Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplemental Information

for

Reactivity Patterns for the Activation of CO_2 and CS_2 with Alumoxane and Aluminum Hydrides

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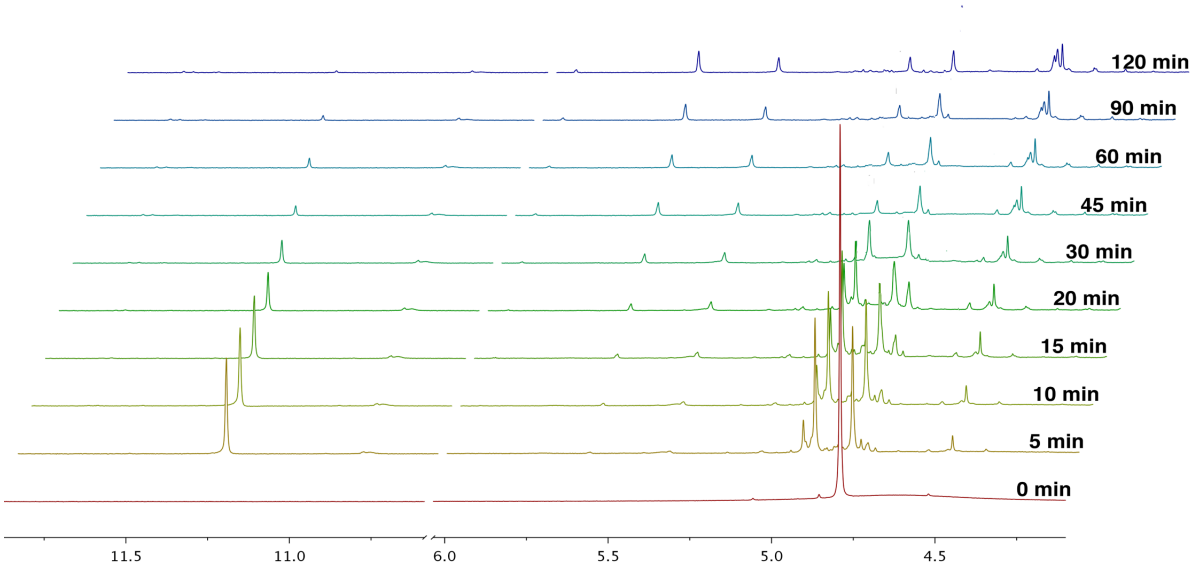


Figure S1. ^{1}H NMR kinetic study of the conversion of **2** to the intermediate **B**. Resonances at δ 11.23 ppm and 4.87 ppm are assigned to the intermediate **B**.

Table S1. Crystal data and structure refinement details for **4** and **5**.

Compound	**4**	**5**
Formula	$C_{48}H_{62}Al_2N_4O_6$	$C_{47.78}H_{61.78}Al_2N_4O_{3.67}$
Formula weight	844.97	804.3
Crystal system	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$
Temperature, K	173(2)	173(2)
λ, Å	0.71073	0.71073
a, Å	8.621(2)	8.7550(6)
b, Å	10.492(2)	9.9863(7)
c, Å	13.350(3)	13.3508(9)
α, °	68.820(3)	70.1027(10)
β, °	81.784(4)	83.2915(11)
γ, °	78.211(4)	79.9565(11)
V, Å^3	1099.0(4)	1078.68(13)
Z	1	1
ρ, g·cm^{-3}	1.277	1.239
μ, mm^{-1}	0.120	0.115
F(000)	452	432
Measured reflns	10698	14497
Independent reflns	3974 [R_{int} = 0.0434]	3902 [R_{int} = 0.0237]
GoF on F^2	1.038	1.034
R_1,[a] wR_2[b] ($I > 2\sigma(I)$)	0.0574, 0.1408	0.0428, 0.1111
R_1,[a] wR_2[b] (all data)	0.0802, 0.1527	0.0475, 0.1150
Largest diff. peak/hole, e·Å^{-3}	0.586 /–0.265	0.471/ –0.234

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma(F_o^2)^2]^{1/2}$

Table S2. Crystal data and structure refinement details for **6** and **7**.

Compound	**6**	**7**
Formula	$C_{46}H_{58}Al_2N_4OS$	$C_{46}H_{58}Al_2N_4O_{0.16}S_{1.84}$
Formula weight	768.98	782.47
Crystal system	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$
T, K	173(2)	173(2)
λ, Å	0.71073	0.71073
a, Å	8.571(1)	8.5925(8)
b, Å	9.899(2)	9.9850(9)
c, Å	13.425(2)	13.4354(12)
α,°	71.329(2)	70.9073(13)
β,°	80.812(2)	81.4316(13)
γ,°	77.725(2)	78.6853(13)
V, Å^3	1049.1(3)	1063.64(17)
Z	1	1
D(cald), g cm^{-3}	1.217	1.221
μ, mm^{-1}	0.159	0.197
Measured reflns	10587	11367
Independent reflns	3787 [R_{int} = 0.0287]	3729 [R_{int} = 0.0352]
GoF on F^2	1.134	1.048
R_1,[a] wR_2[b] ($I > 2\sigma(I)$)	0.0516, 0.1179	0.0471, 0.1168
R_1,[a] wR_2[b] (all data)	0.0568, 0.1208	0.0574, 0.1240
Largest diff. peak/hole, e·Å^{-3}	0.273/ –0.185	0.366 / –0.209

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma(F_o^2)^2]^{1/2}$

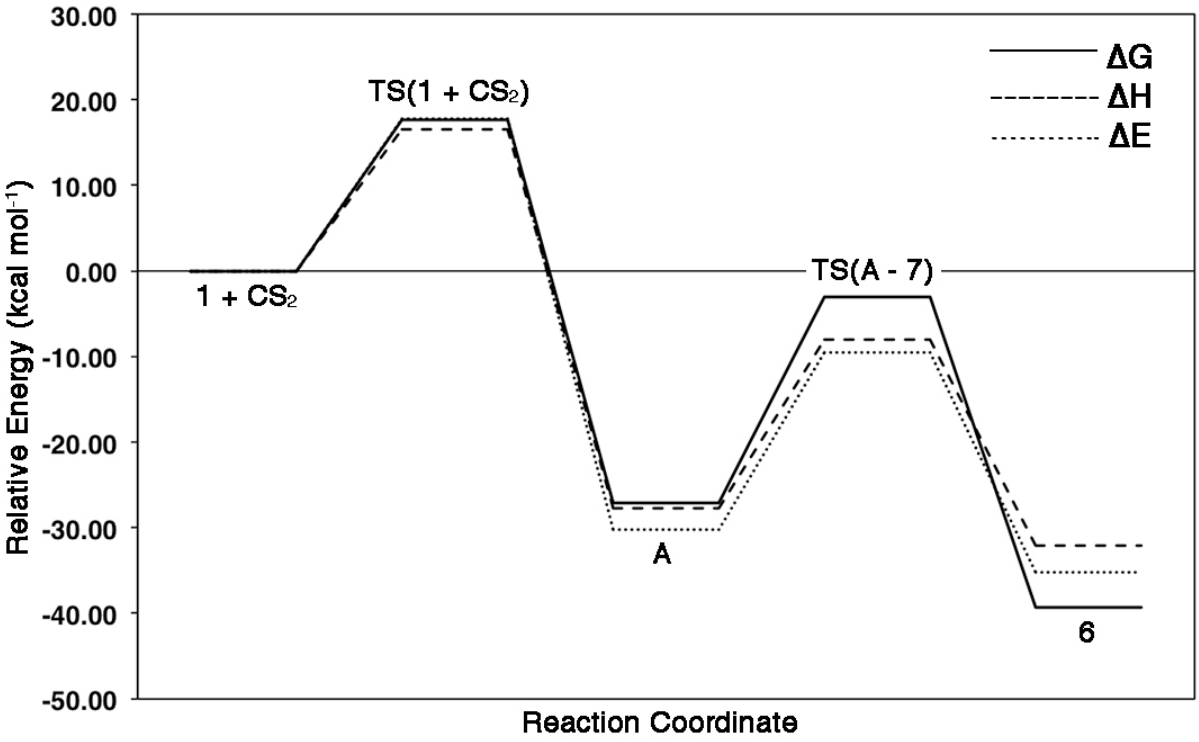


Figure S2. The mechanism of formation of **6**, where ΔG is the free Gibbs energy, ΔH is the enthalpy and ΔE the electronic energy on each step of the mechanism.

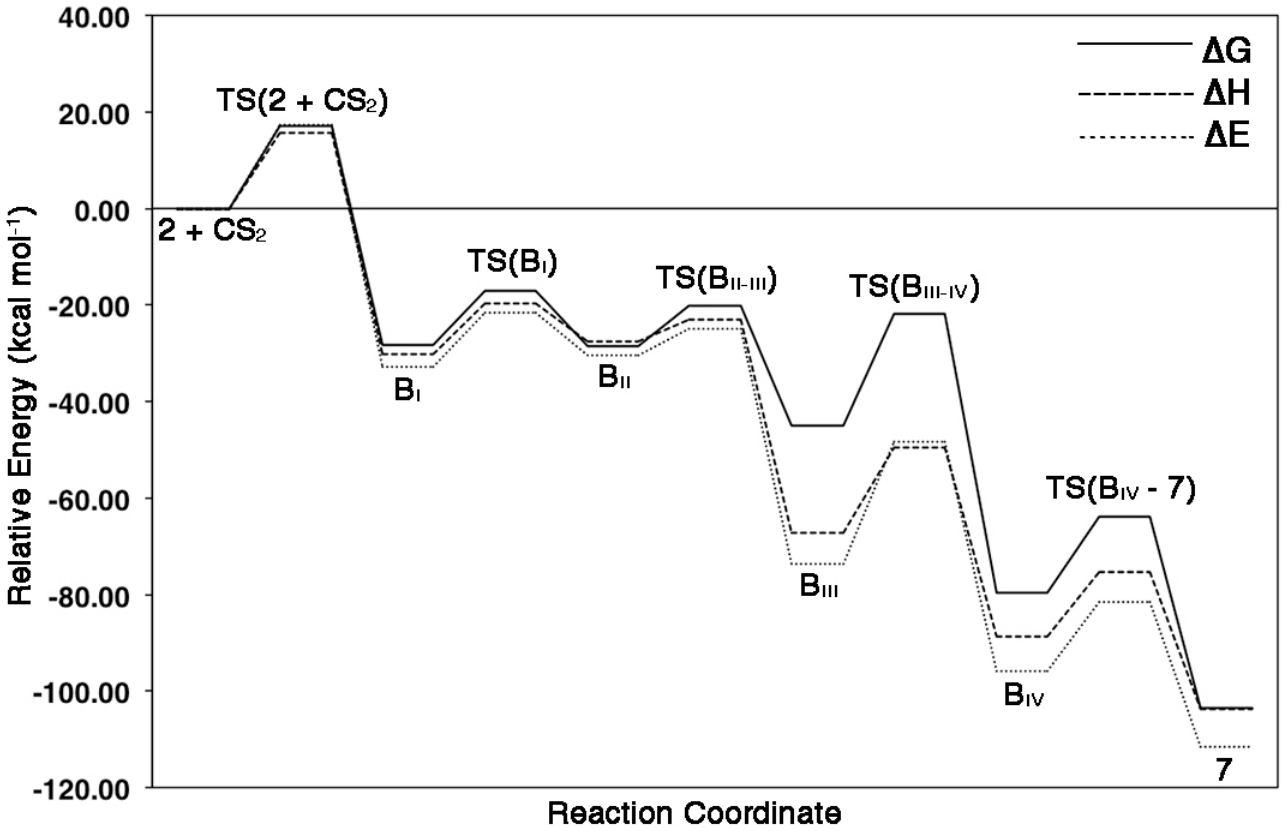
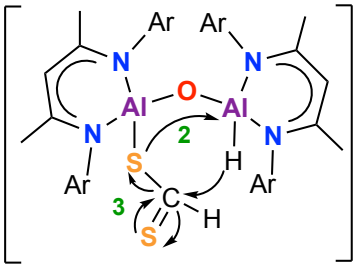


