356192
H	3.157451	-3.019812	0.876085
H	2.774957	-3.212387	-0.837741
C	3.969301	-0.243890	0.012358
C	3.987850	0.976532	-0.674716
C	4.974289	-0.505915	0.948369
C	4.984409	1.907084	-0.414047
H	3.218187	1.178618	-1.402917
C	5.975761	0.429197	1.193015
H	4.966546	-1.436838	1.500150
C	5.986443	1.643098	0.517516
H	4.985610	2.844209	-0.957793
H	6.743879	0.204965	1.923169
H	6.763926	2.371708	0.709220
O	-0.601121	-3.474705	-1.679841
H	0.274353	-3.733559	-1.383725

IM14$_{OH}^{+}$

M05-2X/BS1 SCF energy in gas phase: -365.322549 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -365.497078 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -365.363223 a.u

N	1.621761	-0.090003	-0.074576
C	2.358397	0.941417	0.683823
H	1.980293	0.941754	1.703380
H	3.420589	0.715075	0.660470
H	2.175576	1.909703	0.224092
C	0.175036	-0.032330	-0.038189
C	-0.467596	1.166918	-0.331159
C	-0.523436	-1.187978	0.300235
C	-1.856642	1.193101	-0.302309
H	0.087348	2.052966	-0.609477
C	-1.912428	-1.140210	0.328587
H	0.004348	-2.093522	0.574241
C	-2.575981	0.045674	0.026242
H	-2.376135	2.111003	-0.541509
H	-2.471450	-2.025542	0.599668
H	-3.657063	0.078683	0.052780
C	2.225343	-1.025113	-0.702139
H	3.305379	-1.090436	-0.661250
H	1.642621	-1.738545	-1.270899

TS13$_{OH}$

M05-2X/BS1 SCF energy in gas phase: -1207.260233 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1207.60831 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1207.199616 a.u

N	0.643976	-0.964151	0.072536
C	-0.287781	-1.020511	-1.067891
H	-0.934513	-0.147692	-1.006956
H	0.312421	-1.018696	-1.975766
H	-0.879679	-1.932163	-0.993649
C	1.758781	-1.874865	0.068329
C	3.046466	-1.352736	0.077014
C	1.506223	-3.242054	0.038302
C	4.116945	-2.242576	0.069721
H	3.199800	-0.279086	0.060540
C	2.588108	-4.114426	0.032349
H	0.485782	-3.606028	0.046943
C	3.889533	-3.615468	0.047007
H	5.127741	-1.856384	0.069597
H	2.414872	-5.182436	0.020389
H	4.727605	-4.300326	0.037457
C	0.492313	-0.096387	0.999619
H	-0.353163	0.592282	0.934461

H	1.213475	-0.086578	1.808058
N	0.752582	2.888395	1.044057
H	-0.204328	2.794647	0.705679
O	-1.635494	1.623558	0.208565
O	-3.221906	3.016320	-0.564724
C	-2.806530	1.919804	-0.209901
N	-3.727735	0.807307	-0.305898
C	-4.915377	1.021679	-1.114306
H	-4.744162	0.819549	-2.178343
H	-5.722055	0.379399	-0.758250
H	-5.190303	2.065825	-1.008278
C	-3.390515	-0.492368	0.054199
C	-2.679021	-0.759961	1.240448
C	-3.787775	-1.588918	-0.729689
C	-2.328492	-2.058258	1.582655
H	-2.426495	0.071810	1.881683
C	-3.442902	-2.889478	-0.370213
H	-4.353961	-1.419958	-1.635794
C	-2.694280	-3.139229	0.776153
H	-1.790673	-2.234402	2.507980
H	-3.762766	-3.712287	-0.998806
H	-2.438163	-4.152409	1.060313
C	1.753443	2.538964	0.180795
C	1.419592	2.024589	-1.092914
C	3.115852	2.638067	0.521619
C	2.412123	1.628738	-1.974906
H	0.369921	1.977068	-1.361467
C	4.097491	2.241763	-0.384471
H	3.406514	3.040028	1.483184
C	3.764154	1.729384	-1.634174
H	2.128542	1.253769	-2.951915
H	5.139447	2.343212	-0.103292
H	4.534108	1.430372	-2.332962
C	0.998365	3.642039	2.246973
H	1.543679	4.571448	2.046971
H	0.039520	3.895266	2.694307
H	1.573972	3.067157	2.982019

TBD

M05-2X/BS1 SCF energy in Acetonitrile solution: -438.801453 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -438.912561 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -438.736181 a.u

C	-0.060911	-0.725416	-0.033085
C	2.408216	-0.752993	0.200158
C	2.420116	0.673639	-0.318225
C	1.197828	1.392128	0.225946
H	2.532317	-0.749246	1.290761
H	3.225059	-1.333342	-0.229356
H	3.324591	1.190793	0.003992
H	2.390596	0.666274	-1.410335
H	1.297594	1.524789	1.312159
H	1.103381	2.384625	-0.218976
N	-0.023815	0.654437	-0.086342
N	1.152846	-1.372033	-0.203829
C	-2.432948	0.611636	-0.381666
C	-2.417117	-0.809181	0.170687
C	-1.258178	1.369064	0.211961
H	-2.736325	-0.787604	1.220840
H	-3.153253	-1.421797	-0.358215
H	-2.331202	0.591315	-1.470036
H	-3.369628	1.115440	-0.136754
H	-1.389189	1.483943	1.296660
H	-1.174527	2.368817	-0.219007
N	-1.117981	-1.458560	0.069624
H	1.061192	-2.354179	0.007442

CO_2

M05-2X/BS1 SCF energy in Acetonitrile solution: -188.55078 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -188.618326 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -188.627237 a.u

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.162966
O	0.000000	0.000000	-1.162966

$[Si]H_3$

M05-2X/BS1 SCF energy in Acetonitrile solution: -522.889913 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -522.969647 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -522.884661 a.u

Si	2.338866	0.000088	0.004408
H	2.834185	1.315682	-0.477278
H	2.859769	-1.079023	-0.875587
H	2.877760	-0.228377	1.372620
C	0.463525	-0.000312	-0.009205
C	-0.252601	1.204057	-0.007575
C	-0.253676	-1.205043	-0.007517
C	-1.646172	1.206206	0.002512
H	0.277308	2.150620	-0.017649
C	-1.646154	-1.206614	0.002771
H	0.275101	-2.152654	-0.017738
C	-2.343287	0.000391	0.008158
H	-2.185287	2.145825	0.002446
H	-2.186020	-2.145801	0.003089
H	-3.426747	0.000382	0.013516

[TBD]H$^+$

M05-2X/BS1 SCF energy in Acetonitrile solution: -439.296677 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -439.397846 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -439.208589 a.u

N	1.144287	-1.361567	-0.119948
H	1.086907	-2.368272	-0.125803
N	-1.144291	-1.361561	0.119967
H	-1.086910	-2.368265	0.125849
N	0.000003	0.653473	-0.000010
C	-0.000001	-0.679733	0.000004
C	2.440530	-0.720548	-0.310563
H	2.636977	-0.571950	-1.375308
H	3.199564	-1.386617	0.094177
C	2.426442	0.611649	0.419346
H	2.348722	0.440576	1.494728
H	3.347958	1.157598	0.220273
C	1.243160	1.431261	-0.064421
H	1.100328	2.309068	0.566753
H	1.396371	1.768377	-1.092851
C	-1.243153	1.431258	0.064439
H	-1.100325	2.309089	-0.566701
H	-1.396362	1.768333	1.092883
C	-2.426434	0.611660	-0.419354
H	-3.347949	1.157611	-0.220288
H	-2.348700	0.440602	-1.494738
C	-2.440543	-0.720545	0.310538
H	-2.637032	-0.571962	1.375277
H	-3.199560	-1.386611	-0.094241

[N$_1$]H

M05-2X/BS1 SCF energy in Acetonitrile solution: -135.142302 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -135.179891 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -135.11138 a.u

N	0.000000	0.580503	-0.156742
H	0.000000	1.310227	0.546107
C	1.199905	-0.226072	0.020058
H	1.254688	-0.971907	-0.777272
H	2.087188	0.405219	-0.047351
H	1.228838	-0.763754	0.979820
C	-1.199906	-0.226072	0.020058
H	-2.087187	0.405221	-0.047347
H	-1.254690	-0.971904	-0.777275
H	-1.228835	-0.763757	0.979819

[N$_2$]H

M05-2X/BS1 SCF energy in Acetonitrile solution: -326.888354 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -326.967428 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -326.850807 a.u

