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Electronic Supplementary Information for

**Insight into Reaction Mechanisms for Oxidative Addition of Strong σ
Bonds to an Al(I) Center**

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Table of Contents

Table S1. Predicted detailed thermodynamic data and selected charge populations and bond lengths for the oxidative additions of X–H bonds to the NacNacAl (**1**).

Figure S1. The selected HOMO and LUMO orbitals and their energy levels of reactants by B97–D/6–31G(d) (isovalue=0.02).

Figure S2 Selected optimized structures (Å) of species involved in the synchronous hydrogenation at both Al and N sites and the FLP mechanism.

Figure S3. Selected optimized structures of species involved in the Al–Si bond coupling intra-molecular rotation steps by B97–D/6–31G(d) (the bond angle in degree and the bond length in Å).

Figure S4. Relative free energy profiles and electronic energies (in parentheses) for the hydrogen transfer in the reaction of Si–H bonds (**9** and **11**) to the NacNacAl compound (**1**) (the energy in kcal/mol).

Figure S5. Selected optimized structures of species involved in the hydrogen transfer reaction of Si–H bonds in **9** and **11** to the NacNacAl (**1**) by B97–D/6–31G(d) (the bond length in Å).

Table S2. Predicted detailed thermodynamic data and selected charge populations and bond lengths for the oxidative additions of Si–H bonds in **9** and **11** to the NacNacAl (**1**).

Table S3. The B97–D/6–31G(d)-predicted geometries of species involved in the reaction of **9** and **10** to NacNacAl.

Table S4. The B97–D/6–31G(d)-predicted optimized geometries of the reactants, products, intermediates and transition states

Table S1: Predicted detailed thermodynamic data and selected charge populations and bond lengths for the oxidative additions of X–H bonds to the NacNacAl (1).

Species	ΔE^a	ΔG^b	qAl ^c	qH _a ^c	dAl–H _a ^d	dH _a –X ^d
1+2	-1.1/-0.4/ -1.8	-5.0/1.4/ -6.8	0.19/0.20/ 0.22	0.00/0.00/ 0.00	—	0.74/0.74/ 0.74
IM₁₋₂	0.0/0.0/ 0.0	0.0/0.0/ 0.0	0.22/0.20/ 0.22	0.03/0.00/ 0.03	3.58/6.82/ 3.40	0.74/0.74/ 0.74
TS₁₋₂	34.7/36.9/ 34.3 ^e	37.5/46.0/ 35.6	0.37/0.34/ 0.30	0.02/0.01/ 0.03	1.60/1.60/ 1.59	1.26/1.26/ 1.25
3	-30.9/-31.1/ -34.3	-29.6/-24.6/ -31.0	0.55/0.74/ 0.43	-0.18/-0.28/ -0.14	1.60/1.60/ 1.60	2.72/2.70/ 2.75
1+3	10.2	-5.0	0.19	-0.18	—	1.60
IM₁₋₃	0.0	0.0	0.22	-0.20	3.52	1.60
Peak1	5.9	8.1	0.24	-0.25	2.38	1.62
6	-15.4	-9.9	-2.20	-0.20	1.61	3.54
1+4	3.3	-10.2	0.19	-0.05	—	1.20
IM₁₋₄	0.0	0.0	0.24	-0.04	3.38	1.20
Peak2	12.6	12.8	0.28	-0.09	1.68	1.26
5	-19.6	-18.5	0.46	-0.16	1.60	3.29
1+7	5.1/-0.5/ 4.5 ^e	-4.9/-8.6/ -6.5	0.19/0.20/ 0.18	0.15/0.14/ 0.16	—	1.11/1.10/ 1.10
IM₁₋₇	0.0/0.0/ 0.0	0.0/0.0/ 0.0	0.25/0.19/ 0.22	0.14/0.19/ 0.15	2.92/3.69/ 2.91	1.11/1.10/ 1.10
TS₁₋₇	10.8/29.8/ 15.9	14.6/33.7/ 20.9	0.48/0.46/ 0.40	-0.07/-0.04/ 0.02	1.78/1.78/ 1.83	1.55/1.65/ 1.47
8	-30.7/-6.9/ -30.3	-25.8/-2.2/ -24.1	0.73/0.71/ 0.62	-0.14/-0.15/ -0.09	1.59/1.59/ 1.59	3.11/3.08/ 3.11
1+9	3.8	-6.3	0.19	-0.07	—	1.49
IM₁₋₉	0.0	0.0	0.21	-0.05	3.64	1.49
TS₁₋₉	14.5	16.6	0.43	-0.21	1.96	1.66
10'	-29.4	-27.0	0.59	-0.14	1.61	3.47
10	-30.7	-28.8	0.60	-0.14	1.61	3.44
1+11	4.0	-7.6	0.19	-0.08	—	1.50
IM₁₋₁₁	0.0	0.0	0.24	0.21	5.33	1.50
TS₁₋₁₁	14.6	15.7	0.39	-0.22	1.91	1.69
12'	-28.8	-26.9	0.55	-0.14	1.61	3.47
IM_{12'-12}	-25.7	-24.6	0.57	-0.15	1.61	3.41
12	-30.1	-29.1	0.57	-0.15	1.61	3.46
1+13	6.9	-5.1	0.19	0.29	—	1.03
IM₁₋₁₃	0.0	0.0	0.24	0.34	3.33	1.02
TS₁₋₁₃	25.3	28.0	0.40	0.10	1.73	1.44
14	-41.7	-40.8	0.76	-0.17	1.60	2.96
1+15	8.1	-4.1	0.19	0.32	—	1.02
IM₁₋₁₅	0.0	0.0	0.25	0.35	3.05	1.02

TS₁₋₁₅	29.9	30.9	0.39	0.12	1.72	1.45
16	-44.4	-44.2	0.75	-0.15	1.59	2.96
1+17	4.8	-9.6	0.19	-0.01	—	1.43
IM₁₋₁₇	0.0	0.0	0.29	0.01	3.60	1.43
TS₁₋₁₇	18.8	20.5	0.48	-0.08	2.03	1.61
18	-36.8	-34.7	0.67	-0.17	1.59	3.23
1+19	3.5	-9.5	0.19	0.38	—	0.97
IM₁₋₁₉	0.0	0.0	0.28	0.44	2.73	0.98
TS₁₋₁₉	13.3	13.6	0.38	0.19	1.79	1.25
20	-57.5	-58.7	0.82	-0.19	1.60	2.87

^a the relative energies with the zero-point energy (ZPE) correction in kcal/mol; ^b the relative Gibbs free energy in kcal/mol; ^c Mulliken charge population; ^d bond length; ^e the relative energies by B97-D/B3LYP/M06-2X. ^f the relative energies by B97-D/B3LYP.