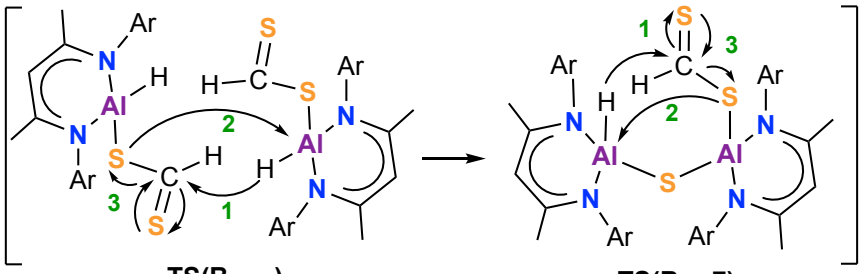
Figure S3. Mechanism of formation of **7**, where ΔG is the free Gibbs energy, ΔH is the enthalpy and ΔE the electronic energy on each step of the mechanism.

Compound **6**



TS(A–6)

Compound **7**



TS($B_{III–IV}$) **TS(B_{IV}–7)**

Figure S4. Graphical representation of the steps involved in the reaction mechanisms to obtain **6** and **7**. The numbers represent the sequence of bond breaking and formation that produce the cyclic structures.

x, y , and z coordinates of every minimum, intermediate and transition state involved in the mechanism of formation of 6.

Label: **1 + CS_2**

Number of atoms: 116
Free Gibs energy: -3401.146353 a.u.
Enthalpy: -3400.984962 a.u.
Electronic energy: -3402.017552 a.u.

Al	0.75329	1.28407	-0.38384
Al	-1.05172	-1.43341	0.32078
N	1.40492	1.72123	-2.13602
N	-2.24213	-2.30334	-0.90373
C	1.46985	2.84016	-4.31213
H	2.52792	3.11717	-4.26131
H	0.93274	3.61370	-4.86082
H	1.41465	1.90063	-4.86989
C	0.90513	2.67315	-2.92349
C	-0.10157	3.56222	-2.51896
C	-0.64709	3.67665	-1.22861
C	-1.59221	4.82028	-0.96261
H	-2.54486	4.45597	-0.56918
H	-1.77803	5.39347	-1.87079
H	-1.16900	5.48762	-0.20458
N	-0.33981	2.85192	-0.23382
C	-0.89827	3.04085	1.07628

C	-2.11863	2.43703	1.41145
C	-2.56874	2.54746	2.72979
C	-1.84762	3.23854	3.70086
C	-0.64384	3.84117	3.33047
C	-0.15085	3.75138	2.03034
C	2.53519	0.95490	-2.58210
C	2.33915	-0.27112	-3.23720
C	3.45972	-1.01536	-3.60305
C	4.75716	-0.57698	-3.33035
C	4.91856	0.64269	-2.67618
C	3.82437	1.42224	-2.29306
C	1.15052	-5.08504	-0.03875
H	2.15521	-4.66797	-0.14998
H	1.02791	-5.90873	-0.74199
H	1.07816	-5.47559	0.98156
C	0.10396	-4.02370	-0.26069
C	-0.86377	-4.24901	-1.25595
C	-1.99476	-3.46126	-1.51659
C	-2.99489	-3.97995	-2.51916
H	-3.19488	-3.22909	-3.28940
H	-3.95013	-4.19419	-2.02894
H	-2.63373	-4.89190	-2.99445
C	-3.50382	-1.64630	-1.10447
C	-4.58068	-1.98418	-0.27248
C	-5.78707	-1.29838	-0.42848
C	-5.94081	-0.29175	-1.37985
C	-4.84813	0.02578	-2.18927
C	-3.62563	-0.63321	-2.06904
N	0.11439	-2.94139	0.50847
C	1.10393	-2.76670	1.53585
C	0.78845	-3.15267	2.84974
C	1.69361	-2.85675	3.86503
C	2.87996	-2.16437	3.61236
C	3.17097	-1.80743	2.29804
C	2.30837	-2.11242	1.24125
H	4.09052	-1.26848	2.08047
H	1.45263	-3.14552	4.88652
H	3.31449	-1.96769	-4.10966
H	5.92167	1.00100	-2.45516
H	-0.43491	4.28510	-3.25127
H	-0.76623	-5.16239	-1.82684
H	-3.50689	2.06799	3.00126
H	-0.06569	4.38393	4.07615
H	-6.62566	-1.55851	0.21379
H	-4.94882	0.81151	-2.93577
O	-0.22756	-0.12391	-0.41662
H	1.97258	1.29495	0.64342
H	-1.84498	-1.11979	1.67020
C	0.94788	-0.77586	-3.50720
H	0.40131	-0.91260	-2.56684
H	0.37080	-0.06156	-4.10622
H	0.97595	-1.72796	-4.04307
C	4.01717	2.73103	-1.57492
H	3.50671	3.55467	-2.08572
H	3.60367	2.67606	-0.56192

H	5.07829	2.97948	-1.50100
C	5.94526	-1.41398	-3.72932
H	5.96495	-2.35898	-3.17659
H	5.91471	-1.66211	-4.79482
H	6.88409	-0.89146	-3.53100
C	1.15410	4.39542	1.64549
H	1.87306	3.64425	1.30142
H	1.02265	5.11257	0.82722
H	1.59079	4.92484	2.49559
C	-2.93763	1.71048	0.37700
H	-2.29367	1.15356	-0.30641
H	-3.63252	1.00904	0.84652
H	-3.53174	2.40918	-0.22593
C	-2.32382	3.29524	5.12909
H	-1.77571	2.57623	5.74840
H	-2.16722	4.28620	5.56471
H	-3.38696	3.05367	5.20424
C	3.79512	-1.78972	4.74925
H	3.29884	-1.09292	5.43351
H	4.08427	-2.66927	5.33361
H	4.70608	-1.30866	4.38507
C	-0.51648	-3.84124	3.14765
H	-1.35798	-3.16059	2.97622
H	-0.67382	-4.71244	2.50322
H	-0.55084	-4.17274	4.18787
C	2.67777	-1.77072	-0.17744
H	1.80419	-1.42803	-0.73524
H	3.44075	-0.98847	-0.20959
H	3.07993	-2.64682	-0.70234
C	-4.42830	-3.05589	0.77392
H	-4.10361	-4.00792	0.33996
H	-3.67232	-2.76614	1.51183
H	-5.37284	-3.22412	1.29607
C	-2.45148	-0.25534	-2.93132
H	-2.72352	0.53983	-3.62998
H	-1.61362	0.08679	-2.31291
H	-2.08774	-1.11268	-3.51028
C	-7.24692	0.44284	-1.53840
H	-7.99670	0.07559	-0.83371
H	-7.11934	1.51613	-1.36455
H	-7.64769	0.32325	-2.54994
C	1.53459	1.08206	3.59892
S	0.20867	0.32565	3.34475
S	2.86860	1.85639	3.85536

Label: **TS(1 + CS_2)**

Number of atoms: 116
Free Gibs energy: -3401.118264 a.u.
Enthalpy: -3400.958674 a.u.
Electronic energy: -3401.98916832 a.u.
Vibrational frequency: -572.32

Al	0.72643	1.40149	0.01724

Al	-0.86616	-1.43651	0.75948
N	1.55021	1.85937	-1.62060
N	-2.02064	-2.28953	-0.51668
C	1.82084	3.03943	-3.74512
H	2.86330	3.33348	-3.58652
H	1.32448	3.81157	-4.33231
H	1.83740	2.10628	-4.31576
C	1.12918	2.84093	-2.42165
C	0.09123	3.72005	-2.08170
C	-0.56296	3.80485	-0.84138
C	-1.51570	4.95041	-0.62215
H	-2.48497	4.58944	-0.26779
H	-1.65682	5.52129	-1.53951
H	-1.12306	5.61830	0.15157
N	-0.35719	2.94441	0.15485
C	-1.00121	3.13613	1.42892
C	-2.23183	2.51508	1.68096
C	-2.78259	2.63975	2.95747
C	-2.14565	3.36032	3.96661
C	-0.92748	3.97682	3.67632
C	-0.33426	3.87118	2.42001
C	2.73609	1.11693	-1.95383
C	2.63132	-0.10607	-2.63116
C	3.80052	-0.82400	-2.88057
C	5.05034	-0.36733	-2.45842
C	5.11843	0.85061	-1.78234
C	3.97565	1.60727	-1.51882
C	1.41374	-5.02932	0.30121
H	2.41415	-4.59896	0.20382
H	1.30176	-5.83605	-0.42298
H	1.34578	-5.44645	1.31094
C	0.35280	-3.97603	0.10354
C	-0.59775	-4.19308	-0.90830
C	-1.74354	-3.42452	-1.15851
C	-2.72565	-3.94358	-2.17861
H	-2.34129	-4.83622	-2.67158
H	-2.94426	-3.18271	-2.93320
H	-3.67603	-4.19123	-1.69444
C	-3.28529	-1.64676	-0.74535
C	-4.37604	-1.99151	0.06510
C	-5.59106	-1.33187	-0.13361
C	-5.74181	-0.35014	-1.11136
C	-4.63633	-0.02848	-1.90153
C	-3.40374	-0.65805	-1.73517
N	0.33727	-2.91807	0.90980
C	1.32214	-2.80530	1.95283
C	0.99333	-3.24601	3.24225
C	1.92818	-3.07119	4.26332
C	3.16585	-2.47295	4.03043
C	3.46651	-2.05685	2.73404
C	2.55989	-2.20086	1.68492
H	4.42297	-1.57794	2.53634
H	1.67577	-3.40248	5.26836
H	3.72940	-1.77447	-3.40561
H	6.08299	1.22150	-1.44336