N	1.783791	-0.616864	-0.152054
H	1.994308	-1.544544	0.180978
C	2.812403	0.370396	0.109924
H	3.778745	-0.130253	0.102212
H	2.822091	1.133066	-0.671613
H	2.683920	0.872790	1.076517
C	0.446904	-0.279207	-0.064563
C	0.011811	1.056240	-0.059909
C	-0.522827	-1.298768	-0.007418
C	-1.349984	1.349806	-0.011490
H	0.730474	1.864136	-0.095019
C	-1.873726	-0.989802	0.044781
H	-0.196271	-2.333217	-0.006989
C	-2.304574	0.338969	0.041555

H	-1.661532	2.388249	-0.010223
H	-2.598371	-1.794799	0.089376
H	-3.359942	0.576818	0.081855

$[N_3]H$

M05-2X/BS1 SCF energy in Acetonitrile solution: -518.626597 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -518.746488 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -518.582607 a.u

N	0.000039	1.033610	0.000978
H	0.000081	2.041699	0.000118
C	1.257557	0.437401	-0.019219
C	1.485891	-0.862099	-0.494676
C	2.354951	1.203801	0.405534
C	2.777868	-1.380360	-0.511626
H	0.665221	-1.457113	-0.870640
C	3.640111	0.679097	0.368265
H	2.184011	2.211773	0.766717
C	3.863490	-0.622149	-0.080696
H	2.932727	-2.387053	-0.881489
H	4.470877	1.290333	0.700455
H	4.864532	-1.033590	-0.100077
C	-1.257528	0.437499	0.020013
C	-2.354540	1.203846	-0.405781
C	-1.486283	-0.861891	0.495591
C	-3.639752	0.679180	-0.369424
H	-2.183289	2.211741	-0.767035
C	-2.778275	-1.380122	0.511603
H	-0.665910	-1.456808	0.872368
C	-3.863526	-0.621957	0.079633
H	-4.470235	1.290368	-0.702409
H	-2.933469	-2.386734	0.881550
H	-4.864596	-1.033364	0.098294

$[Si]H_2(OCHO)$

M05-2X/BS1 SCF energy in Acetonitrile solution: -711.48553 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -711.627321 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -711.529059 a.u

C	-3.248036	-0.000576	-0.799146
O	-3.902342	0.000429	0.216722
O	-1.914472	-0.000728	-0.818282
H	-3.675875	-0.001427	-1.806611
C	0.714796	0.000188	0.296668
C	1.412407	1.206387	0.140900
C	1.412240	-1.206217	0.141697
C	2.768572	1.207635	-0.174274
H	0.896338	2.152164	0.269154
C	2.768393	-1.207860	-0.173511
H	0.896048	-2.151842	0.270580
C	3.445440	-0.000211	-0.333013
H	3.296520	2.145961	-0.292625
H	3.296206	-2.146336	-0.291266
H	4.501227	-0.000360	-0.576225
Si	-1.098291	0.000442	0.698950
H	-1.471350	1.232821	1.428216
H	-1.471412	-1.230851	1.430038

IM6

M05-2X/BS1 SCF energy in Acetonitrile solution: -762.558345 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -762.766706 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -762.492868 a.u

N	0.699793	1.133686	0.151124
H	-0.346234	1.090661	0.067100
N	0.706031	-1.138999	-0.133699
H	-0.340010	-1.099909	-0.063138
N	2.731216	0.003192	0.007124
C	1.387219	-0.000496	0.007846
C	1.353444	2.413556	0.368746
H	1.532191	2.582030	1.435689
H	0.681304	3.192833	0.011650
C	2.672110	2.432984	-0.387958
H	2.477771	2.375057	-1.460977
H	3.218658	3.353723	-0.183999
C	3.507832	1.243871	0.054448
H	4.367399	1.112180	-0.605518
H	3.881948	1.393378	1.071682
C	3.514722	-1.232749	-0.046706
H	4.376104	-1.098136	0.610299
H	3.885728	-1.377148	-1.065859

C	2.687160	-2.427671	0.395229
H	3.238455	-3.344775	0.187730
H	2.495298	-2.373041	1.468872
C	1.366354	-2.414329	-0.357836
H	1.543163	-2.578266	-1.425840
H	0.700086	-3.198870	-0.001289
O	-1.976812	-1.128541	0.055613
O	-1.971573	1.118760	-0.099631
C	-2.550678	-0.006777	-0.064726
C	-4.667129	-1.214974	0.145671
H	-5.628831	-1.217229	-0.372116
H	-4.862051	-1.283622	1.224825
H	-4.092824	-2.084904	-0.158421
N	-3.938114	-0.012783	-0.203468
C	-4.664430	1.223653	0.003234
H	-5.624145	1.170272	-0.515536
H	-4.863894	1.414731	1.066629
H	-4.085140	2.051201	-0.394903

IM12

M05-2X/BS1 SCF energy in Acetonitrile solution: -954.296257 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -954.54527 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -954.222461 a.u

O	0.913940	0.387495	-0.043589
O	0.386946	-1.790795	0.109976
C	1.202518	-0.837090	-0.005321
N	-1.733947	1.068183	0.067869
H	-0.737871	0.774319	0.036208
N	-2.267806	-1.161238	0.044443
H	-1.246025	-1.356056	0.074324
N	-3.971613	0.425844	0.038864
C	-2.666346	0.112545	0.050236
C	-2.062632	2.482450	-0.023042
H	-2.137182	2.796623	-1.069202
H	-1.251613	3.040943	0.442366
C	-3.381855	2.727599	0.690035
H	-3.265107	2.523737	1.756210
H	-3.693935	3.764710	0.568627
C	-4.440178	1.812979	0.096704
H	-5.342790	1.822488	0.709594
H	-4.711591	2.140252	-0.911444
C	-5.015989	-0.596857	-0.058559
H	-5.808891	-0.187488	-0.686626
H	-5.432052	-0.781532	0.936215
C	-4.469705	-1.880938	-0.659012
H	-5.220611	-2.666526	-0.575961
H	-4.239966	-1.729829	-1.715704
C	-3.204556	-2.273705	0.086187
H	-3.445466	-2.538387	1.120638
H	-2.720608	-3.130817	-0.380000
N	2.566472	-1.201526	-0.096664
C	2.900560	-2.604274	0.108993
H	2.993866	-2.864611	1.168588
H	2.109427	-3.208224	-0.322779
H	3.842406	-2.827838	-0.391300
C	3.612399	-0.259939	-0.074493
C	3.529904	0.957162	-0.772174
C	4.802971	-0.554298	0.606970
C	4.598475	1.845061	-0.767203
H	2.622882	1.193576	-1.305084
C	5.871359	0.340164	0.596783
H	4.896272	-1.480649	1.157947
C	5.778856	1.548514	-0.085295
H	4.509973	2.776501	-1.314499
H	6.776861	0.085640	1.135000
H	6.608506	2.244498	-0.090643

IM19

M05-2X/BS1 SCF energy in Acetonitrile solution: -1146.031194 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1146.322221 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1145.950821 a.u

O	0.063744	1.121013	0.084213
O	0.064036	-1.122101	-0.083552
C	0.622112	-0.000474	0.000268
N	-2.679737	1.137279	0.146404
H	-1.643397	1.091912	0.116851
N	-2.679856	-1.137770	-0.146620
H	-1.643563	-1.092590	-0.116722
N	-4.704799	-0.000163	0.000030
C	-3.362987	-0.000205	-0.000065
C	-3.336054	2.434123	0.205023
H	-3.507434	2.827612	-0.802011

H	-2.670027	3.117812	0.729440
C	-4.658483	2.278425	0.936942
H	-4.469819	1.981854	1.970688
H	-5.207502	3.219749	0.940788
C	-5.486796	1.217219	0.232441
H	-6.347787	0.934731	0.840480
H	-5.856811	1.590706	-0.726711
C	-5.486982	-1.217392	-0.232576
H	-6.347786	-0.934739	-0.840802
H	-5.857281	-1.590779	0.726504
C	-4.658747	-2.278788	-0.936872
H	-5.207871	-3.220051	-0.940593
H	-4.469998	-1.982411	-1.970657
C	-3.336338	-2.434542	-0.204933
H	-3.507699	-2.827840	0.802178
H	-2.670454	-3.118411	-0.729299
N	2.046776	-0.000180	0.000219
C	2.779680	-1.215466	0.053293
C	3.849962	-1.412019	-0.824363
C	2.475455	-2.205442	0.992651
C	4.605227	-2.579861	-0.762647
H	4.086070	-0.644958	-1.552353
C	3.224784	-3.376430	1.039312
H	1.646948	-2.052866	1.669921
C	4.294873	-3.569911	0.166479
H	5.431742	-2.716792	-1.449555
H	2.977734	-4.137057	1.770462
H	4.879298	-4.480590	0.211608
C	2.778895	1.215595	-0.053133
C	3.848526	1.413456	0.824999
C	2.474414	2.204749	-0.993255
C	4.602966	2.581820	0.762955
H	4.084759	0.647016	1.553609
C	3.222897	3.376260	-1.040266
H	1.646356	2.051109	-1.670851
C	4.292385	3.571043	-0.166976
H	5.429005	2.719813	1.450222
H	2.975684	4.136255	-1.772018
H	4.876172	4.482118	-0.212363

