Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Dehydrocoupling of dimethylamine borane by titanocene: Elucidation of ten years of inconsistency between theoretical and experimental descriptions.

Jingwen ZHU, [†] Emilie-Laure ZINS, [†] and Mohammad Esmail ALIKHANI [*/†]

[†] Sorbonne Université, CNRS, De la Molécule aux Nano-Objets: Réactivité, Interactions Spectroscopies, MONARIS, 75005, Paris France

Gas phase electronic energy (E), zero-point corrected (E+ZPE), Gibbs (G) and enthalpies (H)

Effect of basis sets

B3LYP-GD3BJ/6-31G*+6-31++G**+LanL2DZ								
	E (a.u.)	E+ZPE (a.u.)	Gibbs free energy (a.u.)	Enthalpy (a.u.)	ΔE (kJ/mol)	Δ(E+ZPE) (kJ/mol)	ΔG (kJ/mol)	ΔH (kJ/mol)
Cp_2Ti	-445.2026	-445.0367	-445.0751	-445.0256				
$HNMe_2BH_3$	-161.8577	-161.7301	-161.7579	-161.7233				
$Cp_2Ti+HNMe_2BH_3$	-607.0603	-606.7668	-606.8330	-606.7489	0.0	0.0	0.0	0.0
S_1	-607.0899	-606.7931	-606.8371	-606.7756	-77.6	-69.1	-10.9	-70.2
TS_{1_2}	-607.0798	-606.7854	-606.8263	-606.7694	-51.1	-48.9	17.4	-54.0

B3LYP-GD3BJ/6-311++G(2d,2p)+LanL2DZ								
	E (a.u.)	E+ZPE (a.u.)	Gibbs free energy (a.u.)	Enthalpy (a.u.)	ΔE (kJ/mol)	Δ(E+ZPE) (kJ/mol)	ΔG (kJ/mol)	ΔH (kJ/mol)
Cp_2Ti	-445.3299	-445.1653	-445.2030	-445.1542				
$HNMe_2BH_3$	-161.9090	-161.7821	-161.8100	-161.7753				
$Cp_2Ti+HNMe_2BH_3$	-607.2389	-606.9475	-607.0129	-606.9295	0.0	0.0	0.0	0.0
S_1	-607.2669	-606.9722	-607.0167	-606.9545	-73.4	-64.9	-10.0	-65.5
TS_{1_2}	-607.2572	-606.9647	-607.0056	-606.9486	-48.0	-45.2	19.1	-50.1

B3LYP-GD3BJ/6-311++G(2d,2p)								
	E (a.u.)	**E+ZPE (a.u.)**	**Gibbs free energy (a.u.)**	**Enthalpy (a.u.)**	**ΔE (kJ/mol)**	**Δ(E+ZPE) (kJ/mol)**	**ΔG (kJ/mol)**	**ΔH (kJ/mol)**
Cp_2Ti	-1236.7054	-1236.5406	-1236.5761	-1236.5304				
$HNMe_2BH_3$	-161.9090	-161.7821	-161.8100	-161.7753				
$Cp_2Ti+HNMe_2BH_3$	-1398.6144	-1398.3227	-1398.3860	-1398.3057	0.0	0.0	0.0	0.0
S_1	-1398.6419	-1398.3471	-1398.3921	-1398.3294	-72.2	-64.1	-15.8	-62.3
TS_{1_2}	-1398.6324	-1398.3399	-1398.3809	-1398.3238	-47.2	-45.2	13.5	-47.6

B3LYP-GD3BJ/6-311++G(3df,3pd)								
	E (a.u.)	**E+ZPE (a.u.)**	**Gibbs free energy (a.u.)**	**Enthalpy (a.u.)**	**ΔE (kJ/mol)**	**Δ(E+ZPE) (kJ/mol)**	**ΔG (kJ/mol)**	**ΔH (kJ/mol)**
Cp_2Ti	-1236.7212	-1236.5561	-1236.5935	-1236.5450				
$HNMe_2BH_3$	-161.9144	-161.7877	-161.8155	-161.7808				
$Cp_2Ti+HNMe_2BH_3$	-1398.6356	-1398.3438	-1398.4090	-1398.3259	0.0	0.0	0.0	0.0
S_1	-1398.6632	-1398.3682	-1398.4125	-1398.3506	-72.6	-64.3	-9.1	-65.0
TS_{1_2}	-1398.6539	-1398.3610	-1398.4019	-1398.3450	-48.0	-45.2	18.6	-50.1

Gas phase electronic energy (E), zero-point corrected (E+ZPE), Gibbs (G) and enthalpies (H)

Path 1: From the [$Cp_2Ti(\eta^1\text{-}BH_3{\cdot}NHMe_2)$] adduct to the linear diborazane

B3LYP-GD3BJ/6-31G*+6-31++G**+LanL2DZ								
	E (a.u.)	E+ZPE (a.u.)	Gibbs free energy (a.u.)	Enthalpy (a.u.)	ΔE (kJ/mol)	Δ(E+ZPE) (kJ/mol)	ΔG (kJ/mol)	ΔH (kJ/mol)
Cp_2Ti	-445.2026	-445.0367	-445.0751	-445.0256				
$HNMe_2BH_3$	-161.8577	-161.7301	-161.7579	-161.7233				
$Cp_2Ti+2HNMe_2BH_3$	-768.9180	-768.4969	-768.5909	-768.4721	0.0	0.0	0.0	0.0
$S_1 + HNMe_2BH_3$	-768.9476	-768.5232	-768.5950	-768.4988	-77.6	-69.1	-10.9	-70.2
$TS_{1\_2} + HNMe_2BH_3$	-768.9375	-768.5155	-768.5842	-768.4927	-51.1	-48.9	17.4	-54.0
$S_2 + HNMe_2BH_3$	-768.9848	-768.5609	-768.6294	-768.5381	-175.3	-168.2	-101.1	-173.3
$S_3 + HNMe_2BH_3$	-768.9544	-768.5377	-768.6122	-768.5133	-95.7	-107.4	-55.9	-108.1
S_4	-768.9915	-768.5667	-768.6194	-768.5435	-192.9	-183.3	-74.9	-187.4
S_5	-769.0004	-768.5763	-768.6263	-768.5535	-216.3	-208.5	-93.2	-213.6

B3LYP-GD3BJ-PCM(toluene)/6-31G*+6-31++G**+LanL2DZ								
	E (a.u.)	E+ZPE (a.u.)	Gibbs free energy (a.u.)	Enthalpy (a.u.)	ΔE (kJ/mol)	Δ(E+ZPE) (kJ/mol)	ΔG (kJ/mol)	ΔH (kJ/mol)
Cp_2Ti	-445.2057	-445.0400	-445.0776	-445.0289				
$HNMe_2BH_3$	-161.8638	-161.7363	-161.7641	-161.7294				
$Cp_2Ti+2HNMe_2BH_3$	-768.9334	-768.5125	-768.6058	-768.4878	0.0	0.0	0.0	0.0
$S_1 + HNMe_2BH_3$	-768.9592	-768.5350	-768.6073	-768.5106	-67.9	-58.9	-3.9	-59.9
$TS_{1\_2} + HNMe_2BH_3$	-768.9477	-768.5261	-768.5951	-768.5032	-37.6	-35.7	28.3	-40.6
$S_2 + HNMe_2BH_3$	-768.9944	-768.5707	-768.6392	-768.5479	-160.1	-152.7	-87.6	-157.8
$S_3 + HNMe_2BH_3$	-768.9638	-768.5473	-768.6239	-768.5220	-79.9	-91.3	-47.5	-89.8
S_4	-769.0002	-768.5753	-768.6278	-768.5522	-175.5	-164.8	-57.6	-169.2