H	-0.17491	4.46442	-2.81961
H	-0.47536	-5.08887	-1.50160
H	-3.73122	2.15082	3.16681
H	-0.41501	4.53979	4.45339
H	-6.44051	-1.59766	0.49177
H	-4.73439	0.73742	-2.66865
O	-0.07997	-0.08989	0.02041
H	1.90431	1.44076	1.20640
H	-1.68253	-1.13870	2.08994
C	1.28458	-0.64548	-3.03075
H	0.68684	-0.86835	-2.13878
H	0.71558	0.08099	-3.62217
H	1.39133	-1.56056	-3.61798
C	4.06047	2.91881	-0.78536
H	3.68083	3.74805	-1.39319
H	3.46617	2.89233	0.13563
H	5.09302	3.14188	-0.50904
C	6.28666	-1.19548	-2.69255
H	6.36345	-1.99516	-1.94773
H	6.26870	-1.66807	-3.67838
H	7.19267	-0.58916	-2.62030
C	0.99549	4.51586	2.13219
H	1.74328	3.77109	1.83775
H	0.92721	5.24129	1.31352
H	1.37286	5.03461	3.01587
C	-2.93904	1.74693	0.59721
H	-2.24494	1.07775	0.08356
H	-3.75583	1.14633	1.00575
H	-3.36123	2.41733	-0.16239
C	-2.73437	3.44117	5.35102
H	-2.26749	2.70424	6.01314
H	-2.57475	4.42742	5.79542
H	-3.80850	3.24070	5.33919
C	4.13896	-2.22659	5.15269
H	4.12914	-1.16895	5.43835
H	3.88718	-2.81561	6.03801
H	5.16190	-2.47479	4.85539
C	-0.34203	-3.88667	3.51482
H	-1.15405	-3.16376	3.38156
H	-0.53938	-4.72073	2.83268
H	-0.38711	-4.26423	4.53878
C	2.90219	-1.71353	0.30220
H	2.02254	-1.29049	-0.18767
H	3.68447	-0.94859	0.33912
H	3.26904	-2.52693	-0.33736
C	-4.23388	-3.05435	1.12169
H	-3.89215	-4.00464	0.69689
H	-3.49571	-2.75567	1.87339
H	-5.18710	-3.22909	1.62537
C	-2.21698	-0.27299	-2.57701
H	-2.48643	0.50732	-3.29306
H	-1.40151	0.09161	-1.94265
H	-1.82225	-1.12966	-3.13625
C	-7.05410	0.36418	-1.30734
H	-7.85768	-0.12049	-0.74804

H	-6.99037	1.40344	-0.96769
H	-7.33945	0.38437	-2.36321
C	2.29512	1.15703	2.68549
S	1.01471	0.58136	3.44644
S	3.84436	1.59342	2.74138

Label: **A**

Number of atoms: 116
Free Gibs energy: -3401.189475 a.u.
Enthalpy: -3401.029126 a.u.
Electronic energy: -3402.065767270 a.u.

Al	-0.26572	1.74525	0.38388
Al	0.32374	-1.62580	0.47328
N	0.21596	2.67289	-1.20175
N	-0.15041	-2.51165	-1.16023
C	-0.16732	3.62937	-3.42767
H	0.34655	4.58070	-3.25799
H	-0.99251	3.79891	-4.11890
H	0.55802	2.95538	-3.89175
C	-0.67041	3.05954	-2.12596
C	-2.05751	2.99307	-1.94105
C	-2.72845	2.66377	-0.75222
C	-4.22202	2.86080	-0.71261
H	-4.72412	1.95564	-0.36059
H	-4.60443	3.12505	-1.69835
H	-4.48088	3.66061	-0.01145
N	-2.10535	2.21994	0.33950
C	-2.85550	2.04279	1.55835
C	-3.38502	0.78175	1.86806
C	-4.04748	0.62334	3.08528
C	-4.19493	1.67799	3.98537
C	-3.68330	2.92607	3.63242
C	-3.00858	3.13170	2.42904
C	1.61287	2.95187	-1.41515
C	2.44541	1.97568	-1.98067
C	3.80048	2.27147	-2.13209
C	4.33920	3.49372	-1.73053
C	3.48178	4.44531	-1.17938
C	2.11916	4.19734	-1.01470
C	4.26976	-2.85226	-0.64169
H	4.81680	-1.96754	-0.30560
H	4.64850	-3.16224	-1.61549
H	4.47586	-3.64689	0.08328
C	2.78769	-2.58147	-0.70152
C	2.11211	-2.91600	-1.88716
C	0.72303	-2.95143	-2.06900
C	0.20417	-3.57423	-3.34066
H	-0.49256	-2.90353	-3.85099
H	-0.34831	-4.49196	-3.11327
H	1.02453	-3.81865	-4.01523
C	-1.55056	-2.76395	-1.36786
C	-2.10367	-3.95355	-0.87198

C	-3.46888	-4.18081	-1.05383
C	-4.28520	-3.26073	-1.70952
C	-3.70485	-2.08470	-2.18737
C	-2.34731	-1.81286	-2.02159
N	2.17716	-2.08838	0.37238
C	2.92709	-1.92445	1.59022
C	2.97437	-2.98904	2.50077
C	3.67610	-2.81081	3.69332
C	4.31906	-1.61085	3.99347
C	4.25179	-0.57109	3.06572
C	3.56221	-0.70386	1.86157
H	4.73779	0.37627	3.28936
H	3.71618	-3.63105	4.40680
H	4.45470	1.52094	-2.57159
H	3.88188	5.40640	-0.86433
H	-2.67200	3.31375	-2.77134
H	2.71789	-3.28759	-2.70261
H	-4.45524	-0.35373	3.33507
H	-3.80288	3.76362	4.31602
H	-3.90230	-5.10259	-0.67212
H	-4.32792	-1.35215	-2.69747
O	0.07009	0.07763	0.38446
H	0.80448	0.40183	2.76300
H	-0.38091	-2.31140	1.72356
C	1.89150	0.64595	-2.41966
H	1.35865	0.15080	-1.60136
H	1.17544	0.76351	-3.24249
H	2.69266	-0.01221	-2.76384
C	1.20901	5.24746	-0.43424
H	0.40365	5.51708	-1.12645
H	0.73027	4.89876	0.48669
H	1.76918	6.15384	-0.19587
C	5.81559	3.76169	-1.86377
H	6.37046	3.29425	-1.04309
H	6.21111	3.35513	-2.79875
H	6.02994	4.83289	-1.83955
C	-2.46697	4.49201	2.07742
H	-1.37262	4.49604	2.11445
H	-2.75736	4.80609	1.06946
H	-2.82808	5.24182	2.78467
C	-3.28677	-0.35054	0.88262
H	-2.26785	-0.45397	0.50431
H	-3.58681	-1.29818	1.33597
H	-3.93255	-0.17552	0.01303
C	-4.87265	1.46739	5.31395
H	-4.15863	1.09854	6.05801
H	-5.29589	2.39944	5.69692
H	-5.67642	0.73007	5.23799
C	5.03505	-1.41787	5.30444
H	4.44531	-0.78248	5.97372
H	5.20215	-2.37188	5.81056
H	6.00434	-0.93138	5.16195
C	2.28079	-4.28910	2.19167
H	1.19705	-4.14286	2.12777
H	2.60595	-4.70600	1.23167

H	2.47932	-5.02883	2.97033
C	3.50347	0.42071	0.86343
H	2.47911	0.57197	0.51233
H	3.86369	1.35691	1.29728
H	4.11420	0.20431	-0.02266
C	-1.23588	-4.95920	-0.16394
H	-0.37985	-5.26159	-0.77746
H	-0.83205	-4.53614	0.76240
H	-1.80752	-5.85462	0.08969
C	-1.74680	-0.52566	-2.52012
H	-2.52492	0.15771	-2.86814
H	-1.17373	-0.03405	-1.72670
H	-1.05324	-0.69935	-3.35223
C	-5.76089	-3.51088	-1.88319
H	-6.01781	-4.54756	-1.65304
H	-6.34981	-2.86707	-1.22121
H	-6.08015	-3.30095	-2.90834
C	1.04849	1.37173	3.20574
S	1.62814	1.45246	4.73060
S	0.75886	2.73183	2.17020

Label: **TS(A – 6)**

Number of atoms: 116
Free Gibs energy: -3401.151245 a.u.
Enthalpy: -3400.997741 a.u.
Electronic energy: -3402.03263812 a.u.
Vibrational frequency: -592.90

Al	-0.16547	-1.42829	-0.32863
Al	0.47762	1.49223	0.43385
N	-1.17060	-2.22775	-1.73172
N	1.86751	2.73185	0.09226
C	-1.80905	-3.98829	-3.33200
H	-2.85667	-3.97525	-3.01810
H	-1.52691	-5.00987	-3.58431
H	-1.74154	-3.37246	-4.23393
C	-0.91460	-3.44783	-2.24224
C	0.14264	-4.26602	-1.84477
C	1.11938	-3.97145	-0.87952
C	2.17077	-5.01380	-0.60439
H	1.98021	-5.49785	0.35915
H	3.16376	-4.56073	-0.54710
H	2.16563	-5.77881	-1.38081
N	1.13654	-2.83242	-0.20040
C	2.08597	-2.65211	0.86366
C	3.16983	-1.79022	0.63527
C	3.98804	-1.45155	1.71223
C	3.76007	-1.95630	2.99363
C	2.71601	-2.86203	3.17028
C	1.86625	-3.22911	2.12449
C	-2.21869	-1.48598	-2.38789
C	-1.89722	-0.76268	-3.54689
C	-2.92930	-0.16597	-4.26960

C	-4.26124	-0.26654	-3.86238
C	-4.54179	-0.95778	-2.68377
C	-3.53813	-1.56633	-1.92517
C	-1.99615	4.96119	0.58122
H	-1.74702	6.00401	0.38693
H	-2.42978	4.88048	1.58174
H	-2.76694	4.63883	-0.12504
C	-0.77742	4.08658	0.45254
C	0.45768	4.70180	0.19462
C	1.69091	4.06485	0.04095
C	2.88883	4.95101	-0.19626
H	3.35164	4.74283	-1.16493
H	3.65324	4.76951	0.56532
H	2.59917	6.00056	-0.16307
C	3.18938	2.24537	-0.20844
C	4.08969	1.97822	0.83016
C	5.40282	1.64053	0.49260
C	5.82255	1.54304	-0.83463
C	4.88153	1.75501	-1.84423
C	3.56142	2.09652	-1.55293
N	-0.90736	2.77183	0.58514
C	-2.16805	2.20392	0.98039
C	-2.47255	2.09509	2.34451
C	-3.63490	1.41285	2.69761
C	-4.47861	0.85218	1.73646
C	-4.15981	1.01548	0.38902
C	-3.00423	1.68665	-0.01091
H	-4.81562	0.60050	-0.37358
H	-3.87030	1.29174	3.75254
H	-2.68748	0.38757	-5.17451
H	-5.57307	-1.03631	-2.34490
H	0.22598	-5.22496	-2.33695
H	0.45522	5.78036	0.11920
H	4.81991	-0.77232	1.54118
H	2.52477	-3.26952	4.16095
H	6.11731	1.45620	1.29285
H	5.18107	1.65077	-2.88491
O	0.42055	0.17117	-0.67478
H	1.16239	-0.84786	2.30679
H	0.42767	0.79567	1.97880
C	-0.46371	-0.65933	-3.99486
H	0.16545	-0.29175	-3.17629
H	-0.06308	-1.63444	-4.29718
H	-0.37073	0.02109	-4.84421
C	-3.86883	-2.31267	-0.66090
H	-3.45290	-1.79906	0.21410
H	-4.95079	-2.38181	-0.52335
H	-3.45744	-3.32741	-0.66854
C	-5.36027	0.40850	-4.64114
H	-5.37253	-0.93307	2.53158
H	-5.12204	0.45523	-5.70678
H	-6.31093	-0.11819	-4.52562
C	0.73272	-4.18005	2.41198
H	0.12357	-3.79580	3.23504
H	0.07266	-4.31971	1.55479