IM8^{-}

M05-2X/BS1 SCF energy in Acetonitrile solution: -1034.751123 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1035.00084 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1034.812943 a.u

O	2.652732	-1.736202	-0.211632
O	1.340278	0.094385	-0.175449
C	2.506691	-0.511763	-0.164715
C	4.888405	-0.207698	0.163549
H	5.086838	-0.240278	1.241832
H	5.655129	0.408917	-0.308412
H	4.942674	-1.217213	-0.232838
N	3.580340	0.346380	-0.127025
C	3.392181	1.746662	0.206648
H	3.257540	1.900679	1.284206
H	4.276524	2.300805	-0.110807
H	2.523513	2.140107	-0.313959
Si	-0.181042	-0.947230	-0.255833
H	-2.022399	-1.954072	1.591038
H	0.166599	-1.591123	1.047006
H	0.184450	-1.438757	-1.613010
C	-1.295812	0.597910	-0.143520
C	-0.841476	1.787677	0.448193
C	-2.608608	0.592617	-0.641269
C	-1.657971	2.912761	0.548885
H	0.169569	1.832195	0.833138
C	-3.425480	1.720095	-0.564599
H	-3.000514	-0.307930	-1.098401
C	-2.953380	2.884148	0.036688
H	-1.281151	3.812905	1.020888
H	-4.430487	1.686922	-0.969156
H	-3.588077	3.759915	0.105634
C	-2.376758	-2.402797	0.643900
O	-1.644663	-2.129356	-0.395652
O	-3.377691	-3.100600	0.631624

TS6^{-}

M05-2X/BS1 SCF energy in Acetonitrile solution: -1169.868985 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1170.156476 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1169.88597 a.u

C	-0.363076	1.461235	-0.890120
O	-0.116592	2.623593	-1.216921
O	0.679597	0.568970	-0.737588

C	-0.304073	0.654538	2.002384
H	-0.716505	0.705560	3.018399
H	-0.365294	-0.374749	1.657237
H	0.742885	0.966289	2.046525
H	-1.973992	1.127088	0.905371
H	-1.292939	0.943678	-1.137015
N	-1.034429	1.503047	1.078050
C	-1.096433	2.892446	1.490659
H	-1.670407	3.460296	0.759075
H	-1.556433	3.010781	2.479109
H	-0.087670	3.310252	1.525181
C	3.359579	-0.141068	-0.300780
C	2.949718	-1.217346	0.498858
C	4.672950	-0.136635	-0.789059
C	3.827277	-2.254331	0.806303
H	1.934426	-1.248013	0.878337
C	5.555932	-1.169791	-0.481356
H	5.012737	0.676903	-1.422597
C	5.132568	-2.229794	0.317604
H	3.494437	-3.080454	1.423340
H	6.567780	-1.151041	-0.867991
H	5.815790	-3.036340	0.555591
O	-3.523299	0.643359	-0.086525
O	-2.856924	-1.105543	1.163821
C	-3.581709	-0.562615	0.296442
C	-5.146140	-0.904962	-1.557673
H	-6.093676	-1.414898	-1.749855
H	-4.475898	-1.109759	-2.406714
H	-5.316536	0.166468	-1.509643
N	-4.597607	-1.358759	-0.296733
C	-4.445903	-2.795810	-0.207839
H	-5.410364	-3.280545	-0.380614
H	-3.733608	-3.190660	-0.948429
H	-4.084290	-3.053570	0.783083
Si	2.206714	1.282707	-0.683775
H	2.628559	1.870713	-1.980276
H	2.284861	2.315850	0.380683

$TS6_{by}^-$

M05-2X/BS1 SCF energy in Acetonitrile solution: -1557.61444 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1557.93988 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1557.645437 a.u

O	-4.769927	-1.511394	0.690219
O	-3.335995	0.174986	0.265632
C	-4.542940	-0.335564	0.396404
N	-5.552691	0.577082	0.207801
C	-5.286512	1.862097	-0.412549
H	-5.231611	1.786781	-1.505370
H	-6.096835	2.546619	-0.157439
H	-4.349771	2.268033	-0.042012
Si	-1.869859	-0.893437	0.528760
H	-0.509932	-1.872126	0.690823
H	-2.231271	-1.815180	-0.588246
H	-2.203775	-1.176814	1.962490
C	-0.695236	0.568929	0.244785
C	-0.939988	1.554772	-0.721220
C	0.466792	0.689602	1.018665
C	-0.046756	2.607075	-0.924063
H	-1.843216	1.500736	-1.318402
C	1.345973	1.757926	0.849697
H	0.692742	-0.072362	1.757250
C	1.096274	2.713990	-0.133882
H	-0.247141	3.348231	-1.689440
H	2.232551	1.834451	1.469030
H	1.787708	3.535312	-0.282443
C	0.503414	-2.664215	-0.286222
O	0.117214	-2.576183	-1.457107
O	1.668431	-2.014386	0.087732
H	0.349890	-3.558165	0.327117
C	3.879471	-0.331313	-0.311161
C	4.441457	-0.862244	0.856940
C	4.459384	0.818096	-0.865690
C	5.552295	-0.266044	1.451453
H	4.001916	-1.742868	1.311458
C	5.572176	1.415451	-0.278553
H	4.031017	1.262720	-1.759179
C	6.119750	0.872371	0.882751
H	5.972834	-0.687087	2.356920
H	6.007026	2.304254	-0.719831
H	6.982678	1.337129	1.344376
Si	2.393932	-1.115139	-1.141105
H	2.853337	-2.024417	-2.226635
H	1.575259	-0.032625	-1.735804
C	-6.908864	0.080655	0.079274
H	-7.162024	-0.144095	-0.963883
H	-7.011030	-0.826337	0.667870

H	-7.606469	0.834618	0.447992

TS9$^-$

M05-2X/BS1 SCF energy in Acetonitrile solution: -1749.351172 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1749.716864 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1749.376029 a.u

O	2.861624	0.595202	1.225035
O	1.738642	1.350429	-0.575265
C	2.794395	0.850618	0.026949
N	3.854174	0.630660	-0.845620
C	3.653820	0.816254	-2.280957
H	3.147524	-0.035216	-2.743906
H	4.624546	0.951449	-2.754508
H	3.054215	1.706518	-2.442126
Si	0.191144	1.721055	0.356975
H	-1.240596	2.172979	1.071464
H	0.895524	2.530527	1.401225
H	-0.323158	2.436503	-0.850825
C	-0.272893	-0.103762	0.664236
C	0.224813	-1.147531	-0.130872
C	-1.158171	-0.444823	1.696465
C	-0.145046	-2.473249	0.093442
H	0.914728	-0.922199	-0.935975
C	-1.514474	-1.769752	1.945085
H	-1.584086	0.342451	2.308585
C	-1.010923	-2.788870	1.139311
H	0.248047	-3.258903	-0.541492
H	-2.191345	-2.005023	2.758333
H	-1.293670	-3.819148	1.321827
Si	-3.847000	1.446913	-0.770575
C	-4.686267	-0.217578	-0.636999
C	-6.069299	-0.329450	-0.439270
C	-3.928515	-1.393722	-0.727202
C	-6.677109	-1.577556	-0.323828
H	-6.680288	0.565523	-0.377391
C	-4.530240	-2.644499	-0.609979
H	-2.856947	-1.334049	-0.891803
C	-5.906179	-2.735842	-0.407814
H	-7.747425	-1.647878	-0.170749
H	-3.928890	-3.543532	-0.677714
H	-6.377728	-3.707345	-0.319150
O	-3.424222	1.872995	0.804682
C	-2.582612	2.974074	0.899700
O	-2.482980	3.748666	-0.058457
H	-2.516815	3.306512	1.941738
H	-2.653658	1.285452	-1.635094
H	-4.814703	2.410086	-1.355887
C	5.024890	-0.033927	-0.410050
C	5.635129	0.286301	0.810175
C	5.619770	-0.997627	-1.232281
C	6.804792	-0.358557	1.195542
H	5.187119	1.033980	1.446604
C	6.797934	-1.629584	-0.841345
H	5.157944	-1.263794	-2.174234
C	7.396636	-1.318581	0.375386
H	7.263769	-0.097562	2.141773
H	7.240511	-2.373414	-1.493100
H	8.310926	-1.812455	0.680013