S_5	-769.0053	-768.5813	-768.6312	-768.5585	-188.9	-180.5	-66.7	-185.8

Path 2: From the [$Cp_2Ti(\eta^2\text{-}BH_3{\cdot}NHMe_2)$] adduct to the linear diborazane

B3LYP-GD3BJ/6-31G*+6-31++G+LanL2DZ**								
	E (a.u.)	**E+ZPE (a.u.)**	**Gibbs free energy (a.u.)**	**Enthalpy (a.u.)**	**ΔE (kJ/mol)**	**Δ(E+ZPE) (kJ/mol)**	**ΔG (kJ/mol)**	**ΔH (kJ/mol)**
$Cp_2Ti+2HNMe_2BH_3$	-768.9180	-768.4969	-768.5909	-768.4721	0.0	0.0	0.0	0.0
S_6	-768.9870	-768.5593	-768.6115	-768.5350	-181.0	-164.0	-54.1	-165.1
TS_{6_7}	-768.9538	-768.5323	-768.5819	-768.5094	-93.9	-93.1	23.5	-97.8
S_7	-768.9582	-768.5351	-768.5859	-768.5119	-105.5	-100.5	12.9	-104.6
TS_{7_8}	-768.9549	-768.5311	-768.5793	-768.5090	-96.8	-90.0	30.2	-96.8
S_8	-768.9839	-768.5614	-768.6143	-768.5384	-172.9	-169.5	-61.4	-173.9

B3LYP-GD3BJ-PCM(toluene)/6-31G*+6-31++G+LanL2DZ**								
	E (a.u.)	**E+ZPE (a.u.)**	**Gibbs free energy (a.u.)**	**Enthalpy (a.u.)**	**ΔE (kJ/mol)**	**Δ(E+ZPE) (kJ/mol)**	**ΔG (kJ/mol)**	**ΔH (kJ/mol)**
$Cp_2Ti+2HNMe_2BH_3$	-768.9334	-768.5125	-768.6058	-768.4878	0.0	0.0	0.0	0.0
S_6	-768.9955	-768.5673	-768.6190	-768.5431	-163.1	-143.8	-34.6	-145.3
TS_{6_7}	-768.9610	-768.5396	-768.5893	-768.5165	-72.6	-71.1	43.3	-75.5
S_7	-768.9694	-768.5462	-768.5968	-768.5229	-94.5	-88.4	23.6	-92.3
TS_{7_8}	-768.9630	-768.5396	-768.5885	-768.5174	-77.9	-71.1	45.6	-77.6
S_8	-768.9906	-768.5687	-768.6220	-768.5455	-150.3	-147.5	-42.6	-151.6

Path 3: From linear diborazane to cyclic diborazane

B3LYP-GD3BJ/6-31G*+6-31++G**+LanL2DZ								
	E (a.u.)	**E+ZPE (a.u.)**	**Gibbs free energy (a.u.)**	**Enthalpy (a.u.)**	**ΔE (kJ/mol)**	**Δ(E+ZPE) (kJ/mol)**	**ΔG (kJ/mol)**	**ΔH (kJ/mol)**
Cp_2Ti	-445.2026	-445.0367	-445.0751	-445.0256				
$HNMe_2BH_2NMe_2BH_3$	-322.5568	-322.3187	-322.3538	-322.3069				
Cp_2Ti +$HNMe_2BH_2NMe_2BH_3$	-767.7595	-767.3554	-767.4289	-767.3325	0.0	0.0	0.0	0.0
S_9	-767.7952	-767.3874	-767.4382	-767.3648	-93.9	-84.1	-24.5	-85.0
TS_{9_10}	-767.7723	-767.3714	-767.4168	-767.3504	-33.6	-42.0	31.6	-47.2
S_{10}	-767.8041	-767.3994	-767.4468	-767.3777	-117.0	-115.5	-47.0	-118.8
TS_{10_11}	-767.7908	-767.3874	-767.4345	-767.3663	-82.2	-84.0	-14.8	-88.8
S_{11}	-767.8101	-767.4060	-767.4539	-767.3850	-132.8	-133.0	-65.7	-138.0

B3LYP-GD3BJ-PCM(toluene)/6-31G*+6-31++G**+LanL2DZ								
	E (a.u.)	**E+ZPE (a.u.)**	**Gibbs free energy (a.u.)**	**Enthalpy (a.u.)**	**ΔE (kJ/mol)**	**Δ(E+ZPE) (kJ/mol)**	**ΔG (kJ/mol)**	**ΔH (kJ/mol)**
Cp_2Ti	-445.2057	-445.0400	-445.0776	-445.0289				
$HNMe_2BH_2NMe_2BH_3$	-322.5622	-322.3241	-322.3593	-322.3123				
Cp_2Ti +$HNMe_2BH_2NMe_2BH_3$	-767.7679	-767.3641	-767.4369	-767.3412	0.0	0.0	0.0	0.0
S_9	-767.8009	-767.3933	-767.4411	-767.3716	-86.5	-76.5	-11.0	-79.7
TS_{9_10}	-767.7767	-767.3760	-767.4240	-767.3542	-23.1	-31.2	33.8	-34.1
S_{10}	-767.8089	-767.4045	-767.4521	-767.3829	-107.7	-106.0	-39.9	-109.3
TS_{10_11}	-767.7946	-767.3914	-767.4384	-767.3703	-70.0	-71.6	-4.0	-76.5
S_{11}	-767.8139	-767.4096	-767.4591	-767.3879	-120.8	-119.5	-58.4	-122.5

Cartesian coordinates of the intermediates and transition states involved in the titanocene-catalyzed dehydrogenation of dimethylamine borane (DMAB)

Optimized at the B3LYP-GD3BJ/ 6-31G*+6-31++G**+LanL2DZ level of theory

Cp_2Ti **E = -445.2026464 Hartree**

C	1.874602	1.153198	0.426824
C	2.155639	0.723239	-0.902267
C	2.160472	-0.688055	-0.928003
C	1.882032	-1.168281	0.383409
C	1.708280	-0.024100	1.243191
H	1.848437	2.179026	0.770003
H	2.294268	1.368758	-1.761329
H	2.301340	-1.300762	-1.810452
H	1.857229	-2.206647	0.686854
H	1.582157	-0.044849	2.317091
C	-1.708282	-0.023518	1.243200
C	-1.874375	1.153488	0.426354
C	-2.155519	0.722984	-0.902576
C	-2.160582	-0.688321	-0.927712
C	-1.882267	-1.168008	0.383888
H	-1.582160	-0.043846	2.317108
H	-1.848166	2.179454	0.769112
H	-2.294107	1.368150	-1.761908
H	-2.301486	-1.301389	-1.809905
H	-1.857514	-2.206251	0.687762
Ti	0.000000	0.002391	-0.140099

HMe_2NBH_3 **E = -161.8576791 Hartree**

B	-1.584780	-0.000034	0.117553
H	-2.055397	1.013548	-0.355820
H	-2.055357	-1.013643	-0.355802
N	-0.004068	-0.000004	-0.341775
H	-1.565867	-0.000023	1.331517
C	0.704851	-1.224345	0.102036
C	0.704793	1.224378	0.102014
H	-0.018681	-0.000012	-1.361745
H	1.747857	-1.217858	-0.233640
H	0.182498	-2.093980	-0.297866
H	0.664663	-1.259491	1.192652
H	1.747792	1.217948	-0.233687
H	0.182382	2.093983	-0.297879
H	0.664630	1.259528	1.192630