H	1.12338	-5.15807	2.71570
C	3.44633	-1.27014	-0.74938
H	3.56929	-2.09641	-1.45919
H	2.62308	-0.64602	-1.11314
H	4.35988	-0.67369	-0.75557
C	4.59536	-1.50798	4.16313
H	4.03228	-0.79963	4.78039
H	4.87247	-2.35021	4.80337
H	5.51226	-1.01376	3.83126
C	-5.68185	0.04679	2.15183
H	-5.50944	1.43655	-4.29227
H	-6.24162	0.54255	2.95014
H	-6.36013	-0.11881	1.31054
C	-1.56709	2.69572	3.38623
H	-0.55031	2.29622	3.30979
H	-1.50238	3.78547	3.28290
H	-1.93254	2.46983	4.38880
C	-2.64202	1.86233	-1.45997
H	-1.69433	1.36122	-1.69136
H	-3.41473	1.44294	-2.10460
H	-2.51697	2.92117	-1.71488
C	3.65515	2.07423	2.26893
H	3.28398	3.07544	2.51347
H	2.84299	1.37105	2.49166
H	4.48610	1.84491	2.94020
C	2.54321	2.29987	-2.64264
H	2.95923	2.03238	-3.61635
H	1.66097	1.67763	-2.45392
H	2.19972	3.33967	-2.69477
C	7.23856	1.14921	-1.16571
H	7.34826	0.05900	-1.17213
H	7.53308	1.51532	-2.15234
H	7.94323	1.54438	-0.42941
C	0.17774	-0.52932	2.63968
S	-0.00186	-0.27960	4.30531
S	-1.17053	-1.29232	1.69654

Label: **6**

Number of atoms: 112
Free Gibs energy: -2963.807315 a.u.
Enthalpy: -2963.661273 a.u.
Electronic energy: -2964.66978494 a.u.

Al	-0.50195	1.46400	1.98555
Al	0.37151	-1.02744	2.01869
N	0.44941	3.11485	2.07100
N	-0.59796	-2.67077	1.97855
C	0.81397	5.53876	1.88804
H	1.26657	5.66198	2.87576
H	0.24515	6.43592	1.64547
H	1.63706	5.43536	1.17443
C	-0.07429	4.31998	1.84214
C	-1.42613	4.52679	1.54399

C	-2.41080	3.54497	1.39622
C	-3.79220	4.02890	1.02476
H	-4.09127	3.63726	0.04779
H	-3.81801	5.11756	0.99056
H	-4.53623	3.67770	1.74536
N	-2.18940	2.23180	1.54623
C	-3.30733	1.37710	1.22884
C	-3.51406	1.01245	-0.10996
C	-4.71609	0.39199	-0.44734
C	-5.70111	0.13123	0.50744
C	-5.42903	0.43797	1.83942
C	-4.23394	1.04870	2.22476
C	1.84317	3.06725	2.42840
C	2.79636	2.87936	1.42101
C	4.14474	2.93700	1.77287
C	4.55253	3.13447	3.09004
C	3.57474	3.28235	4.07430
C	2.21581	3.26463	3.76661
C	3.73962	-3.61212	1.45356
H	4.16121	-3.21185	0.52653
H	3.75701	-4.70050	1.40792
H	4.39366	-3.28059	2.26528
C	2.32825	-3.11604	1.66131
C	1.32904	-4.09190	1.71221
C	-0.04928	-3.87873	1.82997
C	-0.93531	-5.09891	1.76807
H	-1.67388	-4.99611	0.96710
H	-1.49695	-5.22628	2.69784
H	-0.34031	-5.99423	1.59016
C	-2.03199	-2.63754	2.11716
C	-2.61063	-2.86679	3.37281
C	-3.99914	-2.98292	3.44499
C	-4.80504	-2.89513	2.31110
C	-4.19651	-2.63616	1.08318
C	-2.81628	-2.48343	0.96631
N	2.09756	-1.79947	1.76510
C	3.25198	-0.96036	1.55146
C	4.09241	-0.64325	2.62475
C	5.33365	-0.06763	2.34368
C	5.72898	0.22594	1.04060
C	4.82561	-0.01497	0.00309
C	3.58559	-0.60776	0.23497
H	5.10459	0.23839	-1.01860
H	6.01139	0.14532	3.16794
H	4.89335	2.81059	0.99517
H	3.87669	3.42959	5.10959
H	-1.73600	5.55067	1.38855
H	1.65138	-5.11882	1.61273
H	-4.90049	0.13357	-1.48899
H	-6.17445	0.22201	2.60236
H	-4.45921	-3.17449	4.41219
H	-4.80848	-2.55900	0.18727
O	-0.00324	0.22473	0.84774
C	2.36508	2.64974	-0.00326
H	1.70212	1.77873	-0.06889

H	1.81173	3.50992	-0.39961
H	3.23281	2.47775	-0.64507
C	1.17912	3.48253	4.83589
H	0.52005	2.61307	4.91663
H	1.65642	3.64581	5.80480
H	0.54719	4.35161	4.62008
C	6.01407	3.18679	3.45236
H	6.24259	2.49566	4.27001
H	6.64078	2.92176	2.59706
H	6.30561	4.18870	3.78561
C	-3.97480	1.41551	3.66061
H	-3.04242	0.96140	4.01319
H	-3.87544	2.49967	3.78902
H	-4.79039	1.07050	4.30016
C	-2.48716	1.35398	-1.15669
H	-1.49595	0.99858	-0.85442
H	-2.75006	0.90324	-2.11701
H	-2.41437	2.43905	-1.30410
C	-7.00706	-0.49871	0.09985
H	-6.89115	-1.57327	-0.08435
H	-7.76822	-0.37783	0.87523
H	-7.38875	-0.05228	-0.82318
C	7.08091	0.82233	0.74582
H	7.60940	0.24175	-0.01700
H	6.99107	1.84537	0.36156
H	7.70794	0.85354	1.64060
C	3.68414	-0.97009	4.03517
H	4.46000	-0.66769	4.74238
H	2.75616	-0.44859	4.29469
H	3.49825	-2.04229	4.16614
C	2.64942	-0.93297	-0.89819
H	1.64029	-0.56329	-0.68544
H	3.00332	-0.48555	-1.83043
H	2.57571	-2.01694	-1.05307
C	-1.75964	-3.03830	4.60215
H	-2.38277	-3.26250	5.47111
H	-1.03461	-3.85232	4.48874
H	-1.19144	-2.12562	4.80628
C	-2.16428	-2.22200	-0.36510
H	-2.91844	-2.06631	-1.14053
H	-1.52317	-1.33459	-0.31233
H	-1.53074	-3.06356	-0.67173
C	-6.29906	-3.05146	2.41664
H	-6.57341	-3.65694	3.28454
H	-6.78902	-2.07729	2.52682
H	-6.71481	-3.52838	1.52422
S	-0.15781	0.21059	3.81468

*Thioformaldehyde (**SCH_2**) coordinates*

Number of atoms: 4
Free Gibs energy: -437.401677 a.u.
Enthalpy: -437.374843 a.u.
Electronic energy: -437.4039648 a.u.

C	0.00000	-1.02383	0.00000
H	-0.92477	-1.60269	0.00000
H	0.92477	-1.60270	0.00000
S	0.00000	0.58427	0.00000

x, y , and z coordinates of every minimum, intermediate and transition state involved in the mechanism of formation of 7.

Label: **2 + CS_2**

Number of atoms: 60
Free Gibs energy: -2080.699285 a.u.
Enthalpy: -2080.598207 a.u.
Electronic energy: -2081.124754 a.u.

Al	-0.37811	0.08551	0.38610
H	-0.15660	1.42884	-0.45000
H	-0.34786	0.27988	1.97220
N	0.82399	-1.29538	-0.18588
N	-1.96842	-0.83519	-0.16429
C	0.46509	-2.46613	-0.70801
C	-0.86956	-2.83908	-0.92735
C	-2.01161	-2.06029	-0.68422
C	-3.18492	-0.09255	0.01749
C	-3.63863	0.73985	-1.01535
C	-3.86583	-0.16874	1.24266
C	-4.79498	1.49196	-0.80288
C	-5.01574	0.60142	1.41011
C	-5.49307	1.44094	0.40244
H	-5.15426	2.13836	-1.60059
H	-5.55212	0.54578	2.35533
C	2.21527	-0.97300	-0.03581
C	2.87522	-0.30089	-1.07417
C	2.86741	-1.26724	1.17082
C	4.20465	0.07788	-0.88076
C	4.19706	-0.87430	1.31806
C	4.88053	-0.19529	0.30776
H	4.72120	0.60419	-1.68082
H	4.71040	-1.09832	2.25097
C	-3.35142	-2.65028	-1.04466
H	-3.86012	-2.02322	-1.78320
H	-3.23802	-3.65438	-1.45255
H	-4.00219	-2.69454	-0.16609
C	1.54065	-3.44815	-1.09648
H	1.10656	-4.36083	-1.50387
H	2.20968	-3.01049	-1.84343
H	2.15862	-3.70476	-0.23067
H	-1.03398	-3.82117	-1.34934
C	2.52782	2.87490	0.20802
S	2.42382	2.28645	1.63969
S	2.63439	3.49039	-1.21933
C	-2.89646	0.80862	-2.32361
H	-2.80612	-0.17795	-2.79104