TS10$_{by}^-$

M05-2X/BS1 SCF energy in Acetonitrile solution: -1553.361825 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1553.718821 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1553.340316 a.u

C	1.892215	-0.195537	-1.435606
O	0.680844	0.410961	-1.829671
O	2.689575	0.911406	-1.205311
H	-0.603136	-0.868610	-0.891948
H	2.281931	-0.841832	-2.233333
N	1.640263	-1.058940	-0.295427
C	1.244743	-0.342263	0.918928
H	0.489922	0.401164	0.663740
H	0.802691	-1.046552	1.622320
H	2.091307	0.164797	1.393003
C	1.480366	3.188675	-0.200945
C	2.555169	3.103577	0.699003
C	0.529363	4.192042	0.030076
C	2.677605	3.981981	1.774088
H	3.294154	2.326261	0.546223
C	0.640296	5.077686	1.102052
H	-0.318999	4.280365	-0.640996
C	1.718155	4.973567	1.978025
H	3.517371	3.894892	2.454259

H	-0.112572	5.842380	1.255598
H	1.808856	5.656520	2.814641
O	-1.553637	-0.854551	-0.660110
O	-1.082663	-2.735067	0.502753
C	-1.859263	-1.851203	0.172758
N	-3.150803	-1.803392	0.620508
C	-3.613394	-2.953536	1.394422
H	-4.509755	-2.666818	1.939244
H	-3.836061	-3.810065	0.754119
H	-2.836776	-3.237788	2.100192
Si	1.329535	2.044005	-1.728187
H	2.092007	2.605730	-2.905600
H	-0.047833	2.614688	-2.149316
C	2.619234	-2.057170	-0.056953
C	3.942795	-1.925956	-0.493726
C	2.244148	-3.209461	0.647066
C	4.864180	-2.944641	-0.251132
H	4.248910	-1.020194	-1.002023
C	3.174762	-4.209047	0.904363
H	1.209888	-3.308183	0.953900
C	4.489482	-4.086034	0.451263
H	5.883913	-2.833094	-0.600656
H	2.870111	-5.096812	1.446349
H	5.210270	-4.871105	0.644296
C	-4.095508	-0.821840	0.212217
C	-3.812482	0.541799	0.330674
C	-5.346899	-1.229999	-0.253534
C	-4.767660	1.481985	-0.038740
H	-2.848623	0.855880	0.707559
C	-6.303685	-0.281346	-0.606520
H	-5.567647	-2.286440	-0.345252
C	-6.017558	1.077120	-0.506017
H	-4.537483	2.536512	0.052965
H	-7.270908	-0.609688	-0.966975
H	-6.760588	1.813863	-0.785115

TS16^{-}

M05-2X/BS1 SCF energy in Acetonitrile solution: -1941.085295 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1941.492882 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1941.103299 a.u

O	-1.937763	-0.640988	-1.875452
O	-1.485687	1.118285	-0.540520
C	-2.242575	0.148092	-0.990416
N	-3.476385	0.069023	-0.341190
Si	0.274993	1.238299	-1.076677
H	1.846760	1.483057	-1.547545
H	0.384559	2.546882	-0.360374
H	-0.072992	1.276824	-2.532470
C	0.825327	-0.351225	-0.171566
C	0.070079	-0.928562	0.861593
C	2.047966	-0.958600	-0.491784
C	0.513853	-2.062093	1.540525
H	-0.877030	-0.485550	1.148096
C	2.495767	-2.099029	0.175617
H	2.668969	-0.522528	-1.267120
C	1.728054	-2.653717	1.196646
H	-0.086815	-2.481580	2.339419
H	3.445832	-2.545840	-0.095749
H	2.073878	-3.535458	1.723225
C	-4.340691	-1.037584	-0.575325
C	-3.852086	-2.346505	-0.557462
C	-5.702884	-0.808308	-0.777905
C	-4.723669	-3.411762	-0.757970
H	-2.797188	-2.518187	-0.392020
C	-6.570537	-1.881049	-0.963573
H	-6.075931	0.208634	-0.787477
C	-6.084869	-3.186360	-0.959188
H	-4.337560	-4.423777	-0.744741
H	-7.625688	-1.692237	-1.119427
H	-6.759497	-4.020216	-1.108495
C	3.009488	2.443496	-1.931938
O	2.864719	3.521331	-1.347653
O	4.036436	1.582657	-1.544225
H	2.801568	2.311714	-3.000657
C	5.434447	0.132435	0.409913
C	5.979885	-0.623267	-0.636388
C	5.599129	-0.329695	1.722723
C	6.673252	-1.804815	-0.378662
H	5.851162	-0.292669	-1.660910
C	6.292338	-1.508952	1.985607
H	5.173139	0.226840	2.552209
C	6.829994	-2.248157	0.933300
H	7.087612	-2.379047	-1.198834
H	6.407178	-1.853811	3.006185
H	7.365890	-3.167949	1.134858
Si	4.470232	1.702382	0.075893

H	5.315049	2.898122	0.335544
H	3.283333	1.739624	0.966270
C	-3.898236	1.060212	0.595781
C	-4.021252	2.395785	0.212254
C	-4.228608	0.672447	1.894563
C	-4.454512	3.342385	1.135361
H	-3.770335	2.681281	-0.801423
C	-4.674888	1.622066	2.809623
H	-4.133583	-0.369218	2.178243
C	-4.785643	2.959143	2.434430
H	-4.543981	4.379446	0.835600
H	-4.929522	1.316666	3.817153
H	-5.129688	3.697716	3.147964

TS17$_{by}^-$

M05-2X/BS1 SCF energy in Acetonitrile solution: -1936.820912 a.u.

M05-2X/BS2 SCF energy in Acetonitrile solution: -1937.266326 a.u.

M05-2X/BS2 Free energy in Acetonitrile solution: -1936.791952 a.u

C	-2.202089	0.215781	-0.790129
O	-1.861368	-0.859208	-0.049203
O	-3.338111	0.675015	-0.447879
H	0.034528	0.884051	-0.391092
H	-1.854273	0.220876	-1.824028
N	-0.837488	1.474178	-0.259412
O	1.301882	-0.066749	-0.738475
O	2.580390	1.380873	0.413630
C	2.364927	0.300148	-0.160797
N	3.435895	-0.656672	-0.186317
Si	-3.242734	-0.925344	1.017495
H	-3.470392	0.128679	2.038894
C	-0.774602	2.602008	-1.155730
C	-1.924686	3.111845	-1.757837
C	0.477958	3.150439	-1.437096
C	-1.814827	4.183775	-2.642373
H	-2.886442	2.668965	-1.533750
C	0.574907	4.216758	-2.326464
H	1.350841	2.736950	-0.941179
C	-0.569570	4.736206	-2.930205
H	-2.706971	4.583410	-3.108893
H	1.545636	4.644887	-2.546045
H	-0.490573	5.566754	-3.620964
C	3.258455	-1.960084	-0.716519
C	2.132137	-2.732523	-0.409745
C	4.248376	-2.503558	-1.543248
C	2.001952	-4.015530	-0.931425
H	1.359396	-2.314006	0.218413
C	4.118344	-3.793680	-2.049099
H	5.121352	-1.909230	-1.785279
C	2.992300	-4.556909	-1.749809
H	1.122364	-4.599341	-0.686826
H	4.896184	-4.196547	-2.686811
H	2.887581	-5.558845	-2.147334
C	4.703743	-0.329917	0.360772
C	5.338995	-1.234706	1.217829
C	5.347061	0.870450	0.041330
C	6.595610	-0.947159	1.742379
H	4.842302	-2.164030	1.469363
C	6.596570	1.158380	0.580630
H	4.853829	1.572250	-0.615761
C	7.230757	0.252655	1.430164
H	7.072247	-1.660337	2.404375
H	7.082251	2.093062	0.326449
H	8.206325	0.479544	1.842201
C	-1.057745	1.737417	1.121121
C	-0.473126	0.869806	2.048851
C	-1.905045	2.757992	1.553440
C	-0.735994	1.028713	3.405715
H	0.182696	0.086635	1.691413
C	-2.160304	2.907564	2.914213
H	-2.359284	3.428783	0.836512
C	-1.582921	2.045363	3.844271
H	-0.275874	0.357345	4.120798
H	-2.817729	3.701855	3.246613
H	-1.787237	2.167927	4.900668
H	-2.708168	-2.062346	1.852518
C	-4.812314	-1.706790	0.326221
C	-5.109763	-3.029095	0.689186
C	-5.732382	-1.031112	-0.490529
C	-6.276001	-3.657252	0.254865
H	-4.419546	-3.580690	1.318386
C	-6.901081	-1.651345	-0.924880
H	-5.519616	-0.014752	-0.794623
C	-7.175111	-2.966901	-0.553469
H	-6.480644	-4.680932	0.545479
H	-7.597768	-1.110272	-1.554476
H	-8.083116	-3.450249	-0.894232