$HNMe_2BH_2NMe_2BH_3$ **E = -322.5568378 Hartree**

B	-0.133806	-0.523750	-0.734973
N	1.202548	-0.056826	-0.009896
H	-0.238878	-0.035076	-1.836875
N	-1.424688	-0.050502	0.132352
H	-0.172130	-1.726122	-0.739955
C	1.694913	1.250599	-0.515530
B	1.027572	0.020564	1.604404
C	2.246869	-1.071853	-0.319293
H	2.610373	1.524057	0.017728
H	1.892282	1.190784	-1.591012
H	0.950043	2.025065	-0.332841
H	1.967690	-2.018792	0.142267
H	2.334934	-1.207259	-1.403983
H	3.205317	-0.740992	0.090739
H	-1.082530	-0.079232	1.103351
C	-1.881883	1.335176	-0.137163
C	-2.542199	-1.015920	-0.010164
H	2.124812	0.163555	2.097515
H	0.318811	0.987376	1.852958
H	0.500503	-1.022398	1.959291
H	-2.747754	1.576461	0.487380
H	-1.073723	2.027237	0.093309
H	-2.146951	1.417853	-1.193129
H	-3.410996	-0.676371	0.562376
H	-2.806462	-1.095588	-1.067633
H	-2.212703	-1.990361	0.349535

S_1 **E = -607.0898753 Hartree**

C	-2.106411	-1.196661	1.048270
C	-0.911452	-1.982450	0.957768
C	-0.739257	-2.349036	-0.395856
C	-1.799605	-1.804526	-1.155894
C	-2.667352	-1.085672	-0.273176
H	-2.554864	-0.830087	1.960541
H	-0.275816	-2.269837	1.785445
H	0.107636	-2.882991	-0.807203
H	-1.913259	-1.897945	-2.228941
H	-3.617008	-0.638570	-0.531844
C	-1.891311	2.023377	-0.026711
C	-1.244358	1.709552	1.222889
C	0.176341	1.853272	1.035279
C	0.383174	2.258064	-0.311551
C	-0.862658	2.358199	-0.958813

H	-2.956388	2.090329	-0.198840
H	-1.739428	1.515777	2.163660
H	0.926498	1.810450	1.816635
H	1.340592	2.393136	-0.797128
H	-1.004592	2.597613	-2.005892
Ti	-0.778378	0.089718	-0.204069
B	2.018166	-0.378812	-1.403673
H	2.370171	-1.431072	-1.878966
H	0.798870	-0.404067	-1.231050
N	2.698245	-0.238727	0.068098
H	2.323936	0.589134	-2.050800
C	3.998569	0.472306	0.032080
C	2.810134	-1.543536	0.764971
H	2.015827	0.321834	0.592159
H	4.435759	0.528814	1.034337
H	3.842152	1.475113	-0.366464
H	4.672172	-0.071321	-0.634954
H	3.178422	-1.402144	1.786601
H	1.822588	-2.001517	0.785077
H	3.497633	-2.178617	0.203302

TS_{1_2} **E = -607.0797969 Hartree**

C	-1.566525	1.600611	-1.164796
C	-0.252277	2.083602	-0.966493
C	-0.081797	2.271320	0.439428
C	-1.299065	1.919563	1.096254
C	-2.210536	1.517481	0.097152
H	-1.998199	1.317777	-2.115634
H	0.458786	2.313511	-1.746973
H	0.792454	2.652639	0.944889
H	-1.489147	1.969180	2.158822
H	-3.218318	1.164848	0.266249
C	-2.210445	-1.517577	0.097050
C	-1.566329	-1.600762	-1.164841
C	-0.252076	-2.083677	-0.966401
C	-0.081696	-2.271301	0.439550
C	-1.299036	-1.919548	1.096263
H	-3.218259	-1.164980	0.266033
H	-1.997935	-1.318007	-2.115733
H	0.459062	-2.313592	-1.746810
H	0.792538	-2.652542	0.945102
H	-1.489213	-1.969125	2.158815
Ti	-0.337724	-0.000005	0.157025
B	1.803342	0.000077	1.557600
H	2.242152	1.013833	2.035446

H	0.554451	0.000053	1.809343
N	2.121527	0.000054	-0.034149
H	2.242194	-1.013654	2.035462
C	2.887579	-1.197374	-0.470637
C	2.887521	1.197497	-0.470698
H	1.204931	0.000021	-0.820405
H	2.977229	-1.201258	-1.563106
H	2.389227	-2.102668	-0.142843
H	3.881211	-1.156530	-0.018490
H	2.977178	1.201323	-1.563167
H	2.389119	2.102784	-0.142963
H	3.881151	1.156731	-0.018541

S_2 **E = -607.1271044 Hartree**

C	1.944460	-1.305114	-0.958769
C	0.746715	-2.063103	-1.064260
C	0.318666	-2.362344	0.248315
C	1.256459	-1.813246	1.165462
C	2.269314	-1.185400	0.419284
H	2.505079	-0.892889	-1.786482
H	0.254080	-2.346386	-1.982325
H	-0.559735	-2.915621	0.536373
H	1.185441	-1.861619	2.242747
H	3.118948	-0.660884	0.832123
C	1.967548	1.656205	-0.163754
C	1.062389	1.928195	-1.211397
C	-0.172772	2.315652	-0.626702
C	-0.036268	2.251234	0.774730
C	1.284039	1.810284	1.068378
H	2.993102	1.341479	-0.288465
H	1.265721	1.858498	-2.270538
H	-1.060530	2.578696	-1.178912
H	-0.808123	2.437604	1.507278
H	1.693555	1.648717	2.056020
Ti	0.206568	0.010742	-0.020946
B	-1.771014	-0.383272	1.552054
H	-1.902103	-1.511461	1.956597
H	-0.508227	-0.125839	1.688153
N	-2.046204	-0.228254	0.047926
H	-2.286673	0.474823	2.228245
C	-2.891441	0.927534	-0.296599
C	-2.616978	-1.379735	-0.669145
H	-0.365096	-0.061648	-1.574790
H	-2.830476	1.140079	-1.370547
H	-2.597203	1.809088	0.266980

H	-3.937587	0.704388	-0.041671
H	-2.550984	-1.213340	-1.750582
H	-2.094532	-2.299003	-0.426943
H	-3.673434	-1.507831	-0.391471

S_4 **E = -768.9914829 Hartree**

C	0.006834	0.084823	0.334484
C	0.114856	0.239549	1.741461
C	1.488308	0.231283	2.069153
C	2.235619	0.136466	0.866606
C	1.307477	0.016742	-0.205313
H	-0.927987	0.066831	-0.200158
H	-0.719117	0.348155	2.419764
H	1.896665	0.328460	3.064541
H	3.313438	0.135944	0.777028
H	1.568050	-0.046315	-1.252240
C	0.800665	4.159404	2.066154
C	1.350089	3.153250	2.905916
C	2.671779	2.881004	2.461108
C	2.924210	3.670859	1.325477
C	1.770049	4.466146	1.084594
H	-0.182922	4.595319	2.159165
H	0.841538	2.676293	3.732452
H	3.349922	2.152912	2.882906
H	3.821768	3.665623	0.723412
H	1.679239	5.177508	0.280418
C	-5.786499	1.131710	-0.061585
H	-5.543386	2.051538	-0.597579
H	-6.872699	1.037207	0.044788
H	-5.385259	0.283648	-0.617504
C	-5.689742	2.269803	2.106596
H	-5.452569	3.223539	1.630842
H	-6.775162	2.162446	2.208964
H	-5.211284	2.236850	3.086027
C	-0.784566	2.000412	-1.898391
H	-0.289011	1.051085	-2.086599
H	-1.032941	2.442258	-2.875246
H	-1.710048	1.832075	-1.338192
C	-0.617264	4.200277	-1.082764
H	-0.861853	4.556609	-2.094981
H	-1.545978	4.065233	-0.517001
H	-0.019463	4.963738	-0.595725
Ti	1.097861	2.199066	0.744048
B	1.554516	2.931405	-1.665641