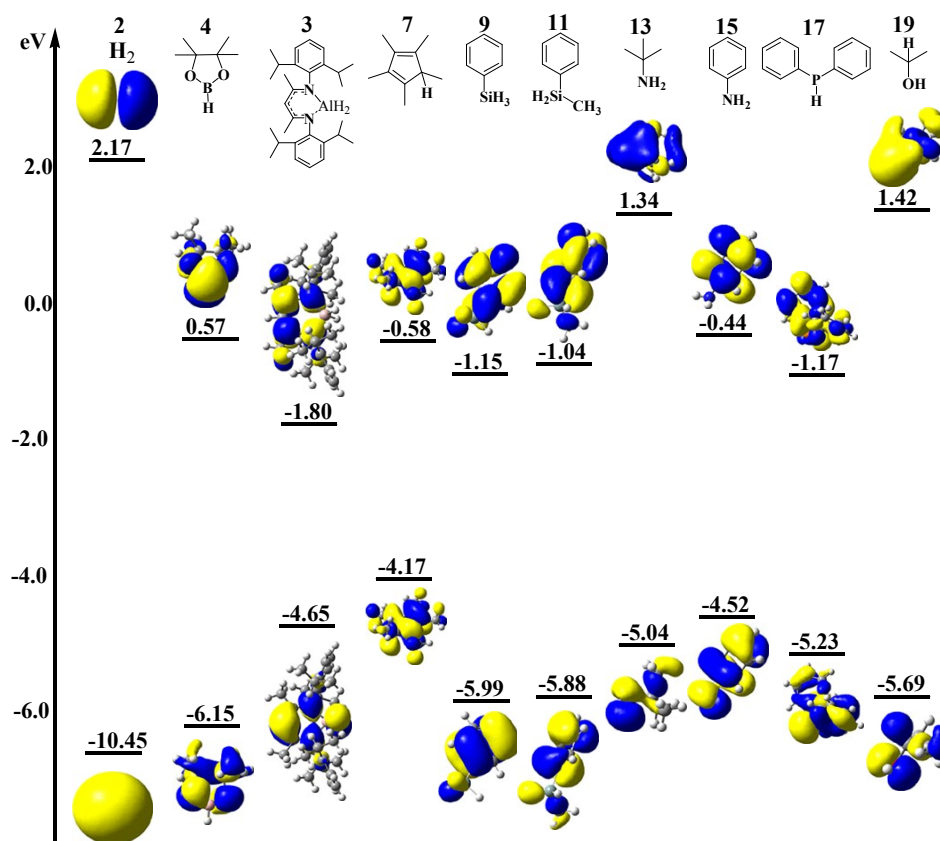


Figure S1 The selected HOMO and LUMO orbitals and their energy levels of reactants by B97-D/6-31G(d) (isovalue=0.02).

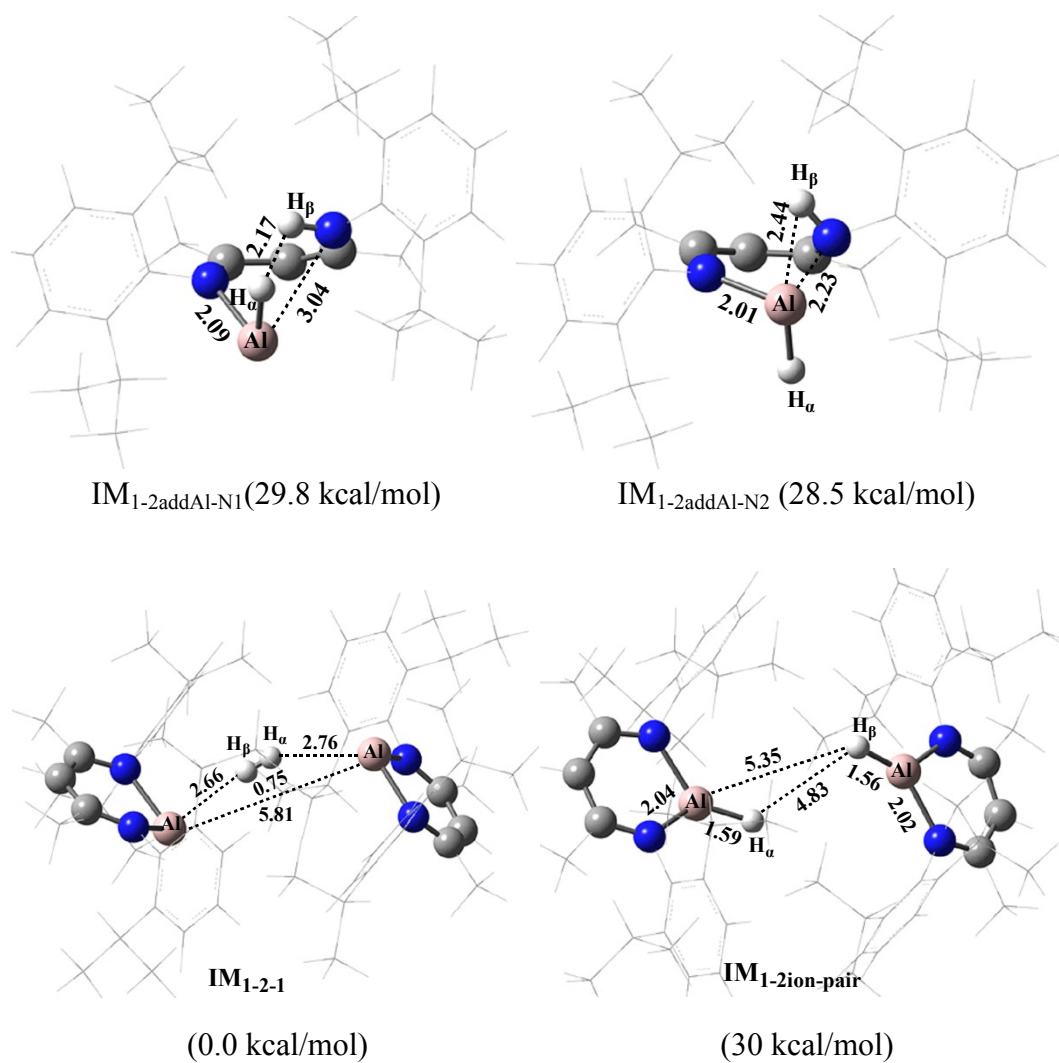


Figure S2 Selected optimized structures (Å) of species involved in the synchronous hydrogenation at both Al and N sites and the FLP mechanism.