[TBD]

M06-2X/BS1 SCF energy in Acetonitrile solution: -438.66092 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -438.775932 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -438.600838 a.u

C	-0.061817	-0.726926	-0.030750
C	2.411576	-0.754585	0.194361
C	2.421508	0.675590	-0.315529
C	1.198014	1.393223	0.227570
H	2.546828	-0.757788	1.286644
H	3.228160	-1.333747	-0.244116
H	3.327713	1.192821	0.009391
H	2.395357	0.674829	-1.410220
H	1.297443	1.529483	1.316592
H	1.102835	2.388935	-0.217252
N	-0.023912	0.656091	-0.083134
N	1.154205	-1.373253	-0.202054
C	-2.436237	0.610652	-0.379827
C	-2.417765	-0.811435	0.170103
C	-1.259873	1.371711	0.206666
H	-2.739334	-0.794099	1.222476
H	-3.155349	-1.426048	-0.360047
H	-2.340567	0.590697	-1.471289
H	-3.374377	1.115536	-0.132638
H	-1.390901	1.498676	1.293194
H	-1.175526	2.371235	-0.232064
N	-1.118886	-1.460075	0.070303
H	1.065425	-2.359253	0.007965

CO_2

M06-2X/BS1 SCF energy in Acetonitrile solution: -188.507577 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -188.575223 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -188.584099 a.u

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.162966
O	0.000000	0.000000	-1.162966

$[Si]H_3$

M06-2X/BS1 SCF energy in Acetonitrile solution: -522.794661 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -522.878772 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -522.794386 a.u

Si	2.341462	0.000112	0.004040
H	2.830965	1.324199	-0.448088
H	2.858723	-1.056654	-0.897912
H	2.875936	-0.258414	1.363842
C	0.465817	-0.000061	-0.009054
C	-0.253517	1.204049	-0.007203
C	-0.254259	-1.204863	-0.007254
C	-1.647590	1.206367	0.002619
H	0.276908	2.153639	-0.016862
C	-1.647095	-1.207083	0.002819
H	0.275145	-2.155517	-0.017181
C	-2.345162	0.000194	0.008114
H	-2.188118	2.148125	0.002662
H	-2.188107	-2.148554	0.003228
H	-3.431081	-0.000013	0.013505

$[TBD]H^+$

M06-2X/BS1 SCF energy in Acetonitrile solution: -439.15302 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -439.259807 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -439.071932 a.u

N	1.145238	-1.362057	-0.120531
H	1.087745	-2.372030	-0.124741
N	-1.145241	-1.362052	0.120546
H	-1.087747	-2.372025	0.124778
N	0.000002	0.655095	-0.000008
C	0.000000	-0.679982	0.000003
C	2.441258	-0.721996	-0.312477
H	2.637104	-0.574880	-1.380684
H	3.202621	-1.391030	0.090075
C	2.430513	0.610945	0.416681
H	2.360833	0.439468	1.495094
H	3.352900	1.158496	0.213604
C	1.244121	1.432781	-0.056552

H	1.101403	2.307645	0.583612
H	1.394173	1.783411	-1.084225
C	-1.244115	1.432778	0.056566
H	-1.101401	2.307663	-0.583570
H	-1.394167	1.783374	1.084251
C	-2.430506	0.610953	-0.416688
H	-3.352894	1.158505	-0.213617
H	-2.360814	0.439487	-1.495103
C	-2.441268	-0.721993	0.312458
H	-2.637146	-0.574888	1.380660
H	-3.202618	-1.391026	-0.090123

$[N_1]H$

M06-2X/BS1 SCF energy in Acetonitrile solution: -135.096623 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -135.135919 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -135.06818 a.u

N	0.000000	0.577364	-0.156832
H	0.000000	1.313914	0.543822
C	1.201401	-0.224890	0.020205
H	1.259718	-0.973190	-0.777997
H	2.089189	0.409426	-0.047899
H	1.235248	-0.764627	0.981668
C	-1.201401	-0.224890	0.020205
H	-2.089189	0.409426	-0.047899
H	-1.259717	-0.973190	-0.777997
H	-1.235248	-0.764627	0.981668

$[N_2]H$

M06-2X/BS1 SCF energy in Acetonitrile solution: -326.77794 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -326.862265 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -326.746779 a.u

N	1.785343	-0.619325	-0.149246
H	1.999742	-1.547881	0.189563
C	2.811721	0.371027	0.104482
H	3.783558	-0.123712	0.087477
H	2.810626	1.136753	-0.677938
H	2.690815	0.876059	1.073916
C	0.446326	-0.282134	-0.060659
C	0.013643	1.054447	-0.055507
C	-0.525705	-1.300320	-0.006215
C	-1.347791	1.351563	-0.011134
H	0.736913	1.862067	-0.086523
C	-1.876493	-0.988362	0.042556
H	-0.199730	-2.337530	-0.005177
C	-2.304205	0.341871	0.038490
H	-1.658049	2.392855	-0.009696
H	-2.604640	-1.793634	0.085584
H	-3.361615	0.581755	0.075443

$[N_3]H$

M06-2X/BS1 SCF energy in Acetonitrile solution: -518.451935 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -518.58044 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -518.418388 a.u

N	0.000008	1.040695	0.000170
H	0.000017	2.052216	0.000050
C	1.257815	0.442269	-0.019038
C	1.482098	-0.857640	-0.497482
C	2.358820	1.203833	0.407106
C	2.771957	-1.381514	-0.514804
H	0.656677	-1.449364	-0.876311
C	3.642194	0.673831	0.369762
H	2.191044	2.214379	0.770214
C	3.860425	-0.627915	-0.081437
H	2.923296	-2.389937	-0.888718
H	4.477514	1.282654	0.702989
H	4.862167	-1.044025	-0.101314
C	-1.257810	0.442288	0.019182
C	-2.358746	1.203841	-0.407151
C	-1.482170	-0.857597	0.497654
C	-3.642129	0.673845	-0.369974
H	-2.190914	2.214372	-0.770275
C	-2.772031	-1.381468	0.514803
H	-0.656804	-1.449300	0.876639
C	-3.860431	-0.627882	0.081241
H	-4.477397	1.282659	-0.703348
H	-2.923429	-2.389877	0.888733
H	-4.862177	-1.043989	0.100974

IM6

M06-2X/BS1 SCF energy in Acetonitrile solution: -762.325814 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -762.539706 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -762.267935 a.u

N	0.692233	1.133620	0.153178
H	-0.360801	1.091419	0.065969
N	0.699128	-1.139828	-0.134613
H	-0.354031	-1.101689	-0.061723
N	2.727346	0.003563	0.006769
C	1.380558	-0.000695	0.008054
C	1.345296	2.412854	0.371573
H	1.523351	2.581483	1.441841
H	0.670058	3.194810	0.017555
C	2.664371	2.437369	-0.384769
H	2.469104	2.388331	-1.460633
H	3.212264	3.359094	-0.176593
C	3.503115	1.245350	0.045556
H	4.358677	1.114907	-0.624658
H	3.892561	1.392025	1.060859
C	3.510925	-1.232947	-0.039154
H	4.368814	-1.099052	0.627394
H	3.896506	-1.374177	-1.056748
C	2.681499	-2.431381	0.391296
H	3.234650	-3.349026	0.179099
H	2.489475	-2.385786	1.467898
C	1.359637	-2.413964	-0.360369
H	1.535014	-2.577720	-1.431873
H	0.691223	-3.201837	-0.006530
O	-1.964987	-1.128089	0.059093
O	-1.960450	1.118493	-0.101599
C	-2.536498	-0.006736	-0.061619
C	-4.658932	-1.215767	0.142911
H	-5.617027	-1.222050	-0.386828
H	-4.868641	-1.287878	1.221782
H	-4.080149	-2.087959	-0.155183
N	-3.928242	-0.012839	-0.195927
C	-4.655920	1.223468	-0.000734
H	-5.614518	1.169872	-0.526951
H	-4.865497	1.421825	1.062175
H	-4.075098	2.053256	-0.399127

IM12

M06-2X/BS1 SCF energy in Acetonitrile solution: -953.999726 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -954.257765 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -953.936735 a.u