H	-3.41047	1.47013	-3.02450
H	-1.87941	1.18688	-2.17633
C	-3.37143	-1.07439	2.33953
H	-2.37434	-0.77528	2.67767
H	-4.04781	-1.04662	3.19648
H	-3.29533	-2.11333	2.00107
C	-6.71946	2.28633	0.62773
H	-7.49983	1.72439	1.14866
H	-6.48242	3.16161	1.24201
H	-7.13250	2.64732	-0.31731
C	2.13971	-1.98324	2.27779
H	1.29554	-1.38647	2.63896
H	1.73046	-2.94123	1.93895
H	2.80972	-2.17684	3.11837
C	2.16047	-0.00432	-2.36567
H	1.26945	0.60764	-2.18929
H	2.81562	0.53148	-3.05637
H	1.82479	-0.92416	-2.85836
C	6.29869	0.26758	0.51543
H	6.31952	1.22565	1.04692
H	6.86924	-0.44934	1.11209
H	6.81503	0.40758	-0.43753

Label: **TS(2 + CS_2)**

Number of atoms: 60
Free Gibs energy: -2080.672050 a.u.
Enthalpy: -2080.573137 a.u.
Electronic energy: -2081.097231 a.u.
Vibrational frequency: -620.18

Al	-0.40086	0.10557	0.10313
H	-0.40612	-1.46185	0.29945
H	-0.39032	0.39033	-1.54557
N	1.01364	1.04680	0.93061
N	-1.81535	1.07143	0.90627
C	0.85998	2.11736	1.71338
C	-0.39313	2.64725	2.05194
C	-1.64980	2.13952	1.69059
C	-3.14272	0.58768	0.62253
C	-3.67387	-0.42650	1.43288
C	-3.84827	1.08002	-0.48494
C	-4.93520	-0.93316	1.12184
C	-5.10542	0.54109	-0.75828
C	-5.66510	-0.46375	0.03037
H	-5.35352	-1.71897	1.74631
H	-5.65667	0.91092	-1.62053
C	2.33137	0.53788	0.65604
C	2.86591	-0.45412	1.48955
C	3.02863	1.00207	-0.46961
C	4.12868	-0.96398	1.18616
C	4.28738	0.46316	-0.73310
C	4.85270	-0.51994	0.08046
H	4.55380	-1.73018	1.83032

H	4.83906	0.81959	-1.60013
C	-2.87103	2.82721	2.24103
H	-3.46773	2.12538	2.83168
H	-2.59171	3.67237	2.86910
H	-3.51059	3.18279	1.42805
C	2.08619	2.77993	2.28264
H	1.81695	3.65244	2.87687
H	2.63748	2.07590	2.91378
H	2.76532	3.08692	1.48203
H	-0.39134	3.52036	2.68991
C	-2.89847	-0.94802	2.61376
H	-2.62125	-0.14333	3.30344
H	-3.48759	-1.68233	3.16706
H	-1.96971	-1.43246	2.29279
C	-3.28634	2.17067	-1.35895
H	-2.19437	2.15561	-1.38853
H	-3.65438	2.06979	-2.38303
H	-3.58804	3.16106	-0.99659
C	-7.01874	-1.03266	-0.30659
H	-7.76940	-0.24134	-0.39397
H	-6.99235	-1.56338	-1.26350
H	-7.35573	-1.73624	0.45807
C	2.43219	2.05785	-1.36193
H	1.51538	1.70131	-1.84672
H	2.16671	2.96081	-0.80171
H	3.13578	2.34004	-2.14779
C	2.09293	-0.94901	2.68313
H	1.15770	-1.42888	2.37385
H	2.67769	-1.68022	3.24505
H	1.82617	-0.13144	3.36158
C	6.20116	-1.10426	-0.24961
H	6.11744	-1.85617	-1.04149
H	6.89156	-0.33396	-0.60364
H	6.64787	-1.58960	0.62140
C	-1.10133	-0.00013	-2.91003
S	-2.06103	-1.24553	-2.61807
S	-0.48997	1.05730	-3.94873

Label: **B_I**

Number of atoms: 60
Free Gibs energy: -2080.744456 a.u.
Enthalpy: -2080.646282 a.u.
Electronic energy: -2081.176993 a.u.

Al	0.00009	-0.23107	-0.61845
H	0.00009	2.29549	0.68762
H	0.00030	-1.35698	-1.72233
N	-1.41528	-0.28649	0.63966
N	1.41518	-0.28644	0.63998
C	-1.25570	-0.16753	1.96050
C	-0.00027	-0.04942	2.57705
C	1.25530	-0.16750	1.96078
C	2.72602	-0.53891	0.09451
C	3.58682	0.51452	-0.23444

C	3.09247	-1.87793	-0.13998
C	4.81862	0.20175	-0.81962
C	4.32819	-2.13846	-0.72202
C	5.20360	-1.10865	-1.07889
H	5.49158	1.01720	-1.07611
H	4.61657	-3.17141	-0.90548
C	-2.72601	-0.53880	0.09385
C	-3.58670	0.51476	-0.23498
C	-3.09244	-1.87774	-0.14118
C	-4.81837	0.20222	-0.82054
C	-4.32806	-2.13803	-0.72355
C	-5.20337	-1.10809	-1.08027
H	-5.49123	1.01779	-1.07695
H	-4.61643	-3.17092	-0.90741
C	2.47522	-0.18922	2.84293
H	3.03447	-1.11790	2.69225
H	3.14914	0.63439	2.58783
H	2.19689	-0.10813	3.89315
C	-2.47582	-0.18924	2.84239
H	-3.14962	0.63445	2.58723
H	-3.03511	-1.11786	2.69150
H	-2.19770	-0.10827	3.89266
H	-0.00040	0.05904	3.65285
C	0.00013	2.82112	-0.27456
S	0.00005	1.79662	-1.67166
S	0.00010	4.45402	-0.26499
C	2.16736	-3.00306	0.24233
H	1.84176	-2.92733	1.28541
H	1.26418	-2.99961	-0.37812
H	2.66057	-3.96819	0.10883
C	6.52879	-1.42412	-1.72106
H	7.11770	-2.10489	-1.09860
H	6.38776	-1.90995	-2.69171
H	7.11728	-0.51794	-1.88161
C	3.24172	1.95793	0.02686
H	2.88077	2.44783	-0.88355
H	2.46525	2.07019	0.78684
H	4.12799	2.50275	0.36401
C	-2.16739	-3.00306	0.24070
H	-1.26470	-2.99998	-0.38046
H	-1.84098	-2.92726	1.28352
H	-2.66098	-3.96807	0.10770
C	-3.24157	1.95808	0.02674
H	-2.46507	2.07012	0.78672
H	-2.88066	2.44823	-0.88356
H	-4.12782	2.50283	0.36407
C	-6.52848	-1.42332	-1.72272
H	-6.38733	-1.90949	-2.69318
H	-7.11778	-2.10373	-1.10022
H	-7.11664	-0.51701	-1.88369

Label: **TS(B_{I-II})**

Number of atoms: 60

Free Gibs energy: -2080.726303 a.u.
Enthalpy: -2080.629604 a.u.
Electronic energy: -2081.159287 a.u.
Vibrational frequency: -131.48

Al	0.05511	0.87870	-0.35115
H	-1.71919	3.61895	0.10030
H	-0.02564	0.52868	-1.88403
N	-1.37668	0.19609	0.67723
N	1.44879	0.04939	0.64125
C	-1.19778	0.18316	2.01014
C	0.06865	0.24734	2.60565
C	1.29702	-0.02793	1.96214
C	2.63705	-0.46517	0.01018
C	3.77077	0.33957	-0.15626
C	2.61043	-1.78585	-0.47160
C	4.88682	-0.21410	-0.79211
C	3.74239	-2.29148	-1.10303
C	4.89529	-1.52052	-1.27012
H	5.77221	0.40523	-0.91695
H	3.72418	-3.31353	-1.47515
C	-2.53248	-0.43646	0.10341
C	-3.42356	0.32015	-0.68297
C	-2.73851	-1.81623	0.26626
C	-4.50686	-0.31239	-1.28153
C	-3.84588	-2.40796	-0.35154
C	-4.73953	-1.68157	-1.12774
H	-5.19354	0.28077	-1.88138
H	-3.99954	-3.47751	-0.22156
C	2.45093	-0.48793	2.81218
H	2.70658	-1.52241	2.55884
H	3.34298	0.11597	2.62576
H	2.19800	-0.43942	3.87070
C	-2.38965	0.01234	2.91543
H	-3.28047	0.47250	2.48284
H	-2.60448	-1.04815	3.08117
H	-2.18209	0.46513	3.88636
H	0.08905	0.27763	3.68733
C	-0.75383	4.09963	0.24079
S	0.62576	3.06610	0.15733
S	-0.71379	5.70754	0.53600
C	1.38362	-2.63710	-0.28868
H	1.18409	-2.81936	0.77321
H	0.49279	-2.15435	-0.70659
H	1.50770	-3.60491	-0.77934
C	6.11496	-2.10332	-1.93492
H	6.59147	-2.85112	-1.29241
H	5.85344	-2.60043	-2.87338
H	6.85500	-1.33056	-2.15450
C	3.81417	1.77181	0.30681
H	3.44364	2.44682	-0.47239
H	3.20220	1.94667	1.19439
H	4.84121	2.06806	0.53370
C	-1.82314	-2.70499	1.07185
H	-0.92877	-2.18878	1.41976

H	-2.34562	-3.10468	1.94808
H	-1.50425	-3.56291	0.47189
C	-3.23486	1.80208	-0.84341
H	-3.23323	2.29667	0.13302
H	-2.29488	2.04515	-1.35605
H	-4.04145	2.23482	-1.43847
C	-5.92698	-2.33439	-1.78454
H	-5.91608	-2.17298	-2.86671
H	-5.93862	-3.41145	-1.60288
H	-6.86489	-1.91761	-1.40406

Label: **B_{II}**

Number of atoms: 60
Free Gibs energy: -2080.744810 a.u.
Enthalpy: -2080.642260 a.u.
Electronic energy: -2081.173250 a.u.