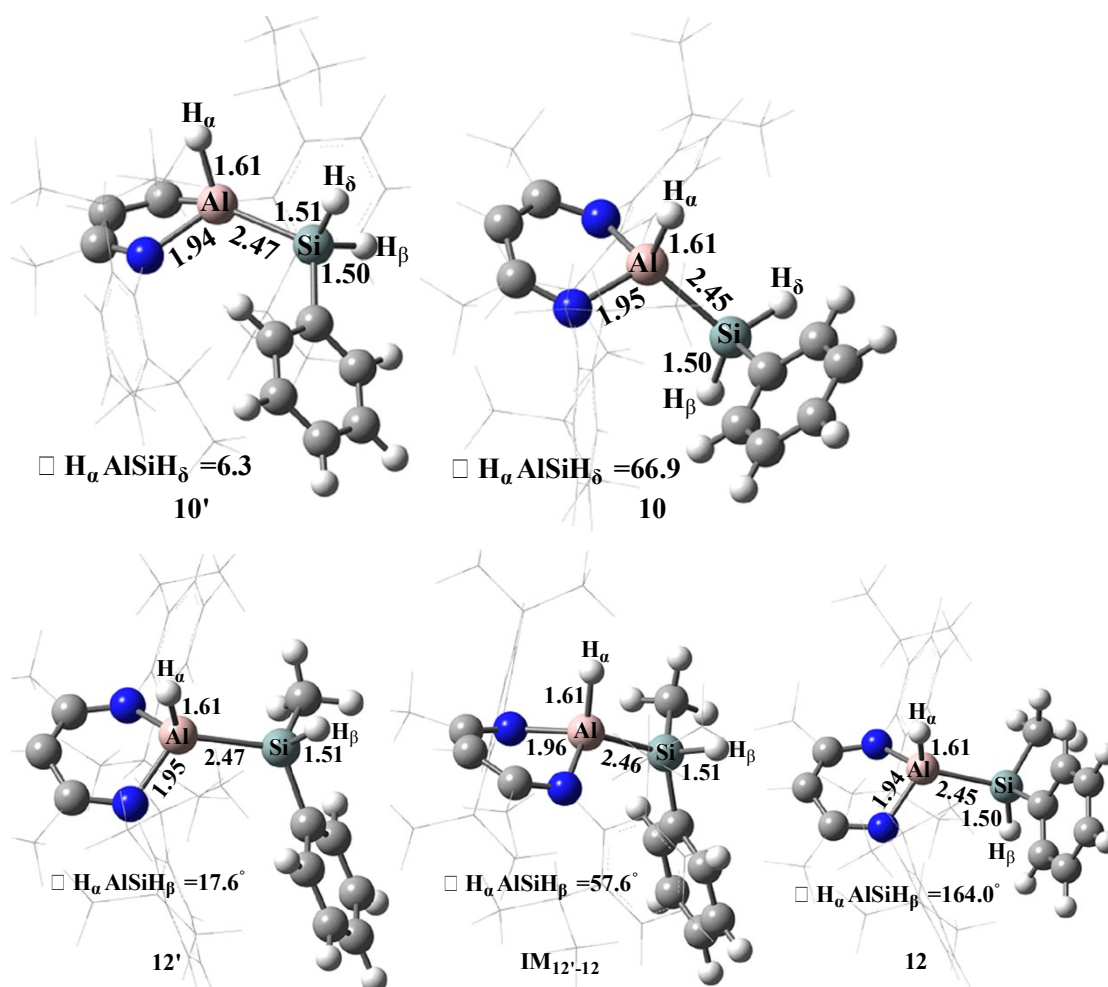


Figure S3 Selected optimized structures of species involved in the Al-Si bond coupling intra-molecular rotation steps by B97-D/6-31G(d) (the bond angle in degree and the bond length in Å).

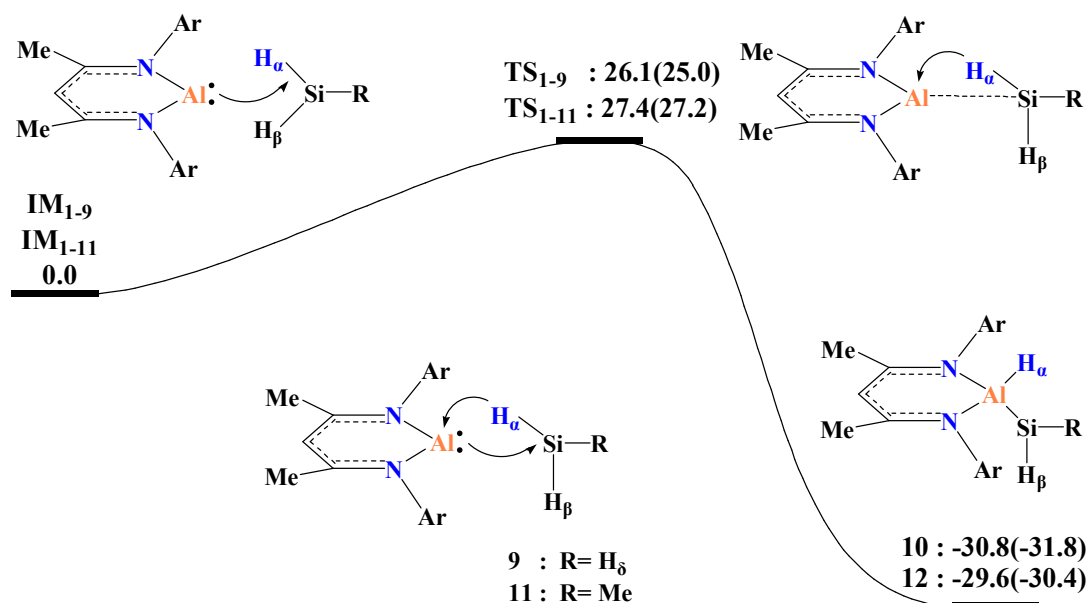


Figure S4 Relative free energy profiles and electronic energies (in parentheses) for the hydrogen transfer in the reaction of Si-H bonds (9 and 11) to the NacNacAl compound (1) (the energy in kcal/mol).