H	1.748013	2.185105	-2.597180
H	2.017712	4.039126	-1.788961
H	2.243737	2.381100	-0.718177
N	0.102287	2.919306	-1.162368
B	-3.490606	1.306656	1.131015
H	-3.068719	1.270227	2.267731
H	-3.290020	2.367360	0.580279
H	-3.155462	0.348710	0.465241
H	-0.489595	2.500689	1.059967
N	-5.124487	1.187024	1.264854
H	-5.299273	0.300223	1.737961

S_5 **E = -769.0003728 Hartree**

C	0.003423	0.020152	-0.015680
C	0.012817	-0.000411	1.410127
C	1.366384	-0.004379	1.827717
C	2.191707	0.034709	0.668065
C	1.351108	0.069640	-0.461415
H	-0.880487	0.035512	-0.636728
H	-0.854480	0.008604	2.052959
H	1.712460	-0.041365	2.851389
H	3.272679	0.023361	0.650354
H	1.688405	0.060006	-1.486172
C	2.713230	-3.612888	0.602184
C	1.472591	-4.292431	0.795756
C	0.971346	-3.936058	2.073450
C	1.877366	-3.010506	2.650167
C	2.958335	-2.829782	1.747344
H	3.331263	-3.665382	-0.281923
H	3.800772	-2.167524	1.893783
H	1.752396	-2.518782	3.605404
H	0.053544	-4.286501	2.522256
H	1.016064	-4.975712	0.096160
C	1.504278	-2.833316	-4.778387
H	2.292831	-2.080394	-4.865046
H	1.956372	-3.824721	-4.738676
H	0.834193	-2.773027	-5.642956
C	0.211169	-1.215214	-3.561090
H	1.043320	-0.509852	-3.646899
H	-0.324290	-1.002338	-2.635921
H	-0.464554	-1.090692	-4.413663
C	-1.415157	-5.067369	-1.610819
H	-0.443965	-5.555053	-1.541093
H	-2.043854	-5.622927	-2.311034
H	-1.889166	-5.031047	-0.625347

C	-2.512620	-2.960636	-2.140367
H	-2.354607	-1.949735	-2.515306
H	-2.920501	-2.911132	-1.126591
H	-3.204909	-3.480668	-2.805736
Ti	0.968415	-2.015571	0.669281
H	-0.447686	-2.217087	1.484006
H	-0.485201	-2.553839	-0.034632
B	1.766003	-2.783766	-2.301155
N	0.734954	-2.602747	-3.523508
B	-0.437333	-3.679646	-3.535689
N	-1.217677	-3.687486	-2.122626
H	2.712686	-2.050078	-2.474407
H	1.171573	-2.421777	-1.264751
H	2.048141	-3.952101	-2.216315
H	0.052013	-4.765532	-3.694386
H	-1.239276	-3.389990	-4.396120
H	-0.650589	-3.205062	-1.382985

S_6 **E = -768.9869567 Hartree**

C	-0.147010	-0.077641	0.001619
C	-0.146313	-0.063576	1.413839
C	1.194720	0.035924	1.864683
C	2.022184	0.105290	0.698330
C	1.192391	0.010036	-0.464215
C	2.139825	-4.022556	-0.278365
C	1.969971	-4.223362	1.110381
C	2.757468	-3.264278	1.814788
C	3.415298	-2.472262	0.819880
C	3.017021	-2.934231	-0.473330
H	2.957674	-3.249702	2.876269
H	1.316955	-4.959288	1.560021
H	1.610631	-4.554219	-1.058659
H	3.335060	-2.532355	-1.425391
H	4.138438	-1.694471	1.016569
H	1.508557	0.086136	-1.494621
H	3.088437	0.274483	0.692403
H	1.503923	0.168961	2.891134
H	-0.998662	-0.150134	2.077573
H	1.218877	-4.304435	4.256036
C	-3.170723	-3.060762	1.648876
C	-2.923071	-2.555081	-0.745597
H	-2.269506	-2.068617	-1.470459
H	-3.898241	-2.059785	-0.720495
H	-3.046218	-3.604086	-1.023395
H	-2.687865	-2.922637	2.617053

H	-4.134310	-2.542675	1.640226
H	-3.314117	-4.123724	1.445671
C	1.652485	-1.868892	5.226552
C	0.297890	-3.754806	4.473885
H	1.832741	-0.805595	5.065907
H	2.556312	-2.439489	4.989264
H	1.377252	-2.025717	6.272347
H	-0.471066	-4.039028	3.754863
H	-0.049030	-3.984907	5.483720
H	-1.015955	-0.169726	-0.640441
Ti	1.188951	-2.001513	0.693906
B	-0.839197	-3.211197	0.585405
N	-2.281456	-2.501208	0.593428
H	-0.294909	-2.877125	1.658028
H	-0.243790	-2.795525	-0.426285
H	-1.017139	-4.397894	0.521491
H	-2.107703	-1.521855	0.824274
N	0.521774	-2.295119	4.372124
H	0.786730	-2.103271	3.384240
B	-0.825564	-1.448825	4.699078
H	-1.657555	-1.796524	3.881846
H	-0.541604	-0.275675	4.584249
H	-1.151590	-1.748005	5.830936

TS_{6_7} **E = -768.95377 Hartree**

C	-2.140605	-0.097352	1.922682
C	-0.838129	0.412350	2.152176
C	0.065408	-0.682967	2.069416
C	-0.686154	-1.859727	1.821307
C	-2.045147	-1.501783	1.702533
H	-3.053996	0.478355	1.943802
H	-0.581408	1.427789	2.399341
H	1.137386	-0.596562	2.176353
H	-0.294494	-2.857444	1.675506
H	-2.864445	-2.174235	1.488953
C	-1.757952	-0.884053	-2.247770
C	-2.840480	-0.822201	-1.342217
C	-2.921052	0.516212	-0.860068
C	-1.875562	1.274062	-1.453218
C	-1.157762	0.397777	-2.309434
H	-1.401943	-1.771760	-2.752824
H	-3.492129	-1.640573	-1.069176
H	-3.668471	0.898551	-0.180907
H	-1.686671	2.327059	-1.316206
H	-0.276830	0.655885	-2.878748

Ti	-0.916191	-0.358775	-0.058948
B	1.104175	-1.216289	-1.067877
H	1.218272	-1.365286	-2.250565
H	0.214876	-1.960506	-0.625247
N	2.510817	-1.467262	-0.346261
H	0.824999	-0.043522	-0.783176
C	3.630152	-1.474842	-1.328644
C	2.580304	-2.662999	0.526758
H	2.644397	-0.605894	0.229438
H	4.584808	-1.519557	-0.796223
H	3.582473	-0.556539	-1.911338
H	3.520577	-2.342764	-1.983216
H	3.574894	-2.739324	0.975814
H	1.833974	-2.582715	1.313217
H	2.379741	-3.554719	-0.072787
B	2.619580	1.663023	0.271338
H	3.519343	2.448257	0.550386
H	2.631275	0.755008	1.129323
N	1.230576	2.371074	0.280695
H	2.820454	1.195446	-0.840678
C	1.034863	3.197533	-0.901959
C	1.020089	3.165648	1.481811
H	-0.088602	1.206318	0.156997
H	0.063486	3.712317	-0.865026
H	1.067336	2.570020	-1.797726
H	1.821171	3.968234	-1.000953
H	-0.020348	3.522071	1.545218
H	1.245519	2.564193	2.367685
H	1.684215	4.048642	1.511043

S_7 **E = -768.9581845 Hartree**

C	2.832454	-1.073118	-1.328723
C	1.638456	-1.045998	-2.087908
C	0.671480	-1.820209	-1.392944
C	1.277613	-2.338101	-0.220143
C	2.605276	-1.857894	-0.162389
H	3.762262	-0.593743	-1.595833
H	1.490006	-0.549944	-3.035349
H	-0.343882	-1.976021	-1.718087
H	0.803028	-2.957736	0.527376
H	3.324215	-2.067362	0.617116
C	1.702118	1.293826	1.935046
C	2.925600	0.882759	1.360387
C	3.045559	1.520884	0.092882
C	1.888529	2.310091	-0.119991