Al	0.00728	0.12518	0.15776
H	-0.38634	2.84751	1.10219
H	-0.08005	0.57013	1.67362
N	1.42141	-1.01371	-0.36129
N	-1.40023	-1.01939	-0.38182
C	1.26729	-2.14653	-1.05442
C	0.01773	-2.65969	-1.42658
C	-1.24026	-2.14911	-1.07251
C	-2.71697	-0.61066	0.03764
C	-3.51300	0.20050	-0.77943
C	-3.15551	-1.01235	1.31427
C	-4.75659	0.61371	-0.28810
C	-4.40080	-0.58008	1.75652
C	-5.21441	0.24299	0.97101
H	-5.37985	1.24512	-0.91822
H	-4.74767	-0.89078	2.73975
C	2.73887	-0.59756	0.04838
C	3.54029	0.18055	-0.79497
C	3.17535	-0.96134	1.33661
C	4.78926	0.59645	-0.32006
C	4.42625	-0.52853	1.76207
C	5.24737	0.25867	0.94809
H	5.41729	1.20189	-0.97063
H	4.77220	-0.81129	2.75404
C	-2.46137	-2.92987	-1.47855
H	-3.04448	-3.21157	-0.59632
H	-3.11397	-2.31800	-2.10894
H	-2.18439	-3.83106	-2.02465
C	2.49404	-2.92704	-1.44451
H	3.15213	-2.31949	-2.07313
H	3.06904	-3.20328	-0.55527
H	2.22276	-3.83169	-1.98769
H	0.02309	-3.57663	-1.99958
C	-0.33060	3.22345	0.07706
S	0.04022	2.02358	-1.11654
S	-0.59195	4.80945	-0.21047

C	-2.29299	-1.90141	2.17122
H	-1.99370	-2.81100	1.63935
H	-1.37332	-1.38624	2.47101
H	-2.82546	-2.19635	3.07790
C	-6.54395	0.72207	1.49217
H	-7.11216	-0.09686	1.94281
H	-6.40749	1.48653	2.26423
H	-7.14893	1.15962	0.69474
C	-3.09143	0.62640	-2.16275
H	-2.90007	1.70341	-2.19401
H	-2.18106	0.12381	-2.49337
H	-3.88623	0.41117	-2.88380
C	2.30570	-1.81275	2.22426
H	1.40014	-1.27312	2.52359
H	1.98217	-2.72804	1.71720
H	2.84312	-2.09699	3.13141
C	3.12443	0.55638	-2.19456
H	2.15083	0.14458	-2.46536
H	3.06652	1.64326	-2.30315
H	3.86108	0.19454	-2.91966
C	6.58660	0.73284	1.44855
H	6.46593	1.50001	2.22046
H	7.15682	-0.08810	1.89316
H	7.18244	1.16408	0.64089

Label: **TS($B_{II\text{-}iii}$)**

Number of atoms: 60
Free Gibs energy: -2080.731563 a.u.
Enthalpy: -2080.634888 a.u.
Electronic energy: -2081.164583 a.u.
Vibrational frequency: -136.85

Al	-0.05159	0.16869	-0.15872
H	-0.18707	3.64230	-0.80153
H	0.03506	0.55998	-1.68650
N	-1.45490	-0.99077	0.36181
N	1.37707	-0.94474	0.40620
C	-1.28587	-2.11092	1.07150
C	-0.02965	-2.60471	1.44573
C	1.22232	-2.08654	1.07977
C	2.69667	-0.55297	-0.02565
C	3.50407	0.23579	0.80821
C	3.13164	-0.95321	-1.29706
C	4.75460	0.62726	0.33205
C	4.39115	-0.53613	-1.73014
C	5.21258	0.25965	-0.93408
H	5.38598	1.24386	0.96835
H	4.73601	-0.84288	-2.71490
C	-2.77844	-0.60363	-0.05505
C	-3.60842	0.13916	0.79186
C	-3.19705	-0.96200	-1.35119
C	-4.86446	0.52860	0.31377
C	-4.45490	-0.55349	-1.78145

C	-5.30309	0.19989	-0.96368
H	-5.51294	1.10688	0.96889
H	-4.78536	-0.83083	-2.78023
C	2.44225	-2.89861	1.42808
H	2.93409	-3.24044	0.51130
H	3.17463	-2.29943	1.97493
H	2.17173	-3.76775	2.02678
C	-2.50072	-2.90484	1.47286
H	-3.15794	-2.30370	2.10860
H	-3.08182	-3.18716	0.58979
H	-2.21425	-3.80616	2.01362
H	-0.02298	-3.52412	2.01478
C	0.48748	3.15696	-0.09290
S	-0.34641	2.08925	1.04187
S	2.07228	3.49586	-0.15207
C	2.26478	-1.82466	-2.16742
H	1.94383	-2.73087	-1.64234
H	1.35860	-1.29321	-2.47768
H	2.80328	-2.12681	-3.06813
C	6.55643	0.72892	-1.42695
H	7.32953	0.59069	-0.66561
H	6.86169	0.18716	-2.32528
H	6.52973	1.79542	-1.67344
C	3.03857	0.64969	2.17789
H	2.16876	1.30988	2.11106
H	2.74810	-0.21190	2.78895
H	3.83102	1.18689	2.70339
C	-2.30527	-1.78784	-2.24101
H	-1.41076	-1.22785	-2.53429
H	-1.96435	-2.69838	-1.73691
H	-2.83335	-2.07925	-3.15134
C	-3.21306	0.50957	2.19855
H	-2.21453	0.15419	2.45930
H	-3.22387	1.59545	2.32805
H	-3.92296	0.08768	2.91825
C	-6.65156	0.64316	-1.46780
H	-6.54700	1.39212	-2.25954
H	-7.21287	-0.19670	-1.88786
H	-7.24886	1.08496	-0.66704

Label: **B_{iii}**

Number of atoms: 120
Free Gibs energy: -4161.470400 a.u.
Enthalpy: -4161.303388 a.u.
Electronic energy: -4162.366895 a.u.

Al	-0.94917	0.70702	0.39361
H	-2.66920	2.73251	-0.71650
H	-1.25430	0.37685	-1.10948
N	-2.28991	0.08490	1.58064
N	0.49653	-0.20750	1.18068
C	-2.06133	-0.63989	2.67136
C	-0.77770	-1.08051	3.03910

C	0.41144	-0.90868	2.31772
C	1.72287	-0.21706	0.42325
C	2.70649	0.75385	0.63919
C	1.87976	-1.20519	-0.56662
C	3.86998	0.69938	-0.13434
C	3.04688	-1.20815	-1.32451
C	4.05914	-0.26710	-1.11697
H	4.64789	1.43931	0.04297
H	3.17080	-1.96797	-2.09336
C	-3.60958	0.53229	1.22307
C	-4.14516	1.69787	1.79295
C	-4.28779	-0.15503	0.19985
C	-5.35482	2.18181	1.29004
C	-5.49294	0.36808	-0.26649
C	-6.03468	1.54389	0.25495
H	-5.76493	3.09700	1.71363
H	-6.01892	-0.15796	-1.06023
C	1.65699	-1.57058	2.84396
H	2.03813	-2.29600	2.11791
H	2.44823	-0.83035	2.99853
H	1.45829	-2.08313	3.78469
C	-3.22562	-1.01649	3.54735
H	-3.65323	-0.12397	4.01552
H	-4.01796	-1.47569	2.94865
H	-2.91814	-1.70978	4.32967
H	-0.71064	-1.65940	3.95019
C	-2.14952	3.49949	-0.13158
S	-0.71917	2.97620	0.68812
S	-2.76140	5.01969	-0.10509
C	0.80704	-2.23642	-0.79264
H	0.58862	-2.80149	0.12101
H	-0.12902	-1.76586	-1.11456
H	1.10622	-2.94204	-1.57061
C	5.31747	-0.30649	-1.94517
H	5.80096	-1.28668	-1.88406
H	5.10039	-0.11968	-3.00244
H	6.03861	0.44338	-1.60855
C	2.54213	1.84925	1.66053
H	2.21162	2.77574	1.17642
H	1.80496	1.59917	2.42724
H	3.49406	2.05699	2.15803
C	-3.73658	-1.43700	-0.36522
H	-3.58338	-2.18656	0.41908
H	-4.41811	-1.85619	-1.10860
H	-2.76925	-1.28212	-0.85421
C	-3.46702	2.44633	2.91266
H	-2.51939	1.99338	3.20706
H	-3.26198	3.47963	2.61297
H	-4.11831	2.48471	3.79253
C	-7.31475	2.12343	-0.28849
H	-7.12393	3.06437	-0.81571
H	-7.79940	1.43583	-0.98618
H	-8.02335	2.34329	0.51571
Al	-0.67990	2.09482	-3.95964
H	-2.19321	-0.20755	-3.14327

H	-1.25014	2.34735	-2.52076
N	-1.91725	2.49232	-5.34151
N	0.68203	3.26309	-4.53033
C	-1.66036	3.26780	-6.39040
C	-0.43624	3.93727	-6.56314
C	0.64468	3.96116	-5.67156
C	1.74864	3.48233	-3.58635
C	2.90690	2.69945	-3.61718
C	1.56259	4.47039	-2.60027
C	3.89815	2.94725	-2.66193
C	2.56688	4.66627	-1.65812
C	3.74834	3.91932	-1.67857
H	4.81085	2.35547	-2.69363
H	2.42706	5.42616	-0.89205
C	-3.16382	1.78865	-5.19996
C	-3.36565	0.56529	-5.85868
C	-4.11235	2.28917	-4.28881
C	-4.52134	-0.16035	-5.56251
C	-5.24890	1.52588	-4.02730
C	-5.46513	0.29252	-4.64405
H	-4.67319	-1.11990	-6.05386
H	-5.98093	1.90601	-3.31801
C	1.81725	4.84219	-6.01020
H	1.94158	5.61816	-5.24805
H	2.74328	4.25934	-6.02563
H	1.67841	5.31913	-6.97994
C	-2.72500	3.44497	-7.43913
H	-2.88869	2.50535	-7.97687
H	-3.67617	3.71901	-6.97345
H	-2.44005	4.21393	-8.15667
H	-0.33824	4.53640	-7.45822
C	-1.46102	-0.86747	-3.62090
S	-0.02202	-0.09741	-4.19529
S	-1.79886	-2.46766	-3.73018
C	0.30378	5.29489	-2.57255
H	0.14097	5.81853	-3.52170
H	-0.57541	4.66498	-2.39506
H	0.34501	6.03750	-1.77283
C	4.82263	4.16940	-0.65217
H	5.12517	5.22129	-0.64574
H	4.46763	3.93120	0.35656
H	5.71259	3.56607	-0.85109
C	3.10867	1.60178	-4.62931
H	2.94296	0.62215	-4.16563
H	2.42337	1.68529	-5.47582
H	4.13273	1.61538	-5.01448
C	-3.92083	3.62847	-3.62787
H	-2.99333	3.66780	-3.04848
H	-3.87185	4.43498	-4.36811
H	-4.74569	3.84438	-2.94497
C	-2.38412	0.00045	-6.85421
H	-1.48582	0.61174	-6.95174
H	-2.07013	-1.00307	-6.54860
H	-2.85066	-0.09026	-7.84120
C	-6.67251	-0.54596	-4.31572

H	-6.38752	-1.41824	-3.71751
H	-7.41463	0.02491	-3.75190
H	-7.15311	-0.92091	-5.22415

Label: **TS(B_{iii-IV})**

Number of atoms: 120
Free Gibs energy: -4161.433528 a.u.
Enthalpy: -4161.275351 a.u.
Electronic energy: -4162.326457 a.u.
Vibrational frequency: -368.65