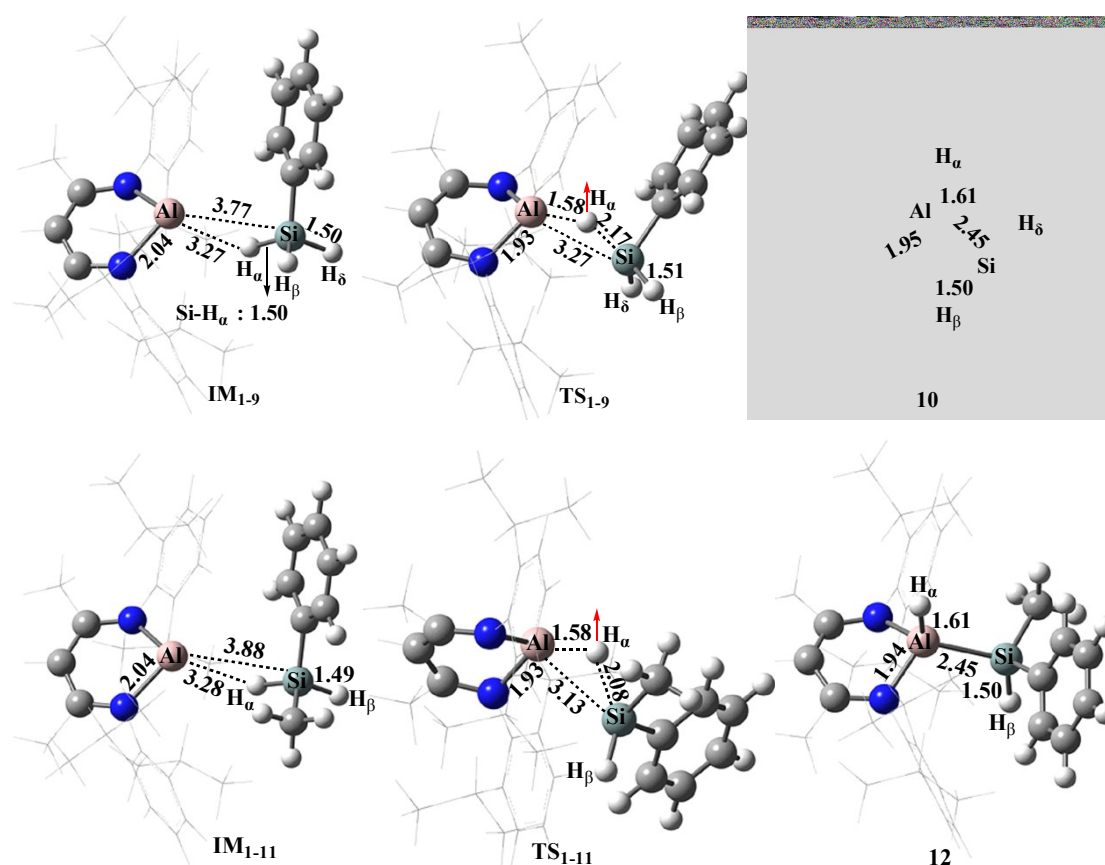


Figure S5 Selected optimized structures of species involved in the hydrogen transfer reaction of Si-H bonds in 9 and 11 to the NacNacAl (1) by B97-D/6-31G(d) (the bond length in Å).

Table S2: Predicted detailed thermodynamic data and selected charge populations and bond lengths for the oxidative additions of Si–H bonds in **9** and **11** to the NacNacAl (1).

	ΔE^a	ΔG^b	q_{Al}^c	$q_{H_a}^c$	$d_{Al-H_a}^d$	$d_{H_a-X}^d$
1+9	2.7/-0.1 ^e	-10.0/-6.4	0.19/0.20	-0.07/-0.07	—	1.49/1.49
SIM₁₋₉	0.0/0.0	0.0/0.0	0.26/0.19	-0.09/-0.07	3.27/5.73	1.49/1.49
STS₁₋₉	25.0/36.1	26.1/39.5	0.50/0.51	-0.04/-0.02	1.59/1.58	2.17/2.20
10	-31.8/-22.2	-30.8/-17.2	0.60/0.59	-0.14/-0.15	1.61/1.60	3.44/3.42
1+11	3.7/-0.1	-9.8/-6.5	0.19/0.20	-0.08/-0.09	—	1.50/1.50
SIM₁₋₁₁	0.0/0.0	0.0/0.0	0.24/0.19	-0.10/-0.09	3.28/5.56	1.49/1.49
STS₁₋₁₁	27.2/41.0	27.4/44.6	0.48/0.48	-0.04/-0.03	1.58/1.58	2.08/2.12
12	-30.4/-18.8	-29.6/-13.0	0.57/0.56	-0.15/-0.15	1.61/1.61	3.46/3.44

^a The relative energies with the zero-point energy (ZPE) correction in kcal/mol; ^b the relative Gibbs free energy in kcal/mol; ^c Mulliken charge population; ^d bond length in Å; ^e the relative energies by B97–D/B3LYP/M06–2X.

Table S3: The B97-D/6-31G(d)-predicted optimized geometries in terms of Cartesian coordinates for the intermediates (SIM), transition states (STS) and products located in the hydrogen transfer reaction of Si-H (**9** and **11**) bonds added to the NacNacAl(I) compound.

SIM₁₋₉

Al	-0.319168	0.217865	-0.686849
N	0.599641	-1.516716	-0.163047
N	-2.088725	-0.702406	-0.261453
C	0.072151	-2.757025	-0.194343
C	-2.337351	-2.021543	-0.185382
C	-1.314214	-2.989875	-0.258516
H	-1.631621	-4.031070	-0.268509
C	1.991267	-1.393261	0.188669
C	2.319608	-1.195751	1.557587
C	2.990669	-1.433794	-0.811967
C	3.678815	-1.097930	1.905109
C	4.334942	-1.313771	-0.416125
C	4.682741	-1.162078	0.929531
H	3.955894	-0.959195	2.950795
H	5.115527	-1.339068	-1.178628
H	5.732582	-1.080930	1.219739
C	-3.185756	0.217134	-0.100146
C	-4.060327	0.473641	-1.185270
C	-3.317495	0.907862	1.135368
C	-5.104208	1.396810	-0.996650
C	-4.385027	1.811947	1.278041
C	-5.278526	2.051400	0.226462
H	-5.782657	1.608079	-1.825045
H	-4.511833	2.348022	2.218771
H	-6.098004	2.761404	0.356809
C	1.228534	-1.112867	2.626568
H	0.334451	-0.685959	2.149231
C	2.642897	-1.569252	-2.290549
H	1.581141	-1.846922	-2.367547
C	-3.848028	-0.160061	-2.558204
H	-3.156834	-1.007247	-2.449263
C	-2.325223	0.669002	2.274506
H	-1.326328	0.577055	1.817202