C	1.050997	2.156873	1.016858
H	1.302929	0.966708	2.884728
H	3.646223	0.211601	1.806491
H	3.880460	1.432316	-0.586335
H	1.686379	2.934307	-0.977551
H	0.079546	2.607849	1.144813
Ti	1.208265	0.047660	-0.039183
B	-0.933551	-0.090160	0.974971
H	-1.157873	0.809418	1.722711
H	0.142541	-0.684332	1.347139
N	-2.134744	-1.087958	1.102802
H	-0.671374	0.275868	-0.200876
C	-2.262084	-1.595071	2.492825
C	-2.264569	-2.188553	0.121609
H	-2.969170	-0.458542	0.938632
H	-3.201653	-2.144752	2.595396
H	-2.259921	-0.746909	3.178759
H	-1.419723	-2.254038	2.721852
H	-3.215062	-2.701940	0.281818
H	-2.268804	-1.755547	-0.875092
H	-1.438201	-2.892090	0.242163
B	-4.201881	0.570161	-0.262199
H	-5.111649	1.346429	-0.533434
H	-4.446997	-0.548950	-0.699938
N	-2.816991	1.039603	-0.784303
H	-4.141355	0.518511	0.989998
C	-2.494960	2.411790	-0.448417
C	-2.560295	0.795250	-2.187251
H	0.641196	0.871994	-1.352037
H	-1.444288	2.640226	-0.693048
H	-2.647583	2.577931	0.623418
H	-3.130574	3.136515	-0.993783
H	-1.495712	0.962971	-2.427854
H	-2.817821	-0.238542	-2.443894
H	-3.156708	1.452613	-2.851671

TS_{7_8} **E = -768.9548676 Hartree**

C	2.820557	-1.182201	-1.240959
C	1.639455	-1.247298	-2.015624
C	0.659290	-1.927769	-1.246710
C	1.247527	-2.303218	-0.007526
C	2.576893	-1.828583	0.003126
H	3.749405	-0.723031	-1.546240
H	1.506736	-0.862951	-3.015597
H	-0.349674	-2.127060	-1.569797

H	0.770351	-2.841903	0.798075
H	3.285201	-1.941907	0.811409
C	1.492725	1.451396	1.820886
C	2.750318	0.935142	1.435740
C	3.065663	1.466989	0.152900
C	1.996228	2.296509	-0.259206
C	1.016756	2.275650	0.769657
H	0.964758	1.226728	2.736450
H	3.368084	0.264983	2.017060
H	3.968222	1.274202	-0.408432
H	1.938262	2.856361	-1.180687
H	0.071198	2.793499	0.749200
Ti	1.165291	0.077306	-0.104918
B	-1.160196	0.119669	0.617726
H	-1.316507	1.051014	1.336122
H	0.037067	-0.431333	1.161731
N	-2.150915	-1.029549	1.092955
H	-0.606660	0.248651	-0.519655
C	-1.960292	-1.346053	2.531848
C	-2.270667	-2.271292	0.293608
H	-3.071075	-0.544105	1.011671
H	-2.760108	-2.011373	2.869346
H	-1.990243	-0.416045	3.100446
H	-0.989831	-1.827228	2.671783
H	-3.132308	-2.843679	0.647040
H	-2.430309	-2.007434	-0.748455
H	-1.364940	-2.866637	0.402495
B	-4.139329	0.638220	-0.133893
H	-4.984886	1.363683	-0.628118
H	-4.416243	-0.536443	-0.359698
N	-2.708911	0.942880	-0.721257
H	-4.093455	0.835421	1.086136
C	-2.399325	2.371059	-0.672860
C	-2.552460	0.484040	-2.101023
H	0.748457	0.816291	-1.533837
H	-1.368412	2.552389	-1.007783
H	-2.516352	2.738333	0.349934
H	-3.081148	2.941486	-1.322289
H	-1.514537	0.614917	-2.439965
H	-2.824518	-0.571933	-2.182615
H	-3.212532	1.045379	-2.781720

S_8 **E = -768.9838718 Hartree**

C	-4.043922	-0.779105	1.130758
C	-3.148884	-1.859681	0.901161

C	-3.006363	-2.015006	-0.503549
C	-3.812920	-1.028022	-1.134406
C	-4.462747	-0.278042	-0.124723
H	-4.334617	-0.390788	2.098759
H	-2.670523	-2.459497	1.660669
H	-2.402424	-2.756467	-1.004648
H	-3.899065	-0.865213	-2.201276
H	-5.132604	0.555483	-0.284358
C	-1.786120	1.957784	-1.295196
C	-2.688698	2.351145	-0.277357
C	-2.018193	2.246608	0.965071
C	-0.688061	1.809496	0.715581
C	-0.542794	1.631376	-0.686440
H	-2.010407	1.895865	-2.352670
H	-3.719563	2.644348	-0.420422
H	-2.451312	2.441539	1.938139
H	0.084317	1.647733	1.451814
H	0.360022	1.318407	-1.188453
Ti	-2.103975	0.065310	0.074196
B	2.841243	0.165986	-0.215085
H	2.581198	0.503579	-1.340509
H	-0.922370	-0.775138	-0.764665
N	2.537514	-1.422323	-0.092687
H	2.190839	0.746850	0.621098
C	1.892907	-1.978681	-1.312276
C	1.784884	-1.807709	1.128769
H	3.483333	-1.836559	-0.047349
H	1.774388	-3.062462	-1.207163
H	2.528824	-1.754076	-2.168348
H	0.913092	-1.512112	-1.433173
H	1.714054	-2.898635	1.195499
H	2.303935	-1.420754	2.006651
H	0.784627	-1.372632	1.080354
B	5.311796	-0.753868	-0.653859
H	6.472972	-0.426229	-0.531910
H	5.124741	-1.807061	-0.042073
N	4.393642	0.387632	0.048680
H	4.961470	-0.848712	-1.812657
C	4.750658	1.708246	-0.529677
C	4.697537	0.427346	1.501562
H	-1.147717	-0.513133	1.327192
H	4.093504	2.487989	-0.125357
H	4.634888	1.661303	-1.612617
H	5.792170	1.941765	-0.289889
H	4.137804	1.234650	1.986162
H	4.422877	-0.524760	1.960115

H	5.771994	0.575612	1.645877

S_9 **E = -767.7952438 Hartree**

C	0.083855	0.079906	0.055569
C	-0.003579	-0.024026	1.458338
C	1.303663	-0.107632	2.000517
C	2.220889	-0.041542	0.898764
C	1.459287	0.069764	-0.317832
H	-0.760790	0.092317	-0.622898
H	-0.928259	-0.096581	2.012930
H	1.562398	-0.125564	3.050320
H	3.297236	0.006457	0.978466
H	1.855191	0.208827	-1.314045
C	1.469136	-3.972783	-0.613085
C	1.672030	-4.361360	0.730990
C	2.758077	-3.626363	1.257663
C	3.243712	-2.769321	0.219599
C	2.444640	-2.984608	-0.956161
H	0.671043	-4.332762	-1.250318
H	1.034409	-5.043672	1.276969
H	3.176733	-3.719752	2.250663
H	4.110805	-2.128263	0.286671
H	2.615051	-2.560170	-1.935736
C	-3.189151	-4.450909	2.451479
C	-2.658081	-2.245420	3.206883
H	-3.890554	-4.032119	1.723417
H	-2.792206	-5.389976	2.067951
H	-3.704353	-4.630337	3.401510
H	-3.479553	-1.917791	2.563980
H	-3.025465	-2.417382	4.224306
H	-1.911382	-1.454201	3.216628
C	0.263994	-2.269907	4.835074
C	1.343670	-4.392581	4.376027
H	-0.371318	-1.490661	4.422602
H	1.267258	-1.861207	4.984694
H	-0.147672	-2.612797	5.786642
H	2.286264	-3.875131	4.574199
H	0.978169	-4.860457	5.293596
H	1.491013	-5.158478	3.617091
Ti	1.165382	-1.977208	0.576058
B	-1.408696	-3.203871	1.209145
N	-2.065411	-3.491303	2.655783
B	-1.069044	-4.214904	3.662880
N	0.324388	-3.420678	3.897830
H	-2.125978	-2.446909	0.596911