O	0.904286	0.392969	-0.080907
O	0.367532	-1.783154	0.074644
C	1.184745	-0.832222	-0.038232
N	-1.713341	1.060622	0.060101
H	-0.710609	0.760010	0.015616
N	-2.264169	-1.166299	0.051532
H	-1.235584	-1.368037	0.064941
N	-3.959538	0.434850	0.048164
C	-2.653572	0.111179	0.052491
C	-2.032931	2.475608	-0.040239
H	-2.108532	2.783750	-1.091418
H	-1.212862	3.034193	0.415842
C	-3.346714	2.739577	0.676679
H	-3.224023	2.549353	1.747333
H	-3.652665	3.779815	0.545927
C	-4.417150	1.825539	0.104672
H	-5.315264	1.845729	0.729053
H	-4.703314	2.147699	-0.904525
C	-5.011255	-0.580955	-0.039924
H	-5.805192	-0.170442	-0.671039
H	-5.430997	-0.751116	0.959428
C	-4.478857	-1.876341	-0.628609
H	-5.236583	-2.656893	-0.531959
H	-4.258013	-1.738837	-1.691743
C	-3.208355	-2.271149	0.107044
H	-3.441133	-2.530285	1.148038
H	-2.732766	-3.137610	-0.357196
N	2.551008	-1.203859	-0.120743
C	2.875198	-2.606732	0.094147
H	2.936918	-2.870636	1.158113
H	2.096597	-3.214186	-0.361882
H	3.833781	-2.833599	-0.377445
C	3.600762	-0.265038	-0.079804
C	3.537355	0.950881	-0.782828
C	4.776404	-0.561711	0.627227
C	4.609362	1.834926	-0.758119
H	2.642609	1.189482	-1.340853

C	5.848187	0.328674	0.637692
H	4.854084	-1.490334	1.182380
C	5.774023	1.535728	-0.049935
H	4.536615	2.766695	-1.312104
H	6.743173	0.071949	1.196926
H	6.608286	2.229800	-0.040278

IM19

M06-2X/BS1 SCF energy in Acetonitrile solution: -1145.670312 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -1145.973504 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -1145.604947 a.u

O	0.042052	1.110450	0.241121
O	0.062188	-1.130496	0.052081
C	0.607632	-0.002982	0.120293
N	-2.670884	1.130275	0.170600
H	-1.626788	1.085416	0.198096
N	-2.653981	-1.148277	-0.103293
H	-1.612703	-1.101477	-0.031234
N	-4.689804	-0.015702	-0.035119
C	-3.345920	-0.011014	0.012338
C	-3.331894	2.424991	0.204756
H	-3.463932	2.820031	-0.810918
H	-2.685471	3.113186	0.753104
C	-4.681960	2.270938	0.885586
H	-4.531630	1.981968	1.930550
H	-5.234206	3.212770	0.864011
C	-5.481501	1.201593	0.160835
H	-6.366418	0.921930	0.740288
H	-5.821651	1.566683	-0.816238
C	-5.457894	-1.236634	-0.294199
H	-6.298003	-0.959907	-0.938391
H	-5.869496	-1.605566	0.653382
C	-4.601650	-2.302110	-0.957766
H	-5.148726	-3.247120	-0.972283
H	-4.379851	-2.016879	-1.990817
C	-3.302835	-2.447284	-0.182215
H	-3.505385	-2.842337	0.821910
H	-2.614369	-3.132195	-0.681345
N	2.034406	0.012181	0.051672
C	2.769336	-1.205929	0.063425
C	3.763528	-1.418465	-0.896894
C	2.543961	-2.179878	1.041359
C	4.524407	-2.584253	-0.876836
H	3.937591	-0.661567	-1.656234
C	3.299460	-3.348766	1.049444
H	1.770992	-2.015353	1.783524
C	4.295572	-3.556113	0.095175
H	5.293512	-2.733679	-1.628458
H	3.116740	-4.097199	1.814788
H	4.887499	-4.465698	0.110703
C	2.762098	1.228282	-0.036589
C	3.937386	1.385052	0.707755
C	2.352417	2.265192	-0.883685
C	4.686840	2.554002	0.607974
H	4.262339	0.583157	1.364096
C	3.099568	3.435926	-0.967614
H	1.443414	2.148060	-1.460711
C	4.271126	3.588833	-0.226968
H	5.596252	2.655345	1.192862
H	2.767346	4.231007	-1.628776
H	4.852791	4.502175	-0.301587

[Si]H_2(OCHO)

M06-2X/BS1 SCF energy in Acetonitrile solution: -711.341173 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -711.488107 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -711.389018 a.u

C	-3.242181	-0.000006	-0.805144
O	-3.914168	-0.000021	0.197633
O	-1.908840	0.000020	-0.807114
H	-3.653342	-0.000013	-1.823376
C	0.714390	0.000006	0.304747
C	1.413214	1.206159	0.144713
C	1.413199	-1.206155	0.144720
C	2.768200	1.207750	-0.177851
H	0.898011	2.155177	0.275648
C	2.768184	-1.207766	-0.177845
H	0.897983	-2.155166	0.275659
C	3.444962	-0.000013	-0.341010
H	3.295755	2.148814	-0.299319
H	3.295728	-2.148837	-0.299309
H	4.501666	-0.000020	-0.591089
Si	-1.098586	0.000013	0.708168

H	-1.475664	1.228373	1.434652
H	-1.475669	-1.228354	1.434641

IM8^{-}

M06-2X/BS1 SCF energy in Acetonitrile solution: -1034.518883 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -1034.773742 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -1034.587341 a.u

O	2.650618	-1.742386	-0.212512
O	1.336526	0.086443	-0.171485
C	2.500655	-0.520488	-0.161848
C	4.885848	-0.208564	0.163754
H	5.096646	-0.230105	1.242780
H	5.653515	0.400824	-0.322062
H	4.937022	-1.225288	-0.222126
N	3.576724	0.342879	-0.121151
C	3.384304	1.742126	0.209117
H	3.253138	1.901471	1.289298
H	4.264907	2.304236	-0.113589
H	2.508796	2.131581	-0.308997
Si	-0.182443	-0.951930	-0.254975
H	-2.008200	-1.988287	1.596858
H	0.167595	-1.604784	1.037608
H	0.183701	-1.441254	-1.608422
C	-1.291296	0.598791	-0.139389
C	-0.823775	1.799846	0.421749
C	-2.615863	0.589847	-0.608240
C	-1.635836	2.929153	0.518688
H	0.197325	1.850127	0.787298
C	-3.429384	1.720539	-0.533986
H	-3.021377	-0.319013	-1.043427
C	-2.942388	2.894943	0.035152
H	-1.245807	3.839255	0.966167
H	-4.445496	1.681901	-0.916499
H	-3.574712	3.775742	0.100404
C	-2.376961	-2.410453	0.637417
O	-1.649923	-2.119041	-0.399332
O	-3.384940	-3.095515	0.618070

TS6^{-}

M06-2X/BS1 SCF energy in Acetonitrile solution: -1169.591904 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -1169.885151 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -1169.614287 a.u

C	-0.286869	0.585867	-0.966440
O	-0.350781	1.692083	-1.486697
O	0.935953	0.038353	-0.675987
C	-0.657617	-0.312339	1.905286
H	-0.957898	-0.202390	2.960264
H	-1.204594	-1.152756	1.469278
H	0.417251	-0.530003	1.880137
H	-1.955335	0.942300	0.967464
H	-1.083067	-0.166334	-0.983057
N	-0.936787	0.861612	1.105618
C	-0.344976	2.080782	1.607840
H	-0.462412	2.872361	0.860048
H	-0.782235	2.423627	2.558659
H	0.728119	1.926323	1.774269
C	3.715904	0.009478	-0.366297
C	3.560140	-1.321246	0.045584
C	4.999371	0.574298	-0.318743
C	4.652825	-2.066911	0.486779
H	2.573977	-1.777755	0.021794
C	6.094046	-0.166996	0.118944
H	5.152453	1.608203	-0.624558
C	5.920758	-1.490698	0.522157
H	4.514157	-3.096663	0.802744
H	7.080364	0.286377	0.149157
H	6.773040	-2.070470	0.863917
O	-3.791659	0.734180	0.770080
O	-2.984296	-1.110037	-0.249450
C	-3.907836	-0.364337	0.161524
C	-6.312236	0.140073	0.056420
H	-7.265945	-0.376407	0.212988
H	-6.414503	0.759543	-0.851326
H	-6.119876	0.801950	0.899052
N	-5.241194	-0.826831	-0.046144
C	-5.449113	-1.832783	-1.064367
H	-6.402774	-2.344874	-0.893034
H	-5.478471	-1.407912	-2.082666
H	-4.638881	-2.558732	-1.022086
Si	2.268606	1.026126	-0.978663
H	2.405472	1.296482	-2.427946
H	2.226429	2.310114	-0.245833

$TS6_{by}^-$

M06-2X/BS1 SCF energy in Acetonitrile solution: -1557.287916 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -1557.623048 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -1557.329567 a.u