H	0.601593	1.895007	1.964506
C	-3.763224	-2.515918	-0.008559
H	-4.233697	-2.023353	0.855794
H	-4.373210	-2.260331	-0.887780
H	-3.787530	-3.604420	0.138174
C	0.994436	-3.965133	-0.162874
H	1.655795	-3.949024	-1.043328
H	1.647925	-3.944256	0.721385
H	0.419293	-4.901237	-0.163587
Si	0.850455	3.199383	1.294521
H	-0.395960	3.694445	0.646837
C	2.264427	3.073770	0.056073
C	2.287916	3.890131	-1.098064
C	3.353233	2.199350	0.274817
C	3.362852	3.840695	-1.998320
H	1.449772	4.560596	-1.305542
C	4.431696	2.151293	-0.620570
H	3.355458	1.526368	1.134664
C	4.440662	2.973681	-1.757609
H	3.357124	4.474055	-2.888473
H	5.252488	1.457306	-0.434445
H	5.277682	2.932714	-2.458681
C	-3.176858	0.863018	-3.504230
H	-2.214885	1.204607	-3.088701
H	-2.995377	0.411260	-4.493986
H	-3.827000	1.743525	-3.636271
C	-5.152708	-0.701571	-3.181237
H	-4.927631	-1.225407	-4.124134
H	-5.663539	-1.405222	-2.503939
H	-5.856077	0.114169	-3.412990
C	-2.236689	1.832611	3.279303
H	-2.083615	2.793169	2.764284
H	-3.150646	1.908384	3.891361
H	-1.389704	1.662273	3.961518
C	-2.608388	-0.654893	3.019198
H	-2.523419	-1.520699	2.349366
H	-1.885119	-0.787216	3.840590
H	-3.622918	-0.640721	3.451306
C	1.603631	-0.203750	3.814685
H	2.392432	-0.658838	4.435762
H	1.953288	0.781836	3.474204
H	0.720288	-0.057649	4.456396
C	0.833047	-2.512780	3.153144
H	0.386118	-3.130743	2.363618

H 1.717745 -3.035255 3.553690
H 0.092837 -2.414434 3.964082
C 2.824039 -0.211800 -3.007385
H 2.185545 0.559417 -2.550573
H 3.869203 0.127912 -2.933102
H 2.560258 -0.306576 -4.074345
C 3.466103 -2.670691 -2.993164
H 3.366692 -3.640893 -2.479763
H 3.122925 -2.788583 -4.033615
H 4.536685 -2.411694 -3.021633
H 1.205398 4.173985 2.381650

STS₁₋₉

Al 0.432299 0.650798 0.798349
N -0.599400 -0.950590 1.103116
N 2.122242 -0.276340 0.624177
C -0.058416 -1.913240 1.882607
C 2.360547 -1.356350 1.393165
C 1.333139 -2.036523 2.088719
H 1.651759 -2.835668 2.754693
C -1.967836 -1.123992 0.669277
C -2.208629 -1.983634 -0.436636
C -3.018398 -0.475034 1.353618
C -3.544711 -2.232299 -0.792872
C -4.338093 -0.743921 0.945000
C -4.605136 -1.628045 -0.102816
H -3.756606 -2.900069 -1.628938
H -5.160321 -0.245421 1.460603
H -5.636198 -1.832498 -0.398868
C 3.198992 0.307486 -0.141684
C 4.096451 1.204620 0.486644
C 3.297017 -0.007505 -1.522429
C 5.127802 1.760570 -0.292259
C 4.352633 0.565641 -2.252550
C 5.266237 1.436984 -1.645227
H 5.824669 2.459999 0.172546
H 4.452565 0.339056 -3.313932
H 6.076209 1.874380 -2.232607
C -1.062277 -2.632436 -1.215245
H -0.165325 -2.020955 -1.050159
C -2.771922 0.502134 2.497483
H -1.688879 0.535188 2.703373
C 3.940329 1.625660 1.945732
H 3.218795 0.951706 2.430586

C 2.279416 -0.933931 -2.184461
H 1.301986 -0.703511 -1.729081
H 0.012678 1.815995 -0.191259
C 3.778717 -1.872364 1.526970
H 4.221403 -2.038914 0.534100
H 4.408136 -1.124485 2.032474
H 3.803087 -2.810042 2.097418
C -0.974829 -2.888400 2.598565
H -1.566225 -2.336956 3.348008
H -1.693175 -3.354340 1.911701
H -0.395515 -3.672329 3.103880
Si -0.674911 1.361446 -2.196320
H 0.162617 2.456691 -2.806490
C -2.337987 2.147004 -1.740547
C -2.417592 3.498757 -1.319065
C -3.527757 1.380380 -1.686971
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H -1.518846 4.121765 -1.337641
C -4.740928 1.941238 -1.263902
H -3.504927 0.325440 -1.969097
C -4.798696 3.287108 -0.866966
H -3.660832 5.111254 -0.580528
H -5.641759 1.323212 -1.237819
H -5.743650 3.725214 -0.536639
C 3.356763 3.055631 2.023264
H 2.375433 3.103380 1.524606
H 3.230009 3.361225 3.075190
H 4.032634 3.773209 1.529907
C 5.265110 1.540405 2.735280
H 5.083156 1.766962 3.797952
H 5.718375 0.538409 2.664220
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H -2.123777 -3.387452 -2.987987
H -1.607643 -1.678908 -3.116676
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C -0.745623 -4.063204 -0.717337
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 H -3.246375 0.756605 4.613713
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 H -0.950787 0.399374 -3.328815

SIM₁₋₁₁

Al -0.283554 0.066197 -0.745607
 N 0.645990 -1.661508 -0.237109
 N -2.041204 -0.865390 -0.305870
 C 0.130669 -2.905853 -0.276707
 C -2.282897 -2.187082 -0.255135
 C -1.254051 -3.148181 -0.347382
 H -1.564796 -4.191115 -0.374877
 C 2.021654 -1.512305 0.162395
 C 2.296762 -1.340978 1.546381
 C 3.054097 -1.490556 -0.804030
 C 3.637855 -1.196610 1.943130
 C 4.378804 -1.331913 -0.358788
 C 4.675355 -1.197139 1.001300
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 H 5.711032 -1.082083 1.328578
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 C -4.012149 0.339019 -1.191916
 C -3.257605 0.715721 1.135417
 C -5.043535 1.271742 -0.981088
 C -4.314497 1.628514 1.300115
 C -5.206509 1.902679 0.255588
 H -5.721367 1.509188 -1.802970
 H -4.434765 2.144601 2.252762
 H -6.016425 2.620269 0.403008
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 C 2.760924 -1.599262 -2.296306