H	-0.331445	-2.647591	1.505713
H	-1.224973	-4.256728	0.662609
H	-0.767381	-5.272309	3.176040
H	0.653671	-3.045038	2.980244
H	-1.589060	-4.318355	4.752979

TS_{9_10} **E = -767.7722859 Hartree**

C	-0.034745	0.022686	0.084940
C	0.056467	-0.006437	1.508222
C	1.438512	-0.021955	1.836895
C	2.189678	0.027914	0.633479
C	1.284569	0.046802	-0.448448
H	-0.944385	0.029052	-0.498390
H	-0.762391	0.044458	2.206047
H	1.849361	-0.079352	2.836699
H	3.267855	-0.013723	0.556615
H	1.547798	0.042817	-1.498719
C	1.821729	-4.027076	-0.127109
C	1.147133	-4.343393	1.076877
C	1.782021	-3.650711	2.135820
C	2.847391	-2.891670	1.577300
C	2.874009	-3.123519	0.169624
H	1.524182	-4.359370	-1.113601
H	0.250937	-4.942911	1.150013
H	1.507798	-3.689252	3.178801
H	3.525819	-2.253840	2.127418
H	3.576170	-2.700370	-0.535878
C	-3.721199	-4.109930	-0.631326
C	-3.413726	-1.826805	0.022641
H	-4.693699	-4.095489	-0.129724
H	-3.836853	-3.811366	-1.678768
H	-3.308054	-5.117520	-0.584378
H	-2.701565	-1.087289	0.386135
H	-4.308590	-1.813574	0.653599
H	-3.682723	-1.567773	-1.006429
C	-2.410303	-1.767882	3.165648
C	-1.226662	-3.765941	3.609693
H	-3.276110	-2.101528	3.758888
H	-2.768774	-1.060836	2.418744
H	-1.716447	-1.241467	3.834015
H	-0.542708	-3.197040	4.253531
H	-0.697531	-4.620933	3.190709
H	-2.048072	-4.148703	4.236360
Ti	0.916668	-1.999245	0.654009
H	-0.662369	-2.474261	-0.105599

B	-1.451556	-3.165564	-0.786454
H	-1.595308	-2.546361	-1.818863
H	-1.027899	-4.279310	-0.924150
N	-2.789858	-3.171824	0.055503
B	-2.628360	-3.754647	1.566890
H	-2.130573	-4.848619	1.434948
H	-3.761697	-3.817431	2.022061
N	-1.738371	-2.908224	2.534896
H	-0.432798	-2.353413	1.864776

S_{10} **E = -767.8040513 Hartree**

C	0.000754	0.038694	0.000486
C	0.000432	0.041102	1.421646
C	1.352560	0.046441	1.857554
C	2.179201	0.016918	0.705851
C	1.340424	0.005243	-0.444354
H	-0.872152	0.014533	-0.635225
H	-0.859472	-0.049748	2.079039
H	1.683989	0.089543	2.883948
H	3.259513	0.022906	0.703640
H	1.671107	-0.022940	-1.473396
C	1.260092	-3.967438	-0.548996
C	1.544232	-4.288502	0.799749
C	2.688191	-3.546485	1.202077
C	3.088570	-2.749083	0.102703
C	2.193157	-2.994428	-0.977590
H	0.429656	-4.348519	-1.125940
H	0.973111	-4.955883	1.427858
H	3.172679	-3.599452	2.165793
H	3.933543	-2.077006	0.082860
H	2.233536	-2.538120	-1.956693
C	-3.594872	-3.580186	0.835205
C	-3.091016	-1.249255	0.613540
H	-3.442225	-3.787340	-0.231062
H	-3.391927	-4.482197	1.412902
H	-4.630409	-3.274107	1.006400
H	-2.936653	-1.328981	-0.469803
H	-2.521992	-0.413440	1.009129
H	-4.151116	-1.067244	0.813701
C	-3.030086	0.032235	3.847184
C	-1.152287	-1.306972	4.467877
H	-3.794928	0.208626	3.085231
H	-3.554185	-0.116213	4.811466
H	-2.428062	0.950459	3.941959
H	-1.555488	-1.526681	5.475736

H	-0.517645	-0.410353	4.563061
H	-0.511235	-2.141655	4.174963
Ti	0.957929	-1.993078	0.768928
B	-1.218324	-2.946768	1.042580
H	-0.731735	-2.434548	-0.023255
H	-0.407193	-2.526953	1.922737
H	-1.162390	-4.137926	0.979977
N	-2.682095	-2.498519	1.291476
B	-2.909002	-2.331515	2.966807
H	-2.470431	-3.370951	3.415853
H	-4.123174	-2.258566	3.059268
N	-2.195827	-1.100681	3.476789
H	1.349273	-2.119256	2.362436

TS_{10_11} **E = -767.7908104 Hartree**

C	-0.026482	0.047165	-0.036777
C	0.009836	0.098332	1.383696
C	1.368281	0.125185	1.793905
C	2.167287	0.060969	0.629844
C	1.305297	0.007471	-0.502086
H	-0.908808	0.024087	-0.658588
H	-0.838642	0.131062	2.047061
H	1.723562	0.191382	2.811109
H	3.247270	0.058449	0.607194
H	1.614958	-0.051804	-1.535996
C	1.225048	-3.921861	-0.598357
C	1.557173	-4.267786	0.735949
C	2.715829	-3.535920	1.111217
C	3.083582	-2.725748	0.011993
C	2.154265	-2.954021	-1.041887
H	0.379813	-4.296238	-1.157029
H	1.015981	-4.955142	1.367775
H	3.225923	-3.596512	2.061089
H	3.924808	-2.048904	-0.021912
H	2.162105	-2.479955	-2.013357
C	-3.274427	-3.046252	-0.222086
C	-3.053616	-1.179652	1.261937
H	-2.824204	-2.472357	-1.040751
H	-3.064229	-4.106004	-0.362342
H	-4.358692	-2.894318	-0.223624
H	-2.621899	-0.571510	0.463273
H	-2.686655	-0.831655	2.225339
H	-4.141809	-1.068235	1.254491
C	-1.395800	-5.024371	3.358362
H	-0.314306	-5.023982	3.557785

H	-1.598509	-5.683089	2.512058
H	-1.906034	-5.432133	4.246241
C	-1.533083	-2.771847	4.154835
H	-0.448206	-2.743187	4.325660
H	-1.863689	-1.756557	3.925869
H	-2.030347	-3.085960	5.086020
Ti	0.954835	-1.974954	0.758223
H	-0.609478	-2.380224	0.047389
B	-1.207333	-3.052658	1.228043
H	-0.304721	-2.494300	1.950358
H	-1.082230	-4.169604	0.844058
N	-2.715795	-2.606400	1.076892
B	-3.221764	-3.505699	2.354238
N	-1.849320	-3.674119	3.052385
H	-4.035194	-2.874250	2.993757
H	-3.642313	-4.556150	1.934781
H	1.361935	-2.103873	2.369269