O	-4.761931	-1.439762	0.743195
O	-3.294786	0.202535	0.264442
C	-4.509372	-0.282246	0.408654
N	-5.504375	0.646021	0.182884
C	-5.209226	1.897516	-0.488399
H	-5.156698	1.778419	-1.580289
H	-6.002668	2.615133	-0.262195
H	-4.260095	2.296817	-0.134698
Si	-1.857392	-0.893299	0.543285
H	-0.516819	-1.893306	0.705282
H	-2.240735	-1.819190	-0.558050
H	-2.192102	-1.153187	1.976376
C	-0.650318	0.540847	0.250613
C	-0.860767	1.525025	-0.726827
C	0.509276	0.639731	1.033178
C	0.065440	2.548275	-0.936040
H	-1.763471	1.490327	-1.331870
C	1.421352	1.679100	0.857837
H	0.708921	-0.122224	1.784062
C	1.207821	2.629249	-0.140624
H	-0.107469	3.287877	-1.712998
H	2.309413	1.736381	1.482106
H	1.928485	3.427055	-0.296612
C	0.475304	-2.706939	-0.258377
O	0.072176	-2.648901	-1.424181
O	1.645506	-2.053012	0.085279
H	0.332979	-3.590426	0.380187
C	3.817397	-0.339284	-0.331440
C	4.306731	-0.781306	0.905203
C	4.439841	0.762567	-0.936359
C	5.385728	-0.145213	1.518474
H	3.828963	-1.623131	1.399885
C	5.519924	1.400380	-0.330250
H	4.068445	1.141600	-1.887235
C	5.993341	0.946495	0.900914
H	5.749410	-0.497951	2.479090
H	5.987842	2.253934	-0.811789
H	6.831237	1.445364	1.378697
Si	2.346164	-1.155563	-1.154859
H	2.810622	-2.062406	-2.233556
H	1.497346	-0.100090	-1.747566
C	-6.868627	0.171314	0.068773
H	-7.125166	-0.094073	-0.966939
H	-6.995161	-0.709232	0.696451
H	-7.556247	0.954294	0.401653

$IM13^-$

M06-2X/BS1 SCF energy in Acetonitrile solution: -1226.191216 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -1226.490163 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -1226.25506 a.u

C	1.184162	-0.347881	-0.163450
O	1.421445	-1.551538	-0.116513
O	-0.010652	0.178072	-0.175615
C	-3.592334	-2.478301	0.793841
O	-4.581095	-3.189585	0.794625
O	-2.872825	-2.202411	-0.254219
H	-3.234173	-2.015398	1.737959
Si	-1.479579	-0.960511	-0.178532
H	-1.068152	-1.504453	-1.496718
H	-1.075003	-1.503973	1.147690
C	-2.661865	0.536958	-0.141822
C	-2.261696	1.782226	0.372390
C	-3.979945	0.438857	-0.618468
C	-3.131394	2.870854	0.416594
H	-1.248553	1.900980	0.743894
C	-4.850570	1.528379	-0.598024
H	-4.333826	-0.507184	-1.017807
C	-4.429852	2.748918	-0.074790
H	-2.792900	3.816997	0.829782
H	-5.859458	1.421782	-0.986567
H	-5.107382	3.597428	-0.049410
N	2.199964	0.611843	-0.212786
C	1.846975	2.023253	-0.105556
H	1.681082	2.336452	0.932675
H	2.654253	2.623224	-0.529289
H	0.935621	2.205790	-0.671717
C	3.557997	0.244549	-0.070383
C	4.083283	-0.885371	-0.715854

C	4.420948	1.049257	0.685475
C	5.431439	-1.200097	-0.588926
H	3.429288	-1.508389	-1.310961
C	5.772415	0.729481	0.797481
H	4.036764	1.925086	1.197737
C	6.287678	-0.398073	0.165859
H	5.818603	-2.078361	-1.097518
H	6.419719	1.367814	1.391447
H	7.340038	-0.647910	0.255332

TS9$^-$

M06-2X/BS1 SCF energy in Acetonitrile solution: -1748.96159 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -1749.34157 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -1748.998506 a.u

O	3.305330	2.843298	0.120574
O	2.057159	0.995993	0.416563
C	3.175538	1.624118	0.165958
N	4.270597	0.788947	-0.059279
C	5.496999	1.440780	-0.502362
H	5.601735	2.382521	0.033907
H	6.348340	0.797786	-0.273638
H	5.490922	1.655246	-1.577753
Si	0.505058	1.926839	0.718827
H	-0.937006	2.765829	0.916872
H	0.506486	2.560178	-0.630153
H	1.037042	2.641629	1.916375
C	-0.423553	0.304321	1.065848
C	-0.082473	-0.902012	0.433664
C	-1.475309	0.273837	1.992209
C	-0.759781	-2.088301	0.716571
H	0.737656	-0.915368	-0.279083
C	-2.140650	-0.911978	2.302191
H	-1.784729	1.199243	2.473949
C	-1.786527	-2.097807	1.659877
H	-0.483358	-3.005711	0.203297
H	-2.945847	-0.909036	3.032142
H	-2.312298	-3.020921	1.887581
C	4.175213	-0.620287	-0.164100
C	4.878246	-1.286602	-1.176026
C	3.438967	-1.379396	0.757734
C	4.831812	-2.675874	-1.274094
H	5.456399	-0.717593	-1.896860
C	3.385510	-2.763914	0.641266
H	2.905716	-0.878361	1.555469
C	4.080660	-3.423781	-0.372471
H	5.381601	-3.170383	-2.069290
H	2.802700	-3.331771	1.360964
H	4.039989	-4.505308	-0.453526
C	-2.104088	3.366892	0.080879
O	-1.663582	3.837302	-0.973840
O	-2.898324	2.227527	0.041544
H	-2.401509	3.994303	0.934320
C	-3.656935	-0.279706	-0.983405
C	-4.677962	-0.364381	-0.024514
C	-3.269346	-1.454616	-1.642799
C	-5.295034	-1.580436	0.261372
H	-4.983501	0.528601	0.515956
C	-3.885250	-2.674383	-1.363880
H	-2.464020	-1.423726	-2.374919
C	-4.899845	-2.737173	-0.410758
H	-6.081034	-1.628853	1.009505
H	-3.569117	-3.574097	-1.883631
H	-5.379562	-3.685934	-0.188736
Si	-2.813752	1.343390	-1.383463
H	-3.541347	2.043812	-2.472320
H	-1.439532	1.043336	-1.838271

TS10$_{by}^-$

M06-2X/BS1 SCF energy in Acetonitrile solution: -1552.955744 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -1553.326892 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -1552.949122 a.u

C	1.911295	-0.119961	-1.453983
O	0.682341	0.429777	-1.863578
O	2.654639	1.016719	-1.213287
H	-0.545677	-0.861876	-0.950237
H	2.338870	-0.754965	-2.246957
N	1.681960	-0.995977	-0.313482
C	1.215491	-0.304466	0.888120
H	0.433335	0.407622	0.612448
H	0.781268	-1.029330	1.579303
H	2.022270	0.243878	1.392413
C	1.323900	3.205616	-0.183822

C	2.377165	3.136248	0.744006
C	0.334841	4.173846	0.045051
C	2.442301	3.992686	1.842081
H	3.148057	2.385722	0.593903
C	0.389440	5.039440	1.138201
H	-0.501513	4.250835	-0.647164
C	1.446565	4.949395	2.041327
H	3.267440	3.915982	2.545102
H	-0.392108	5.779248	1.287913
H	1.492956	5.616938	2.897050
O	-1.493222	-0.885596	-0.700272
O	-0.922990	-2.709369	0.506158
C	-1.740158	-1.870253	0.163576
N	-3.031666	-1.864550	0.631569
C	-3.431826	-3.013227	1.439350
H	-4.316555	-2.745908	2.017255
H	-3.655289	-3.890486	0.822683
H	-2.619363	-3.265410	2.120147
Si	1.248528	2.087137	-1.737004
H	2.001928	2.703321	-2.885856
H	-0.142151	2.594148	-2.165836
C	2.693288	-1.955384	-0.060538
C	4.003456	-1.802022	-0.533383
C	2.370163	-3.097296	0.688298
C	4.959015	-2.787816	-0.286672
H	4.273998	-0.901506	-1.075926
C	3.335252	-4.062939	0.948671
H	1.345111	-3.218042	1.027071
C	4.634540	-3.918892	0.456989
H	5.967955	-2.657830	-0.667545
H	3.068623	-4.943837	1.525636
H	5.383027	-4.680485	0.651810
C	-4.026987	-0.941107	0.206924
C	-3.788900	0.437539	0.223544
C	-5.284444	-1.417595	-0.173287
C	-4.792128	1.319943	-0.161523
H	-2.820208	0.808844	0.537819
C	-6.288124	-0.525389	-0.543989
H	-5.474948	-2.486434	-0.185190
C	-6.046348	0.845573	-0.545447
H	-4.594091	2.387355	-0.147864
H	-7.259573	-0.909001	-0.840432
H	-6.827737	1.539112	-0.839231