H 1.704681 -1.883496 -2.416640
 C -3.818406 -0.272544 -2.577595
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 H 1.704783 -4.080941 -1.159779
 H 1.742090 -4.076196 0.603731
 H 0.501572 -5.046904 -0.249747
 Si 0.721940 3.238341 1.245321
 C 2.206140 3.116760 0.083519
 C 2.313043 3.959041 -1.046416
 C 3.257197 2.203149 0.329774
 C 3.429539 3.900591 -1.894877
 H 1.509212 4.663641 -1.275064
 C 4.378996 2.147142 -0.509995
 H 3.197381 1.509447 1.171587
 C 4.468760 2.997022 -1.623605
 H 3.487242 4.556956 -2.766504
 H 5.170394 1.426231 -0.300812
 H 5.339485 2.949421 -2.282019
 C -3.159947 0.763372 -3.518217
 H -2.188142 1.091121 -3.115107
 H -2.999467 0.327891 -4.518765
 H -3.807237 1.649653 -3.623173
 C -5.133370 -0.801940 -3.189838
 H -4.923403 -1.310352 -4.144586
 H -5.635483 -1.515703 -2.516712
 H -5.838154 0.019029 -3.397013
 C -2.195781 1.564600 3.321487
 H -2.057958 2.551425 2.855910
 H -3.113573 1.593299 3.931970
 H -1.347234 1.377539 3.996514
 C -2.507261 -0.911462 2.954245
 H -2.392737 -1.750939 2.256673
 H -1.784670 -1.051673 3.774538
 H -3.523621 -0.942242 3.381010
 C 1.405570 -0.347289 3.736003
 H 2.239833 -0.662141 4.384033

H	1.620085	0.661536	3.354568
H	0.501212	-0.296606	4.363148
C	0.937653	-2.762412	3.154660
H	0.620687	-3.464210	2.370879
H	1.860829	-3.147693	3.618826
H	0.148583	-2.733442	3.923987
C	2.957391	-0.227226	-2.980553
H	2.298953	0.531271	-2.530843
H	3.997406	0.116651	-2.864782
H	2.730839	-0.303224	-4.057462
C	3.619357	-2.681757	-2.986357
H	3.501574	-3.663164	-2.498690
H	3.323638	-2.778232	-4.043545
H	4.688828	-2.417650	-2.960431
H	1.049017	4.167824	2.379786
C	-0.829996	3.883797	0.364085
H	-1.135803	3.180663	-0.426545
H	-1.672713	3.997320	1.065371
H	-0.642822	4.868074	-0.097730

STS₁₋₁₁

Al	0.378664	0.304641	1.121119
N	-0.693767	-1.293275	0.933815
N	2.036253	-0.570842	0.628987
C	-0.173895	-2.430586	1.444380
C	2.258145	-1.801432	1.124697
C	1.214153	-2.612552	1.637216
H	1.517796	-3.549327	2.099951
C	-2.037279	-1.318741	0.408212
C	-2.246447	-1.896495	-0.874280
C	-3.105516	-0.787932	1.165374
C	-3.566345	-1.984132	-1.348299
C	-4.405781	-0.882590	0.636008
C	-4.642900	-1.489275	-0.599715
H	-3.750953	-2.440444	-2.322130
H	-5.237686	-0.470957	1.209627
H	-5.660402	-1.563712	-0.989255
C	3.111514	0.164767	0.009357
C	3.990110	0.925808	0.818053
C	3.226517	0.144021	-1.406047
C	5.015332	1.650666	0.182229
C	4.276907	0.873973	-1.989644
C	5.168494	1.619160	-1.206158

H	5.696287	2.248601	0.790527
H	4.391502	0.872365	-3.073465
H	5.973043	2.183410	-1.682298
C	-1.092178	-2.426368	-1.726615
H	-0.157618	-2.022216	-1.317008
C	-2.899488	-0.126251	2.523313
H	-1.828917	-0.180285	2.782279
C	3.833709	1.022395	2.333343
H	3.086893	0.282309	2.657828
C	2.232789	-0.639430	-2.262257
H	1.247939	-0.530047	-1.780153
H	-0.004658	1.713033	0.514723
C	3.671324	-2.347706	1.154521
H	4.144683	-2.257729	0.166330
H	4.283995	-1.758977	1.854884
H	3.679347	-3.400213	1.466800
C	-1.109472	-3.545217	1.875551
H	-1.669439	-3.210773	2.765345
H	-1.854341	-3.777123	1.104037
H	-0.550455	-4.456198	2.127326
Si	-0.425233	1.788793	-1.519727
C	-2.116883	2.516467	-1.091582
C	-2.239308	3.740755	-0.387540
C	-3.306150	1.786875	-1.337666
C	-3.488989	4.223343	0.031446
H	-1.344096	4.329611	-0.169869
C	-4.556343	2.265267	-0.923348
H	-3.252935	0.821113	-1.845879
C	-4.654441	3.488133	-0.238416
H	-3.553817	5.173775	0.567598
H	-5.454154	1.676988	-1.127515
H	-5.628355	3.861551	0.087124
C	3.297871	2.418732	2.725372
H	2.320665	2.606344	2.253373
H	3.175621	2.487821	3.818981
H	4.000100	3.204672	2.401987
C	5.151705	0.723298	3.081873
H	4.974223	0.726047	4.169218
H	5.568545	-0.256369	2.797857
H	5.913816	1.488313	2.863885
C	2.096913	-0.094480	-3.697062
H	1.907845	0.988572	-3.698051
H	3.004240	-0.294568	-4.291197
H	1.251812	-0.591033	-4.194956

C 2.565037 -2.149024 -2.309883
 H 2.502369 -2.614452 -1.317510
 H 1.849521 -2.666921 -2.968635
 H 3.579730 -2.308316 -2.711732
 C -1.197679 -1.966201 -3.196308
 H -2.064991 -2.424152 -3.698614
 H -1.287504 -0.873669 -3.265474
 H -0.294686 -2.278779 -3.744162
 C -0.993583 -3.969366 -1.679060
 H -0.769918 -4.336867 -0.668179
 H -1.939598 -4.426132 -2.013955
 H -0.189381 -4.313578 -2.350015
 C -3.290402 1.366474 2.471343
 H -2.720389 1.901910 1.699167
 H -4.359327 1.481405 2.233817
 H -3.098332 1.839123 3.448843
 C -3.680245 -0.862716 3.634837
 H -3.393260 -1.925530 3.690482
 H -3.481050 -0.393987 4.612114
 H -4.765350 -0.814161 3.448549
 H -0.588498 1.113046 -2.859695
 C 0.865994 3.191389 -1.731861
 H 0.977633 3.756381 -0.790534
 H 1.857618 2.772904 -1.973421
 H 0.588966 3.906408 -2.525262

Table S4: The B97–D/6–31G(d)-predicted optimized geometries in terms of Cartesian coordinates for the reactants, products, intermediates and transition states located for all reactions presented.