S_{11} **E = -767.8100795 Hartree**

C	-0.011787	0.067953	-0.028946
C	-0.009572	0.067873	1.389682
C	1.336957	0.095499	1.840963
C	2.169867	0.087758	0.698034
C	1.336217	0.068603	-0.457766
H	-0.883984	0.065078	-0.664871
H	-0.885960	0.046420	2.020705
H	1.663741	0.119502	2.869517
H	3.250972	0.078519	0.702607
H	1.670351	0.047556	-1.485574
C	1.300803	-4.165374	-0.134967
C	2.217017	-3.989177	0.925157
C	3.148316	-2.987313	0.533982
C	2.823182	-2.583450	-0.785283
C	1.669344	-3.287287	-1.193092
H	0.443027	-4.821357	-0.134123
H	2.196852	-4.497907	1.877379
H	3.957298	-2.604182	1.140465
H	3.334270	-1.819420	-1.354924
H	1.145408	-3.173092	-2.131347
C	-3.148213	-2.205805	1.398031
C	-3.047214	-4.597716	1.124994
H	-2.750854	-2.046586	0.390932
H	-2.857230	-1.363696	2.025257
H	-4.242053	-2.258998	1.374373
H	-4.141724	-4.654230	1.128549

H	-2.641374	-5.524117	1.530789
H	-2.692763	-4.466444	0.096371
C	-0.976634	-1.932933	4.367655
H	-1.571603	-1.201139	3.822639
H	-1.272095	-1.901342	5.421944
H	0.082518	-1.680960	4.259795
C	-0.461730	-4.271794	4.617117
H	-0.785112	-4.237934	5.663759
H	0.608485	-4.044814	4.557168
H	-0.641094	-5.270907	4.220801
Ti	1.022036	-1.958095	0.681380
H	-0.389532	-2.241699	-0.209456
H	1.364355	-2.209767	2.318798
H	-0.538595	-2.431537	1.763018
B	-1.035302	-3.429921	2.249469
H	-0.515851	-4.466531	1.969502
N	-2.599623	-3.461802	1.954252
B	-2.773512	-3.630350	3.548929
N	-1.221284	-3.285760	3.823174
H	-3.015435	-4.773759	3.833494
H	-3.520436	-2.812440	4.022829

Cartesian coordinates of the intermediates and transition states involved in the titanocene-catalyzed dehydrogenation of diisopropylamine borane (D^iPrAB)

Optimized at the B3LYP-GD3BJ/ 6-31G*+6-31++G**+LanL2DZ level of theory

$H^iPr_2NBH_3$ **E = -319.1329862 Hartree**

H	0.112315	-1.302143	2.035699
C	0.674928	-0.527247	2.561927
C	1.488115	0.312184	1.579363
C	0.584992	1.145412	0.671271
H	2.124026	1.000917	2.154612
H	1.305031	-1.002153	3.318499
H	-0.032679	0.125609	3.083205
H	1.162613	1.692336	-0.083299
H	-0.140171	0.518598	0.148506
H	0.047026	1.877999	1.282249
C	3.551526	-1.132319	1.604030
C	4.882581	-0.976273	0.867481
C	3.290556	-2.590585	1.978615
H	3.336843	-3.232383	1.096782
H	2.313610	-2.730249	2.443343
H	4.060575	-2.909403	2.690201
H	4.855248	-1.506096	-0.089522
H	5.116739	0.079665	0.678959
H	5.694964	-1.394009	1.470188
H	3.593984	-0.533400	2.523021
N	2.446250	-0.523596	0.756353
B	1.773990	-1.535412	-0.365061
H	2.916916	0.157131	0.159975
H	1.215108	-0.812916	-1.159376
H	1.020148	-2.291840	0.200397
H	2.711229	-2.108451	-0.877888

S_1 **E = -764.3657097 Hartree**

C	-0.705547	1.833401	1.072937
C	-0.642404	2.375400	-0.240329
C	-1.942413	2.440334	-0.774812
C	-2.862333	1.943735	0.197639
C	-2.092653	1.567176	1.357254
H	0.111116	1.773862	1.783128
H	0.258298	2.625607	-0.784620
H	-2.188798	2.760880	-1.780029
H	-3.940215	1.942924	0.115415

H	-2.492416	1.253158	2.310734
C	-1.517003	-2.052667	0.679816
C	-1.466246	-2.270440	-0.716354
C	-2.633196	-1.737072	-1.306618
C	-3.446491	-1.174307	-0.272964
C	-2.745953	-1.373327	0.969856
H	-0.778554	-2.371793	1.403175
H	-0.633883	-2.694378	-1.263191
H	-2.851483	-1.728702	-2.367474
H	-4.442922	-0.771644	-0.390234
H	-3.121580	-1.136237	1.955052
C	2.053669	-1.315124	0.368407
C	3.280745	-2.074421	-0.122211
C	1.944269	-1.295383	1.895511
H	1.169339	-1.832399	-0.005545
H	1.060484	-0.731957	2.215168
H	2.826625	-0.875523	2.383147
H	1.825851	-2.323865	2.253486
H	3.186731	-3.120077	0.189607
H	3.352827	-2.052126	-1.211874
H	4.208996	-1.686780	0.307975
C	3.055776	1.039760	-0.283548
C	3.712117	1.276255	1.076298
C	4.084145	0.725108	-1.371920
H	2.557672	1.968678	-0.577831
H	3.594956	0.463610	-2.312640
H	4.691395	1.620652	-1.541347
H	4.760474	-0.083362	-1.087166
H	4.389715	2.132693	0.994167
H	2.974258	1.508308	1.852100
H	4.305462	0.418146	1.404281
Ti	-1.632860	0.123830	-0.245264
B	1.106885	-0.015926	-1.667985
N	1.896246	0.065985	-0.243562
H	1.185844	0.510520	0.347424
H	-0.088730	-0.150529	-1.389783
H	1.467465	-0.994747	-2.273573
H	1.266974	1.017994	-2.262663

TS_{1_2} **E = -764.3444493 Hartree**

C	-0.033938	-0.135009	0.060532
C	0.017539	-0.012708	1.476216
C	1.363611	0.128047	1.879248
C	2.171658	0.094447	0.722984
C	1.306682	-0.049596	-0.401870

H	-0.922505	-0.179268	-0.552524
H	-0.836816	0.022542	2.131229
H	1.715338	0.184373	2.900500
H	3.250447	0.163007	0.697666
H	1.615617	-0.077073	-1.436620
C	1.132952	-3.956366	-0.662054
C	2.046130	-4.172273	0.412621
C	3.129035	-3.254979	0.278173
C	2.884372	-2.488083	-0.880071
C	1.651467	-2.902256	-1.445832
H	0.236205	-4.516496	-0.881223
H	1.976125	-4.917850	1.189413
H	3.984940	-3.177123	0.933287
H	3.500524	-1.675665	-1.240585
H	1.168660	-2.463349	-2.309077
Ti	1.175228	-2.052773	0.778213
B	0.799953	-3.069441	3.066340
H	1.729891	-2.404488	2.489256
H	0.557821	-2.429297	4.057511
H	1.293802	-4.141397	3.281811
N	-0.541014	-3.217917	2.176874
H	-0.484728	-2.751302	0.976812
C	-1.673796	-2.387890	2.767318
C	-0.865186	-4.668199	1.837152
C	-2.359950	-3.025224	3.975531
C	-2.709830	-1.899676	1.746269
H	-1.145178	-1.521506	3.150393
H	-1.635786	-3.419337	4.691581
H	-2.940888	-2.243450	4.477680
H	-3.058852	-3.816067	3.692425
H	-2.241483	-1.607790	0.803466
H	-3.217788	-1.020888	2.158902
H	-3.475893	-2.648614	1.535047
C	-2.018813	-4.818823	0.842794
C	-1.050030	-5.608909	3.036634
H	0.035398	-4.998945	1.335062
H	-1.938340	-4.105235	0.017284
H	-1.987431	-5.830198	0.423118
H	-2.994785	-4.695057	1.319536
H	-0.857350	-6.630263	2.688498
H	-2.063157	-5.589893	3.441054
H	-0.341668	-5.391196	3.836819