Al	-0.37767	-1.26557	-0.13915
H	-2.11347	1.16408	-0.43051
H	-0.87511	-1.70592	-1.67448
N	-1.80647	-1.87976	0.92204
N	1.00415	-2.34248	0.53862
C	-1.77444	-3.10355	1.44721
C	-0.61655	-3.90294	1.45124
C	0.69073	-3.50709	1.13502
C	2.37092	-1.87421	0.61163
C	2.80995	-1.24381	1.78669
C	3.25058	-2.07122	-0.46429
C	4.14088	-0.82442	1.86812
C	4.57339	-1.65868	-0.32950
C	5.03847	-1.02589	0.82515
H	4.48001	-0.34256	2.78422
H	5.25608	-1.81889	-1.16152
C	-2.94392	-1.00812	1.08090
C	-2.94346	-0.08523	2.14354
C	-3.95887	-0.99013	0.11279
C	-3.95492	0.87021	2.19476
C	-4.93872	0.00423	0.19492
C	-4.95110	0.94620	1.21890
H	-3.94769	1.59486	3.00674
H	-5.70836	0.03602	-0.57346
C	1.81275	-4.41890	1.55478
H	2.45198	-4.65524	0.69870
H	2.44396	-3.92565	2.29990
H	1.42362	-5.34323	1.97956
C	-3.01702	-3.63663	2.10393
H	-3.29939	-2.99980	2.94875
H	-3.85043	-3.62382	1.39607
H	-2.86752	-4.65502	2.46043
H	-0.72264	-4.88949	1.88076
C	-1.26658	1.73555	-0.05485
S	0.25295	0.89100	0.04979
S	-1.47980	3.30886	0.32525
C	2.77535	-2.69882	-1.74032
H	2.28079	-3.66164	-1.57239
H	2.03949	-2.05642	-2.24352
H	3.60804	-2.85692	-2.42879
C	6.46826	-0.55996	0.91488
H	7.16550	-1.39622	0.80386

H	6.69458	0.15843	0.12029
H	6.66916	-0.07627	1.87356
C	1.91207	-1.03841	2.98016
H	1.76626	0.02974	3.17512
H	0.93108	-1.49360	2.84001
H	2.36199	-1.47523	3.87728
C	-4.04378	-2.02301	-0.97715
H	-4.80780	-2.77103	-0.73327
H	-4.33979	-1.56712	-1.92620
H	-3.10796	-2.56000	-1.13669
C	-1.85543	-0.06993	3.18456
H	-1.39570	-1.05005	3.31816
H	-1.06279	0.63462	2.90319
H	-2.25631	0.25372	4.14822
C	-6.00121	2.02314	1.28625
H	-5.53835	3.01404	1.31825
H	-6.66336	1.98666	0.41828
H	-6.61602	1.91810	2.18573
Al	-0.76718	0.91444	-4.09904
H	-2.08852	-1.23501	-2.91681
H	-1.62681	1.25057	-2.80857
N	-1.82683	1.06330	-5.66615
N	0.55378	2.14984	-4.62875
C	-1.45750	1.70261	-6.77472
C	-0.26780	2.44416	-6.87273
C	0.65563	2.68740	-5.84569
C	1.44377	2.53017	-3.56218
C	2.61374	1.80430	-3.31520
C	1.04115	3.57490	-2.70762
C	3.36348	2.12525	-2.17821
C	1.81679	3.85595	-1.58923
C	2.97525	3.13007	-1.29857
H	4.27001	1.55904	-1.97872
H	1.50047	4.64850	-0.91471
C	-3.07016	0.34178	-5.60280
C	-3.15108	-0.98443	-6.05622
C	-4.16574	0.96462	-4.97955
C	-4.34262	-1.68066	-5.84318
C	-5.33484	0.22851	-4.79313
C	-5.43842	-1.10011	-5.20831
H	-4.40509	-2.71479	-6.17636
H	-6.18538	0.70660	-4.31194
C	1.80949	3.61290	-6.12525
H	1.79967	4.45564	-5.42769
H	2.75974	3.08998	-5.97701
H	1.76807	3.99383	-7.14514
C	-2.36526	1.65310	-7.97510
H	-2.46786	0.62398	-8.33349
H	-3.36816	1.99920	-7.70630
H	-1.97824	2.27176	-8.78412
H	-0.07183	2.92107	-7.82357
C	-1.24353	-1.91662	-3.04784
S	0.13759	-1.14359	-3.89400
S	-1.62234	-3.55496	-3.25444
C	-0.19835	4.37287	-3.01102

H	-0.13596	4.85289	-3.99425
H	-1.08779	3.73483	-3.01706
H	-0.34854	5.15134	-2.26047
C	3.76027	3.43473	-0.05070
H	4.00819	4.49878	0.01253
H	3.17628	3.17945	0.83961
H	4.69062	2.86473	-0.01625
C	3.08582	0.70152	-4.22812
H	2.86109	-0.28129	-3.80210
H	2.61376	0.74414	-5.21203
H	4.16981	0.76175	-4.36383
C	-4.08554	2.40682	-4.55341
H	-3.31796	2.55707	-3.78626
H	-3.83258	3.05898	-5.39643
H	-5.04169	2.73900	-4.14339
C	-2.00191	-1.68357	-6.73578
H	-1.21832	-0.99136	-7.05054
H	-1.54375	-2.40626	-6.05218
H	-2.35875	-2.23070	-7.61389
C	-6.69693	-1.89619	-4.97807
H	-6.49136	-2.78453	-4.37289
H	-7.45481	-1.30262	-4.46138
H	-7.12581	-2.24111	-5.92422

Label: **B_{iv}**

Number of atoms: 116
Free Gibs energy: -3724.123690 a.u.
Enthalpy: -3723.963111 a.u.
Electronic energy: -3724.998439 a.u.

Al	-1.61610	0.75830	-0.14736
H	-3.17433	3.51844	-0.14354
N	-3.08280	0.29273	0.96256
N	-0.34451	-0.36503	0.72287
C	-3.14861	-0.87482	1.60271
C	-2.05091	-1.73843	1.73585
C	-0.71212	-1.42942	1.43901
C	1.04902	-0.00310	0.64152
C	1.60024	0.85255	1.60463
C	1.83132	-0.48811	-0.42483
C	2.92646	1.27116	1.44592
C	3.15271	-0.06294	-0.52524
C	3.71515	0.83342	0.38956
H	3.34597	1.95454	2.18181
H	3.76209	-0.43829	-1.34576
C	-4.14282	1.25848	1.08485
C	-4.09620	2.15535	2.17135
C	-5.12843	1.37241	0.09735
C	-5.01576	3.19669	2.21413
C	-6.01898	2.45111	0.17377
C	-5.97050	3.37839	1.20821
H	-4.96712	3.90648	3.03717
H	-6.76890	2.55781	-0.60814

C	0.35307	-2.30763	2.04058
H	1.15086	-2.52287	1.32650
H	0.81260	-1.78886	2.88965
H	-0.07543	-3.24245	2.40186
C	-4.44648	-1.26144	2.26054
H	-4.67666	-0.57281	3.08007
H	-5.26991	-1.19302	1.54326
H	-4.39595	-2.27520	2.65736
H	-2.22682	-2.66508	2.26533
C	-2.24740	3.93644	0.25164
S	-0.88596	2.87655	0.32104
S	-2.21508	5.50924	0.71599
C	1.26705	-1.46742	-1.41892
H	0.87014	-2.36034	-0.92254
H	0.44113	-1.02845	-1.98526
H	2.04073	-1.78821	-2.12071
C	5.13463	1.30821	0.21753
H	5.83865	0.46976	0.22964
H	5.26377	1.82215	-0.74121
H	5.42138	2.00070	1.01254
C	0.83785	1.30883	2.82296
H	0.78992	2.40089	2.86391
H	-0.18516	0.92974	2.84079
H	1.34469	0.96597	3.73166
C	-5.29095	0.36601	-1.01279
H	-6.27744	-0.10678	-0.94215
H	-5.23274	0.85100	-1.99228
H	-4.52743	-0.41180	-0.98545
C	-3.04135	2.03256	3.23909
H	-2.91823	1.00216	3.58831
H	-2.06909	2.36692	2.85924
H	-3.29608	2.65614	4.09900
C	-6.90032	4.56212	1.24765
H	-6.34773	5.48932	1.06297
H	-7.68252	4.47973	0.48914
H	-7.38086	4.65856	2.22585
Al	-2.44454	2.13796	-3.25768
H	-3.25802	3.08958	-2.28358
N	-3.42128	1.80499	-4.86500
N	-0.96950	2.99471	-4.11910
C	-3.00868	2.10778	-6.09726
C	-1.79220	2.74607	-6.36977
C	-0.84572	3.18643	-5.43021
C	0.03689	3.49799	-3.21904
C	1.14061	2.69855	-2.88943
C	-0.15484	4.75591	-2.62558
C	2.02607	3.16651	-1.91664
C	0.76512	5.18857	-1.67284
C	1.84709	4.39606	-1.28723
H	2.86513	2.53648	-1.62885
H	0.60751	6.15221	-1.19326
C	-4.71786	1.21511	-4.66892
C	-4.87366	-0.17798	-4.68222
C	-5.80755	2.06313	-4.39824
C	-6.13342	-0.70722	-4.38979

C	-7.04811	1.48907	-4.12663
C	-7.22943	0.10448	-4.10781
H	-6.25641	-1.78850	-4.38990
H	-7.89491	2.14091	-3.92137
C	0.35261	3.94178	-5.94451
H	0.35704	4.95773	-5.53668
H	1.28385	3.46838	-5.62276
H	0.33902	3.99808	-7.03275
C	-3.90286	1.77026	-7.26216
H	-4.08838	0.69279	-7.30412
H	-4.87654	2.25729	-7.14977
H	-3.45403	2.08804	-8.20293
H	-1.57328	2.94878	-7.40917
S	-1.89553	0.21560	-2.26196
C	-1.33604	5.61116	-3.00213
H	-1.42243	5.72669	-4.08836
H	-2.27320	5.16705	-2.64855
H	-1.24841	6.60442	-2.55651
C	2.76084	4.83272	-0.17340
H	3.06267	5.87867	-0.28444
H	2.25004	4.74002	0.79173
H	3.66337	4.21586	-0.13423
C	1.38900	1.38212	-3.57712
H	2.16826	0.82340	-3.05208
H	0.48380	0.77015	-3.60815
H	1.72449	1.52723	-4.61155
C	-5.63600	3.55930	-4.40840
H	-5.00568	3.88622	-3.57456
H	-5.15464	3.90415	-5.32969
H	-6.60370	4.05848	-4.32067
C	-3.74252	-1.10397	-5.04532
H	-2.76729	-0.64079	-4.89241
H	-3.78042	-2.01496	-4.44280
H	-3.81187	-1.40083	-6.09905
C	-8.56857	-0.49314	-3.76256
H	-8.67235	-0.62048	-2.67911
H	-9.38855	0.14848	-4.09608
H	-8.69652	-1.47665	-4.22183

Label: **TS(B_{iv} – 7)**

Number of atoms: 116
Free Gibs energy: -3724.098865 a.u.
Enthalpy: -3723.941789 a.u.
Electronic energy: -3724.975516 a.u.
Vibrational frequency: -522.01