1

Al 0.00000000 0.00000000 -1.01530717
 N -1.40550306 0.00000000 0.44615883
 N 1.40550306 0.00000000 0.44615883
 C -1.25988307 0.00000000 1.78459083
 C 1.25988307 0.00000000 1.78459083

C 0.00000000 0.00000000 2.41266583
 H 0.00000000 0.00000000 3.50122083
 C -2.74630606 0.00000000 -0.08689118
 C -3.37697307 -1.23558705 -0.37425913
 C -3.37697307 1.23558705 -0.37425913
 C -4.64893206 -1.21046407 -0.97339313
 C -4.64893206 1.21046407 -0.97339313
 C -5.28416806 0.00000000 -1.27380519
 H -5.14317507 -2.15504808 -1.20880310
 H -5.14317507 2.15504808 -1.20880310
 H -6.27092606 0.00000000 -1.74177419
 C 2.74630606 0.00000000 -0.08689118
 C 3.37697307 1.23558705 -0.37425913
 C 3.37697307 -1.23558705 -0.37425913
 C 4.64893206 1.21046407 -0.97339313
 C 4.64893206 -1.21046407 -0.97339313
 C 5.28416806 0.00000000 -1.27380519
 H 5.14317507 2.15504808 -1.20880310
 H 5.14317507 -2.15504808 -1.20880310
 H 6.27092606 0.00000000 -1.74177419
 C -2.70282907 -2.57304404 -0.07793807
 H -1.80268707 -2.38087602 0.52371493
 C -2.70282907 2.57304404 -0.07793807
 H -1.80268707 2.38087602 0.52371493
 C 2.70282907 2.57304404 -0.07793807
 H 1.80268707 2.38087602 0.52371493
 C 2.70282907 -2.57304404 -0.07793807
 H 1.80268707 -2.38087602 0.52371493
 C 2.49551093 -0.00000000 2.66755084
 H 2.22350592 -0.00000000 3.73193684
 H 3.11861193 -0.88233296 2.45294088
 H 3.11861193 0.88233296 2.45294088
 C -2.49551093 -0.00000000 2.66755084
 H -2.22350592 -0.00000000 3.73193684
 H -3.11861193 0.88233296 2.45294088
 H -3.11861193 -0.88233296 2.45294088
 C 2.24882596 3.24923588 -1.39124030
 H 3.11700196 3.45180385 -2.03972630
 H 1.55385996 2.59555986 -1.94304927
 H 1.74231496 4.20548389 -1.17770434
 C 3.61296095 3.51581697 0.73904470
 H 3.94938994 3.03726500 1.67308072
 H 4.50763995 3.80483594 0.16450169
 H 3.06621495 4.43759298 0.99623165

C 2.24882596 -3.24923588 -1.39124030
 H 1.55385996 -2.59555986 -1.94304927
 H 3.11700196 -3.45180385 -2.03972630
 H 1.74231496 -4.20548389 -1.17770434
 C 3.61296095 -3.51581697 0.73904470
 H 4.50763995 -3.80483594 0.16450169
 H 3.94938994 -3.03726500 1.67308072
 H 3.06621495 -4.43759298 0.99623165
 C -2.24882596 3.24923588 -1.39124030
 H -1.55385996 2.59555986 -1.94304927
 H -3.11700196 3.45180385 -2.03972630
 H -1.74231496 4.20548389 -1.17770434
 C -3.61296095 3.51581697 0.73904470
 H -4.50763995 3.80483594 0.16450169
 H -3.94938994 3.03726500 1.67308072
 H -3.06621495 4.43759298 0.99623165
 C -3.61296095 -3.51581697 0.73904470
 H -4.50763995 -3.80483594 0.16450169
 H -3.06621495 -4.43759298 0.99623165
 H -3.94938994 -3.03726500 1.67308072
 C -2.24882596 -3.24923588 -1.39124030
 H -3.11700196 -3.45180385 -2.03972630
 H -1.55385996 -2.59555986 -1.94304927
 H -1.74231496 -4.20548389 -1.17770434

2

H 0.000000 0.000000 0.372058
 H 0.000000 0.000000 -0.372058

IM₁₋₂

Al 0.009931 -0.448564 -1.047306
 N 1.421639 -0.380780 0.401383
 N -1.383497 -0.284989 0.421945
 C 1.281780 -0.525950 1.732346
 C -1.234822 -0.458213 1.748766
 C 0.024665 -0.641186 2.353853
 H 0.027897 -0.790745 3.432021
 C 2.727888 -0.048492 -0.110524
 C 3.059974 1.320840 -0.265543
 C 3.621740 -1.072952 -0.505597
 C 4.308982 1.645717 -0.824041
 C 4.856089 -0.699869 -1.066321

C 5.203567 0.646998 -1.224952
 H 4.575902 2.697331 -0.948291
 H 5.551701 -1.479418 -1.383057
 H 6.167465 0.916648 -1.661798
 C -2.696772 0.031295 -0.080994
 C -3.642500 -1.000634 -0.298527
 C -2.985642 1.383790 -0.407913
 C -4.904501 -0.650735 -0.810137
 C -4.267803 1.684039 -0.900898
 C -5.223851 0.679917 -1.097063
 H -5.641578 -1.435205 -0.989849
 H -4.518576 2.714950 -1.151416
 H -6.211231 0.935046 -1.487767
 C 2.107901 2.439936 0.152549
 H 1.197381 1.986821 0.568826
 C 3.262690 -2.549173 -0.366349
 H 2.348087 -2.623827 0.239764
 C -3.301657 -2.468486 -0.053521
 H -2.388139 -2.516498 0.555718
 C -1.935235 2.480668 -0.219139
 H -0.952809 2.043789 -0.466586
 H -3.256252 0.087503 -3.808736
 H -2.610284 -0.015250 -3.451495
 C -2.455188 -0.444513 2.654744
 H -3.046649 0.468776 2.491833
 H -3.114417 -1.293800 2.420903
 H -2.161431 -0.501654 3.711829
 C 2.517695 -0.538944 2.614580
 H 3.217764 -1.321381 2.283236
 H 3.055712 0.418302 2.531305
 H 2.252073 -0.711025 3.666704
 C -4.410337 -3.222985 0.711129
 H -4.660597 -2.720926 1.659792
 H -5.333026 -3.293569 0.113432
 H -4.078496 -4.249495 0.935333
 C -2.995221 -3.168087 -1.398086
 H -3.880092 -3.140931 -2.054883
 H -2.166015 -2.664030 -1.919986
 H -2.719209 -4.222483 -1.228738
 C -2.131286 3.686937 -1.156769
 H -2.231136 3.363542 -2.204265
 H -3.027200 4.269430 -0.885626
 H -1.262755 4.358563 -1.078532
 C -1.859149 2.952930 1.250683

H -2.834830 3.351541 1.575370
 H -1.575113 2.131820 1.922917
 H -1.107993 3.754039 1.352373
 C 2.729896 3.326963 1.253721
 H 3.001219 2.730696 2.139637
 H 3.641630 3.825812 0.887061
 H 2.014603 4.106071 1.565034
 C 1.688076 3.292498 -1.064295
 H 2.564933 3.773443 -1.527325
 H 1.196906 2.667588 -1.826670
 H 0.986549 4.082990 -0.751956
 C 2.953766 -3.158902 -1.752639
 H 2.129546 -2.614855 -2.241217
 H 3.840323 -3.098779 -2.405321
 H 2.668416 -4.219493 -1.651671
 C 4.366864 -3.354662 0.352263
 H 5.296465 -3.372148 -0.238901
 H 4.601583 -2.922702 1.338745
 H 4.039927 -4.397248 0.495973