S_2 **E = -764.3912432 Hartree**

C	-1.562094	1.988965	1.152868

C	-0.803356	2.417543	0.033575
H	-1.168910	2.251501	-2.156482
C	-1.509045	2.082573	-1.144996
C	-2.704312	1.432669	-0.762993
C	-2.742598	1.389117	0.659281
H	-3.528160	0.962315	1.265497
H	-3.450571	1.035518	-1.436556
H	-1.299279	2.124958	2.191356
H	0.132959	2.944403	0.083932
C	-0.937585	-2.237054	0.831645
C	-0.919750	-2.340024	-0.574140
C	-2.142143	-1.813549	-1.076313
C	-2.930700	-1.436155	0.030689
C	-2.176847	-1.649804	1.207957
H	-0.149254	-2.521917	1.511814
H	-0.116060	-2.712272	-1.189615
H	-2.415934	-1.737990	-2.119570
H	-3.916561	-0.997048	-0.018953
H	-2.481215	-1.410950	2.217607
C	2.107739	-1.253518	0.110981
C	2.400473	-1.293388	1.613969
C	3.358608	-1.686009	-0.682008
H	1.552613	-0.921082	2.194694
H	3.288245	-0.711795	1.877411
H	2.599086	-2.330637	1.909495
H	3.219791	-1.537919	-1.755392
H	3.522332	-2.756777	-0.508813
H	4.265604	-1.166246	-0.368222
H	1.379860	-2.032967	-0.082290
C	2.140940	1.291039	-0.098340
C	2.119521	1.776912	1.359443
C	3.572543	1.375606	-0.652103
H	1.165221	1.556243	1.840657
H	1.575587	2.006482	-0.690127
H	2.279425	2.862330	1.375934
H	2.914766	1.330012	1.960115
H	3.875981	2.429353	-0.667316
H	4.294872	0.840873	-0.030135
H	3.628343	0.991815	-1.674266
Ti	-0.952122	-0.002040	-0.043860
N	1.429270	-0.002475	-0.371234
B	0.907702	-0.089886	-1.812981
H	-0.262869	0.046511	1.454483
H	1.165172	0.875659	-2.490938
H	1.093040	-1.146480	-2.361565
H	-0.389158	-0.031794	-1.761376

S_3 **E = -764.3750149 Hartree**

C	0.737742	2.215749	0.086915
C	0.981140	1.773975	1.414480
C	2.388215	1.631423	1.571917
C	3.009070	2.007229	0.354041
C	1.992460	2.355332	-0.564878
H	-0.231437	2.403905	-0.348400
H	0.228830	1.584051	2.164527
H	2.896660	1.287115	2.463388
H	4.071001	1.992481	0.150186
H	2.140365	2.642180	-1.598334
C	1.844088	-1.859517	-1.340140
C	1.946376	-2.257852	0.018951
C	3.139637	-1.694177	0.548997
C	3.779331	-0.965561	-0.482224
C	2.975678	-1.053472	-1.643695
H	1.050177	-2.123567	-2.022444
H	3.173216	-0.568855	-2.591419
H	4.698848	-0.404636	-0.386665
H	3.485982	-1.787108	1.570438
H	1.246798	-2.882380	0.553804
C	-3.669508	0.420092	-0.903540
H	-3.945908	-0.497727	-1.434361
C	-2.702360	1.196885	-1.802381
C	-4.960057	1.200059	-0.632798
H	-2.477401	2.178936	-1.372998
H	-1.759098	0.653387	-1.917141
H	-3.147689	1.355688	-2.791743
H	-4.739290	2.136264	-0.109083
H	-5.643249	0.612856	-0.009227
C	-3.016968	-1.477478	0.548294
H	-5.469275	1.442581	-1.572958
C	-2.711385	-1.911489	1.980373
C	-2.028837	-2.135825	-0.426824
H	-2.254133	-1.887581	-1.469052
H	-1.016440	-1.785092	-0.209200
H	-4.032621	-1.826510	0.306270
H	-2.066093	-3.227041	-0.326140
H	-2.841592	-2.996767	2.056221
H	-3.383223	-1.430715	2.698658
H	-1.680335	-1.671051	2.256877
Ti	1.668589	0.065571	-0.019350
B	-2.480532	0.915869	1.248064
N	-3.031399	-0.008832	0.367994

H	0.519465	-0.565756	1.025102
H	0.370884	0.079757	-1.085068
H	-2.526235	2.078152	0.970032
H	-1.982450	0.575106	2.273206

S_4 **E = -1083.5423575 Hartree**

C	-1.721854	-1.330267	-2.367857
C	-0.351796	-1.078537	-2.153195
C	0.188221	-2.176467	-1.426988
C	-0.849790	-3.118146	-1.241253
C	-2.042374	-2.582055	-1.772445
H	-2.434306	-0.684119	-2.856482
H	0.196055	-0.201845	-2.461699
H	1.201703	-2.260632	-1.060277
H	-0.759394	-4.059621	-0.719434
H	-3.021871	-3.039754	-1.752548
C	-1.608746	-0.770925	2.387731
C	-2.596432	-1.712566	2.015594
C	-1.934684	-2.853511	1.508138
C	-0.532580	-2.619934	1.590417
C	-0.331262	-1.329984	2.128427
H	-3.665377	-1.562203	2.063606
H	-2.415876	-3.740065	1.119667
H	0.256725	-3.291504	1.286597
H	0.625793	-0.876158	2.326472
H	-1.788609	0.189777	2.836806
C	-1.679014	1.850616	-1.482839
C	-2.147939	2.028330	1.019126
C	-0.258047	2.418085	-1.409658
C	-2.632099	2.893532	-2.102601
C	-2.943713	3.339829	0.924722
C	-0.766505	2.302673	1.635085
H	0.410963	1.727000	-0.892865
H	0.118633	2.576581	-2.427363
H	-0.223548	3.386098	-0.901415
H	-2.372784	3.010901	-3.162091
H	-3.671550	2.562305	-2.047109
H	-2.550550	3.878363	-1.638523
H	-1.650464	1.041566	-2.203447
H	-2.406347	4.118098	0.376691
H	-3.114320	3.716987	1.940287
H	-3.917594	3.180133	0.454342
H	-0.890722	2.550788	2.696672
H	-0.261646	3.150620	1.166587
H	-0.117304	1.429987	1.553665

H	-2.703325	1.419132	1.727739
C	4.280616	0.432628	-0.961964
C	2.865159	0.892859	1.096047
C	3.157064	0.006813	-1.899714
C	5.641176	-0.128263	-1.375477
C	2.878948	0.677705	2.610369
C	2.967148	2.387483	0.777628
H	4.364976	1.522456	-0.985914
H	3.077216	-1.081471	-1.939530
H	3.364888	0.380248	-2.907878
H	2.193298	0.410672	-1.580051
H	5.904259	0.267762	-2.361867
H	6.427472	0.179136	-0.673744
H	5.631642	-1.218328	-1.424280
H	1.933036	0.492667	0.688713
H	2.800084	-0.378374	2.868652
H	2.041512	1.219816	3.060577
H	3.805970	1.068743	3.051935
H	2.222099	2.921075	1.374453
H	3.954201	2.789353	1.041430
H	2.763214	2.618573	-0.270698
Ti	-1.407025	-1.093159	0.000116
N	-2.156998	1.189024	-0.223778
B	-3.466742	0.400881	-0.389044
H	-3.191570	-0.855153	-0.220493
H	-0.063038	-0.137732	0.108155
H	-3.933791	0.415692	-1.499715
H	-4.271178	0.595498	0.490571
N	3.964671	0.057768	0.468733
B	3.703671	-1.568446	0.725771
H	2.503061	-1.723594	0.711853
H	4.251672	-2.182233	-0.156936
H	4.190003	-1.817447	1.807435
H	4.813895	0.270600	0.994820