Al	-0.56401	0.83369	-0.06185
H	-2.68121	2.86985	-0.64009
N	-1.99028	0.15308	1.00642
N	0.82109	-0.16479	0.77558
C	-1.89923	-0.89781	1.81480
C	-0.68179	-1.53548	2.09805
C	0.59050	-1.14524	1.66421

C	2.19943	0.11955	0.44891
C	2.89608	1.10602	1.15765
C	2.84134	-0.64945	-0.54199
C	4.25439	1.29467	0.87726
C	4.19279	-0.42315	-0.78579
C	4.92134	0.53789	-0.07862
H	4.80196	2.04695	1.44117
H	4.69727	-1.02535	-1.53942
C	-3.23152	0.87333	0.88821
C	-3.46559	1.93903	1.78173
C	-4.12237	0.59316	-0.15404
C	-4.55320	2.77270	1.54686
C	-5.20491	1.46089	-0.34514
C	-5.41768	2.56893	0.46656
H	-4.71584	3.62166	2.20657
H	-5.88893	1.25608	-1.16545
C	1.76577	-1.85349	2.29153
H	2.44984	-2.25479	1.54032
H	2.34029	-1.14402	2.89655
H	1.42519	-2.66407	2.93470
C	-3.14956	-1.42226	2.46889
H	-3.62545	-0.64775	3.07753
H	-3.87449	-1.71451	1.70232
H	-2.92961	-2.28461	3.09762
H	-0.72261	-2.36843	2.78616
C	-1.89477	3.62677	-0.63033
S	-0.37216	3.07417	0.17271
S	-2.37934	5.23967	-0.49304
C	2.10723	-1.73292	-1.28592
H	1.77889	-2.53468	-0.61389
H	1.21234	-1.34251	-1.77760
H	2.75358	-2.17883	-2.04554
C	6.38658	0.74204	-0.36424
H	6.94014	-0.19758	-0.27142
H	6.54535	1.10824	-1.38522
H	6.83059	1.46488	0.32462
C	2.24072	1.94859	2.22131
H	1.94094	2.92087	1.81458
H	1.34711	1.47640	2.63576
H	2.93912	2.13909	3.04081
C	-3.98433	-0.60677	-1.05524
H	-4.88250	-1.23030	-0.97885
H	-3.87851	-0.30038	-2.10052
H	-3.11537	-1.21625	-0.80404
C	-2.55060	2.18648	2.95212
H	-2.41008	1.28396	3.55653
H	-1.56285	2.51372	2.61385
H	-2.96207	2.96624	3.59645
C	-6.52531	3.54765	0.18168
H	-6.10827	4.48708	-0.19684
H	-7.21981	3.15777	-0.56724
H	-7.09450	3.78273	1.08602
Al	-1.08211	2.23429	-3.22513
H	-1.61546	3.34226	-2.08081
N	-2.26138	2.10333	-4.69880

N	0.37134	3.01486	-4.14553
C	-2.01910	2.65712	-5.89481
C	-0.81079	3.27762	-6.23043
C	0.32187	3.42328	-5.41486
C	1.54121	3.31826	-3.35811
C	2.56285	2.37045	-3.23242
C	1.60471	4.55999	-2.70610
C	3.66602	2.69523	-2.43998
C	2.72158	4.83512	-1.92164
C	3.75923	3.91416	-1.77272
H	4.46660	1.96746	-2.33807
H	2.77569	5.79067	-1.40457
C	-3.48420	1.36234	-4.52421
C	-3.52659	0.02648	-4.95274
C	-4.59875	1.97394	-3.93203
C	-4.72045	-0.68144	-4.80595
C	-5.77565	1.23068	-3.82440
C	-5.85803	-0.09462	-4.25199
H	-4.76038	-1.71711	-5.13548
H	-6.65503	1.70695	-3.39429
C	1.53799	4.07781	-6.01568
H	1.79138	4.99531	-5.47656
H	2.40332	3.41344	-5.93312
H	1.37002	4.31710	-7.06514
C	-3.09803	2.61978	-6.94660
H	-3.35100	1.59112	-7.21878
H	-4.01339	3.07916	-6.56081
H	-2.78162	3.15426	-7.84166
H	-0.73571	3.67496	-7.23316
S	-0.83469	0.30205	-2.20548
C	0.49075	5.56253	-2.83753
H	0.24320	5.76978	-3.88425
H	-0.42532	5.21263	-2.34721
H	0.76571	6.50494	-2.35961
C	4.94794	4.24452	-0.90873
H	5.44510	5.15697	-1.25378
H	4.64137	4.41499	0.12843
H	5.68242	3.43514	-0.91711
C	2.48428	1.04360	-3.93924
H	3.39536	0.46481	-3.76844
H	1.63299	0.45833	-3.57486
H	2.35465	1.16691	-5.02063
C	-4.53742	3.38918	-3.42172
H	-3.97060	3.45757	-2.48461
H	-4.05231	4.06349	-4.13419
H	-5.54169	3.76885	-3.21896
C	-2.31224	-0.62662	-5.55755
H	-1.46546	-0.58829	-4.86442
H	-2.51586	-1.67379	-5.79056
H	-1.99643	-0.13099	-6.48229
C	-7.13732	-0.87250	-4.08447
H	-7.31333	-1.11231	-3.03014
H	-7.99975	-0.29793	-4.43455
H	-7.10715	-1.81314	-4.63913

Label: **7**

Number of atoms: 112
Free Gibs energy: -3286.760244 a.u.
Enthalpy: -3286.612071 a.u.
Electronic energy: -3287.619393 a.u.

Al	-0.65890	-0.92859	-0.30140
N	-2.10253	-1.43511	0.84618
N	0.73693	-1.59084	0.83865
C	-1.97402	-2.20035	1.93556
C	-0.74185	-2.61445	2.45046
C	0.52834	-2.27669	1.96665
C	2.10970	-1.44856	0.41701
C	2.81953	-0.28679	0.74373
C	2.73176	-2.52129	-0.24482
C	4.17780	-0.22670	0.42334
C	4.08602	-2.41034	-0.55221
C	4.83036	-1.28024	-0.21200
H	4.73978	0.66360	0.69734
H	4.57959	-3.24338	-1.04908
C	-3.40909	-0.87314	0.60923
C	-3.76357	0.28922	1.31976
C	-4.31120	-1.49789	-0.25611
C	-5.04262	0.80962	1.14722
C	-5.60049	-0.96435	-0.35887
C	-5.98173	0.18840	0.31894
H	-5.31943	1.71364	1.68581
H	-6.32014	-1.47399	-0.99513
C	1.70872	-2.70791	2.80368
H	2.37608	-3.37456	2.25223
H	2.30184	-1.83350	3.08957
H	1.37134	-3.21504	3.70710
C	-3.20907	-2.62905	2.68927
H	-3.71187	-1.76957	3.14294
H	-3.92911	-3.09517	2.01065
H	-2.94876	-3.33652	3.47633
H	-0.77173	-3.21080	3.35172
S	-0.86357	1.22668	-0.84130
C	1.98738	-3.79523	-0.54370
H	1.73825	-4.34245	0.37343
H	1.05118	-3.59410	-1.06912
H	2.59745	-4.45365	-1.16629
C	6.30284	-1.22352	-0.52518
H	6.80797	-2.13732	-0.19694
H	6.47603	-1.12982	-1.60279
H	6.78542	-0.37584	-0.03281
C	2.15290	0.84036	1.48555
H	1.31903	1.25300	0.90894
H	1.74618	0.50023	2.44543
H	2.86532	1.64513	1.68190
C	-3.92548	-2.70932	-1.06126
H	-4.81685	-3.23523	-1.41417
H	-3.33657	-2.41579	-1.93942

H	-3.31274	-3.40831	-0.48399
C	-2.78762	0.93617	2.26590
H	-2.52086	0.26915	3.09439
H	-1.85955	1.19938	1.74853
H	-3.21257	1.84787	2.69198
C	-7.36101	0.77223	0.15279
H	-7.31548	1.74923	-0.34062
H	-7.99824	0.12139	-0.45144
H	-7.85137	0.92172	1.11981
Al	-0.61850	0.34289	-2.87437
N	-1.95966	0.55482	-4.22029
N	0.75181	1.30505	-3.80353
C	-1.85797	1.38906	-5.26055
C	-0.69808	2.10901	-5.56216
C	0.53548	2.03592	-4.90090
C	2.05819	1.41384	-3.20004
C	3.02170	0.43134	-3.47813
C	2.37607	2.53420	-2.41635
C	4.32219	0.62272	-3.01221
C	3.68732	2.67198	-1.95836
C	4.67990	1.74547	-2.26650
H	5.07834	-0.11963	-3.25924
H	3.94228	3.55125	-1.36833
C	-3.13049	-0.28424	-4.17497
C	-3.11276	-1.48080	-4.91340
C	-4.26701	0.11173	-3.46257
C	-4.25485	-2.27765	-4.91859
C	-5.40531	-0.69623	-3.53928
C	-5.41641	-1.89736	-4.24204
H	-4.24283	-3.20997	-5.47931
H	-6.30685	-0.36668	-3.02811
C	1.66151	2.85535	-5.48193
H	1.88909	3.70681	-4.83238
H	2.57644	2.26296	-5.56412
H	1.38756	3.23422	-6.46628
C	-3.03598	1.56109	-6.18710
H	-3.27968	0.61896	-6.68751
H	-3.92538	1.85979	-5.62430
H	-2.82335	2.31610	-6.94358
H	-0.74118	2.75517	-6.42794
S	-0.43797	-1.81081	-2.34109
C	1.37952	3.61965	-2.09639
H	0.42485	3.47673	-2.60336
H	1.17126	3.63690	-1.02281
H	1.77987	4.60070	-2.37424
C	6.09843	1.97150	-1.81185
H	6.44698	2.96770	-2.10236
H	6.18370	1.90635	-0.72158
H	6.78082	1.23668	-2.24574
C	2.67886	-0.77288	-4.31347
H	3.57380	-1.36677	-4.51345
H	1.95415	-1.41086	-3.79593
H	2.23657	-0.48612	-5.27389
C	-4.28217	1.36661	-2.63164
H	-3.79204	1.19335	-1.66529

H	-3.74988	2.18954	-3.11772
H	-5.31017	1.68308	-2.43479
C	-1.89507	-1.86979	-5.70822
H	-1.01035	-1.92863	-5.06625
H	-2.04015	-2.84276	-6.18297
H	-1.67770	-1.13814	-6.49569
C	-6.63673	-2.78095	-4.24494
H	-6.53646	-3.58589	-3.50759
H	-7.53767	-2.21449	-3.99490
H	-6.78883	-3.25218	-5.22001

*Thioformaldehyde (**SCH_2**) coordinates*

Number of atoms: 4
Free Gibs energy: -437.401677 a.u.
Enthalpy: -437.374843 a.u.
Electronic energy: -437.4039648 a.u.

C	0.00000	-1.02383	0.00000
H	-0.92477	-1.60269	0.00000
H	0.92477	-1.60270	0.00000
S	0.00000	0.58427	0.00000