TS₁₋₂

Al -0.348258 -0.339966 0.000000
 N 1.077503 0.133057 1.227106
 N -1.772046 0.244294 1.190186
 C 0.902623 0.102080 2.557736
 C -1.625634 0.179333 2.526631
 C -0.373842 0.005088 3.159112
 H -0.390122 -0.073962 4.244025
 C 2.367713 0.474731 0.684314
 C 2.709343 1.844643 0.543723
 C 3.244595 -0.555415 0.267062
 C 3.963383 2.158462 -0.008182
 C 4.484572 -0.188283 -0.288608
 C 4.847994 1.155348 -0.423259
 H 4.242783 3.208221 -0.117834
 H 5.170623 -0.973600 -0.612464
 H 5.816240 1.421598 -0.852630
 C -3.056421 0.594867 0.635708
 C -4.030707 -0.412128 0.429272
 C -3.292424 1.949557 0.281171
 C -5.270274 -0.032859 -0.117617
 C -4.554385 2.277998 -0.245960
 C -5.538452 1.300293 -0.441607

H -6.030704 -0.797057 -0.288201
 H -4.767806 3.311658 -0.518449
 H -6.509466 1.578683 -0.856909
 C 1.771949 2.975674 0.962711
 H 0.841589 2.535615 1.346604
 C 2.900860 -2.034902 0.417882
 H 1.911433 -2.115326 0.892527
 C -3.763479 -1.881716 0.743331
 H -2.824389 -1.950928 1.311998
 C -2.212745 3.014595 0.477717
 H -1.239980 2.523456 0.311910
 H -0.198979 1.320825 -1.044349
 H -0.272124 0.150412 -1.519133
 C -2.855585 0.290380 3.408052
 H -3.437709 1.189927 3.161724
 H -3.516979 -0.571837 3.232379
 H -2.576297 0.319015 4.469513
 C 2.116014 0.192317 3.461676
 H 2.868542 -0.553427 3.163948
 H 2.596930 1.176933 3.367873
 H 1.835127 0.032745 4.511207
 C -4.882070 -2.515685 1.599907
 H -5.056627 -1.949514 2.528962
 H -5.833149 -2.552019 1.045110
 H -4.609738 -3.549496 1.866675
 C -3.573815 -2.682062 -0.566055
 H -4.487245 -2.633695 -1.181748
 H -2.735078 -2.275272 -1.152507
 H -3.362268 -3.740364 -0.339704
 C -2.311627 4.164729 -0.543547
 H -2.342279 3.776181 -1.573028
 H -3.208127 4.784316 -0.375556
 H -1.432558 4.818652 -0.445746
 C -2.214648 3.583562 1.915434
 H -3.196561 4.022436 2.161242
 H -1.980983 2.809533 2.659593
 H -1.453217 4.376659 2.003843
 C 2.392207 3.846394 2.079639
 H 2.647962 3.254512 2.972387
 H 3.313320 4.336410 1.724539
 H 1.682114 4.633844 2.381404
 C 1.400088 3.859029 -0.248163
 H 2.299082 4.315965 -0.693334
 H 0.885121 3.254519 -1.010684

H 0.727654 4.670853 0.072996
 C 2.811336 -2.727508 -0.959703
 H 2.033413 -2.254986 -1.579100
 H 3.773766 -2.660875 -1.492942
 H 2.559359 -3.793391 -0.833470
 C 3.921137 -2.759778 1.325187
 H 4.928749 -2.734258 0.879733
 H 3.980351 -2.291004 2.320680
 H 3.631400 -3.815392 1.453951

3

Al 0.000000 0.000000 0.875651
 N 0.000000 1.425770 -0.450353
 N 0.000000 -1.425770 -0.450353
 C 0.000000 1.265341 -1.784010
 C 0.000000 -1.265341 -1.784010
 C 0.000000 0.000000 -2.408291
 H 0.000000 0.000000 -3.496336
 C 0.000000 2.754440 0.109873
 C 1.236941 3.379446 0.409927
 C -1.236941 3.379446 0.409927
 C 1.210186 4.651709 1.008726
 C -1.210186 4.651709 1.008726
 C 0.000000 5.288402 1.306284
 H 2.155861 5.144172 1.244322
 H -2.155861 5.144172 1.244322
 H 0.000000 6.276367 1.771794
 C 0.000000 -2.754440 0.109873
 C -1.236941 -3.379446 0.409927
 C 1.236941 -3.379446 0.409927
 C -1.210186 -4.651709 1.008726
 C 1.210186 -4.651709 1.008726
 C 0.000000 -5.288402 1.306284
 H -2.155861 -5.144172 1.244322
 H 2.155861 -5.144172 1.244322
 H 0.000000 -6.276367 1.771794
 C 2.580691 2.722211 0.102362
 H 2.389980 1.750726 -0.374764
 C -2.580691 2.722211 0.102362
 H -2.389980 1.750726 -0.374764
 C -2.580691 -2.722211 0.102362
 H -2.389980 -1.750726 -0.374764
 C 2.580691 -2.722211 0.102362

H 2.389980 -1.750726 -0.374764
 H 1.362082 0.000000 1.715878
 H -1.362082 0.000000 1.715878
 C 0.000000 -2.496960 -2.669036
 H 0.881848 -3.119993 -2.456408
 H -0.881848 -3.119993 -2.456408
 H 0.000000 -2.221062 -3.731702
 C 0.000000 2.496960 -2.669036
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 H 0.881848 3.119993 -2.456408
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 H -4.359169 -3.063754 -1.120555
 C -3.378681 -2.456971 1.398307
 H -3.594390 -3.402078 1.923191
 H -2.811228 -1.798386 2.071283
 H -4.338945 -1.970799 1.158334
 C 3.378681 -2.456971 1.398307
 H 2.811228 -1.798386 2.071283
 H 3.594390 -3.402078 1.923191
 H 4.338945 -1.970799 1.158334
 C 3.415168 -3.578361 -0.877514
 H 3.664951 -4.553928 -0.429744
 H 2.871476 -3.767680 -1.816934
 H 4.359169 -3.063754 -1.120555
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 H 2.871476 3.767680 -1.816934
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C	3.681464	0.011976	-0.985953
C	4.153552	-0.976674	1.615924
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9

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12

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13

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14

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15

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IM₁₋₁₅

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16

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17

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18

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19

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