IM20^{-}

M06-2X/BS1 SCF energy in Acetonitrile solution: -1417.86217 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -1418.206571 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -1417.923773 a.u

C	0.846389	-1.133952	-0.242064
O	1.012132	-2.336526	-0.403060
O	-0.297173	-0.522464	-0.162364
C	-4.207288	-2.729149	0.565261
O	-5.297817	-3.267772	0.510098
O	-3.471897	-2.427603	-0.465635
H	-3.761368	-2.464010	1.547277
Si	-1.907371	-1.432203	-0.284778
H	-1.572273	-1.885501	-1.657481
H	-1.572483	-2.196337	0.950767
C	-2.842526	0.221515	-0.072342
C	-2.231000	1.354480	0.494416
C	-4.178533	0.362269	-0.485610
C	-2.916856	2.557904	0.649963
H	-1.195405	1.295786	0.814203
C	-4.867297	1.567556	-0.348905
H	-4.691580	-0.484959	-0.930680
C	-4.239292	2.670444	0.224912
H	-2.413646	3.410666	1.097929
H	-5.896273	1.643245	-0.689276
H	-4.773921	3.609146	0.338716
N	1.934681	-0.249996	-0.118828
C	3.270812	-0.725883	-0.048590
C	3.599360	-1.871634	0.685503
C	4.285131	-0.013625	-0.698170
C	4.921505	-2.300650	0.747927
H	2.816347	-2.420317	1.193509
C	5.606510	-0.443729	-0.618702
H	4.032283	0.876128	-1.266722
C	5.932297	-1.592252	0.099521
H	5.163466	-3.191642	1.319579
H	6.381863	0.118974	-1.129698
H	6.962131	-1.929959	0.156473
C	1.705747	1.159862	-0.049094
C	1.062485	1.826856	-1.094081
C	2.133673	1.872061	1.071775
C	0.824521	3.194651	-1.002143
H	0.739389	1.262160	-1.962808

C	1.905305	3.244284	1.153044
H	2.637770	1.345157	1.876863
C	1.244523	3.907979	0.120906
H	0.314052	3.705617	-1.812707
H	2.235604	3.792243	2.030203
H	1.059709	4.975419	0.189060

TS16^{-}

M06-2X/BS1 SCF energy in Acetonitrile solution: -1940.632522 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -1941.056885 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -1940.665432 a.u

O	-1.976948	-0.280662	-2.274468
O	-1.219151	1.383653	-0.956161
C	-2.043800	0.416286	-1.272119
N	-3.053508	0.225532	-0.320318
Si	0.437651	1.491863	-1.742074
H	1.987470	1.746933	-2.334542
H	0.677738	2.755021	-0.990943
H	-0.071180	1.582000	-3.139657
C	1.013463	-0.200628	-1.083523
C	0.515523	-0.739403	0.114297
C	1.956673	-0.959184	-1.789889
C	0.939162	-1.982938	0.584152
H	-0.220652	-0.180096	0.688735
C	2.363605	-2.216689	-1.344355
H	2.388035	-0.552810	-2.702306
C	1.859900	-2.730064	-0.149866
H	0.550094	-2.369397	1.522342
H	3.087786	-2.788483	-1.918337
H	2.188962	-3.700718	0.210161
C	-3.977041	-0.849600	-0.460211
C	-3.539221	-2.139859	-0.773315
C	-5.337317	-0.614191	-0.243517
C	-4.462324	-3.174636	-0.888733
H	-2.481642	-2.318551	-0.930490
C	-6.252567	-1.658017	-0.347619
H	-5.671325	0.388807	0.005641
C	-5.820789	-2.941192	-0.676495
H	-4.114810	-4.173026	-1.136578
H	-7.307021	-1.462479	-0.178351
H	-6.535846	-3.752994	-0.763988
C	3.312013	2.467448	-1.994619
O	3.076094	3.543349	-1.432418
O	3.892765	1.432120	-1.271001
H	3.631709	2.403484	-3.045885
C	4.278745	-0.129038	1.019963
C	5.163551	-0.930940	0.283478
C	3.783808	-0.629425	2.232577
C	5.547022	-2.188202	0.744525
H	5.542255	-0.573247	-0.671021
C	4.164719	-1.886571	2.700390
H	3.079873	-0.038907	2.816435
C	5.048606	-2.666347	1.956401
H	6.229297	-2.797245	0.158741
H	3.768466	-2.259946	3.640107
H	5.344985	-3.647108	2.316692
Si	3.764652	1.559938	0.397853
H	4.687069	2.600449	0.917628
H	2.397413	1.839842	0.885822
C	-3.189370	1.080398	0.816230
C	-3.375582	2.455432	0.664053
C	-3.175699	0.515781	2.092931
C	-3.530615	3.260748	1.788452
H	-3.390306	2.881752	-0.333686
C	-3.343955	1.324995	3.213577
H	-3.034831	-0.556588	2.197461
C	-3.519007	2.699372	3.065196
H	-3.671598	4.330210	1.665183
H	-3.331672	0.879875	4.203703
H	-3.647057	3.330394	3.939084

TS17$_{\mathbf{by}}^{-}$

M06-2X/BS1 SCF energy in Acetonitrile solution: -1936.286764 a.u.

M06-2X/BS2 SCF energy in Acetonitrile solution: -1936.751751 a.u.

M06-2X/BS2 Free energy in Acetonitrile solution: -1936.282613 a.u

C	-2.229624	0.203744	-0.802359
O	-1.945854	-0.905345	-0.100470
O	-3.341795	0.703166	-0.439850
H	0.049333	0.777672	-0.364650
H	-1.871677	0.244016	-1.835536
N	-0.801191	1.400193	-0.219857
O	1.285958	-0.231040	-0.652196

O	2.491942	1.270610	0.507081
C	2.329746	0.187870	-0.077904
N	3.458466	-0.711520	-0.121022
Si	-3.350292	-0.909091	0.945610
H	-3.525443	0.113648	2.007166
C	-0.708027	2.552037	-1.081853
C	-1.849889	3.132380	-1.637729
C	0.559747	3.051280	-1.389700
C	-1.715888	4.218853	-2.501199
H	-2.828032	2.729769	-1.395630
C	0.680816	4.132853	-2.258136
H	1.428286	2.591127	-0.922409
C	-0.454732	4.718991	-2.816293
H	-2.604111	4.670527	-2.932335
H	1.666404	4.521275	-2.497225
H	-0.356991	5.561958	-3.493345
C	3.324870	-2.039314	-0.599442
C	2.243838	-2.843900	-0.216514
C	4.298868	-2.575943	-1.450639
C	2.138762	-4.148046	-0.688849
H	1.484262	-2.431734	0.437226
C	4.193989	-3.886488	-1.908793
H	5.140712	-1.959189	-1.751380
C	3.111876	-4.680277	-1.534581
H	1.291799	-4.756305	-0.385029
H	4.958800	-4.282779	-2.570191
H	3.027416	-5.700090	-1.896353
C	4.738479	-0.268448	0.300546
C	5.532204	-1.087145	1.112831
C	5.240902	0.973154	-0.107269
C	6.801274	-0.671882	1.508507
H	5.149224	-2.051989	1.432750
C	6.503758	1.387812	0.302552
H	4.627473	1.609255	-0.734277
C	7.293385	0.569057	1.110159
H	7.402405	-1.320079	2.139263
H	6.877402	2.354494	-0.022296
H	8.280274	0.894485	1.423482
C	-1.016932	1.611593	1.169847
C	-0.483932	0.668152	2.056546
C	-1.825695	2.643099	1.649770
C	-0.761828	0.760661	3.416352
H	0.142007	-0.124722	1.658901
C	-2.095305	2.726927	3.014132
H	-2.240896	3.373963	0.963930
C	-1.572301	1.787096	3.900978
H	-0.343074	0.028121	4.099817
H	-2.725057	3.530854	3.383176
H	-1.790244	1.857273	4.961943
H	-2.902386	-2.106902	1.739968
C	-4.959040	-1.572086	0.214461
C	-5.349469	-2.882503	0.533339
C	-5.823528	-0.815524	-0.594258
C	-6.548176	-3.420699	0.065700
H	-4.704791	-3.497755	1.156802
C	-7.023548	-1.345188	-1.062976
H	-5.544386	0.197171	-0.865514
C	-7.388892	-2.650397	-0.734273
H	-6.823564	-4.438957	0.324544
H	-7.674909	-0.740042	-1.687073
H	-8.323312	-3.063951	-1.102353