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SUPPLEMENTARY INFORMATION

Computational mechanistic elucidation of the rare earth metal-mediated cycloamidination of aminoalkenes with nitriles

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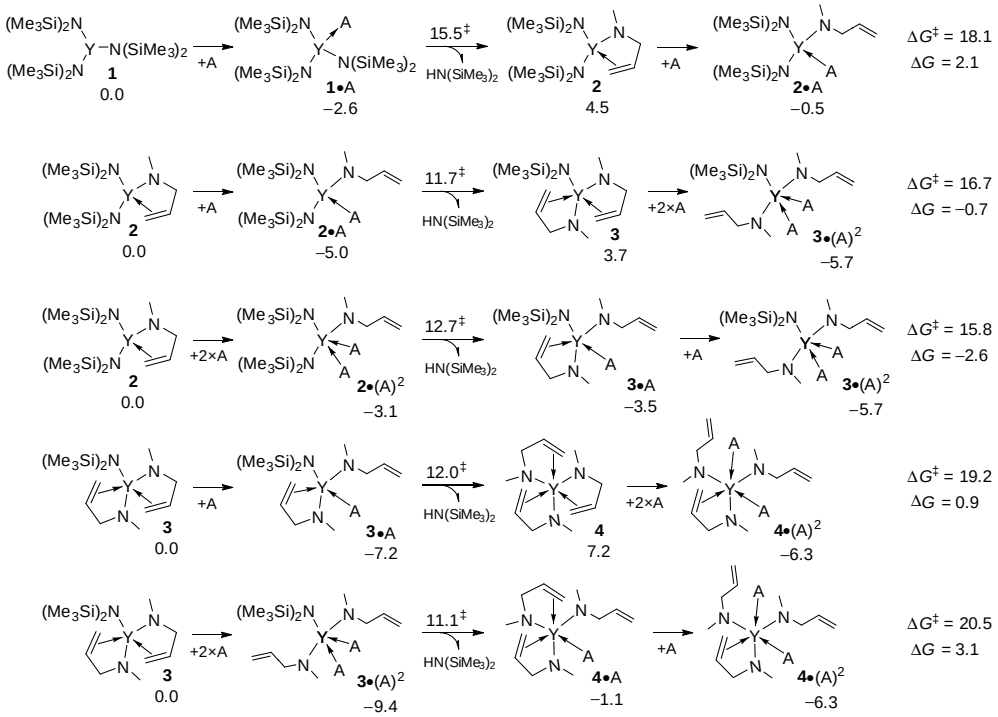
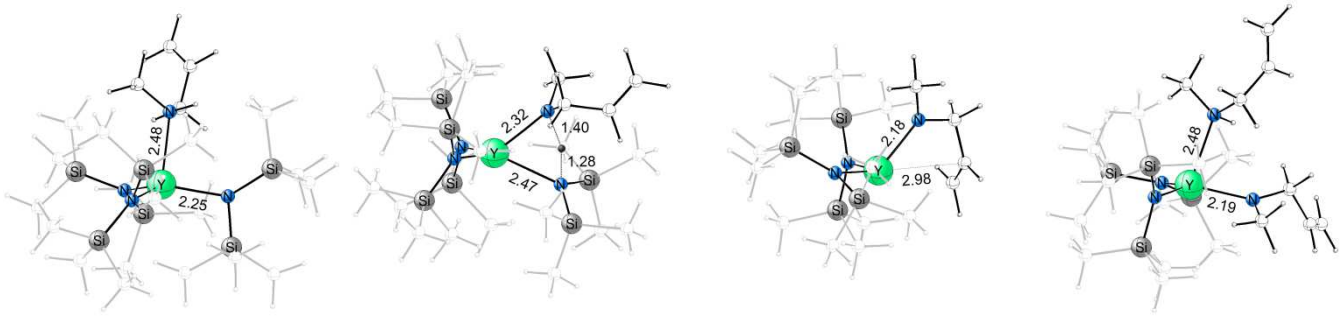


Fig.S1. Sequential Y–N(SiMe$_3$)$_2$σ-bond aminolysis at [Y{N(SiMe$_3$)$_2$}$_3$] starting material **1** by A. Free energies are given in kcal mol^{-1} relative to (reactant ±*n*×A/HN(TMS)$_2$).



1•A TS[**1**•A–**2**] **2** **2**•A

Fig. S2.Selected structural parameter (angstroms) of the optimised structures of key stationary points for Y–N(SiMe$_3$)$_2$σ-bond aminolysis at [Y{N(SiMe$_3$)$_2$}$_3$] starting material **1** by A.

The silylamide ligands are greyed out to enhance the visualisation of crucial structural aspects.

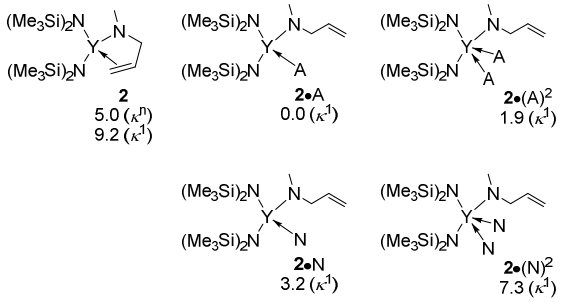


Fig. S3.Reagent association at [Y{N(SiMe$_3$)$_2$}$_2$(NRR')] compound **2**. Free energies are given in kcal mol^{-1} relative to (**2**•A±*n*×A/N).

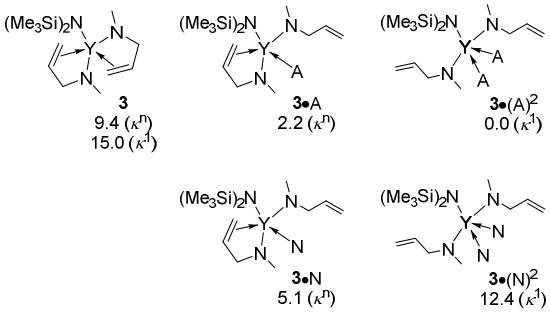


Fig.S4. Reagent association at [Y{N(SiMe$_3$)$_2$}(NRR')$_2$] compound **3**.Free energies are given in kcal mol^{-1} relative to (**3**•(A)^2±*n*×A/N).

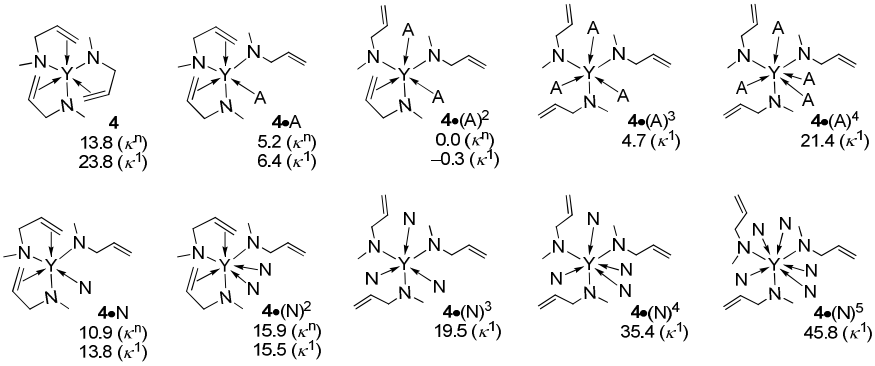
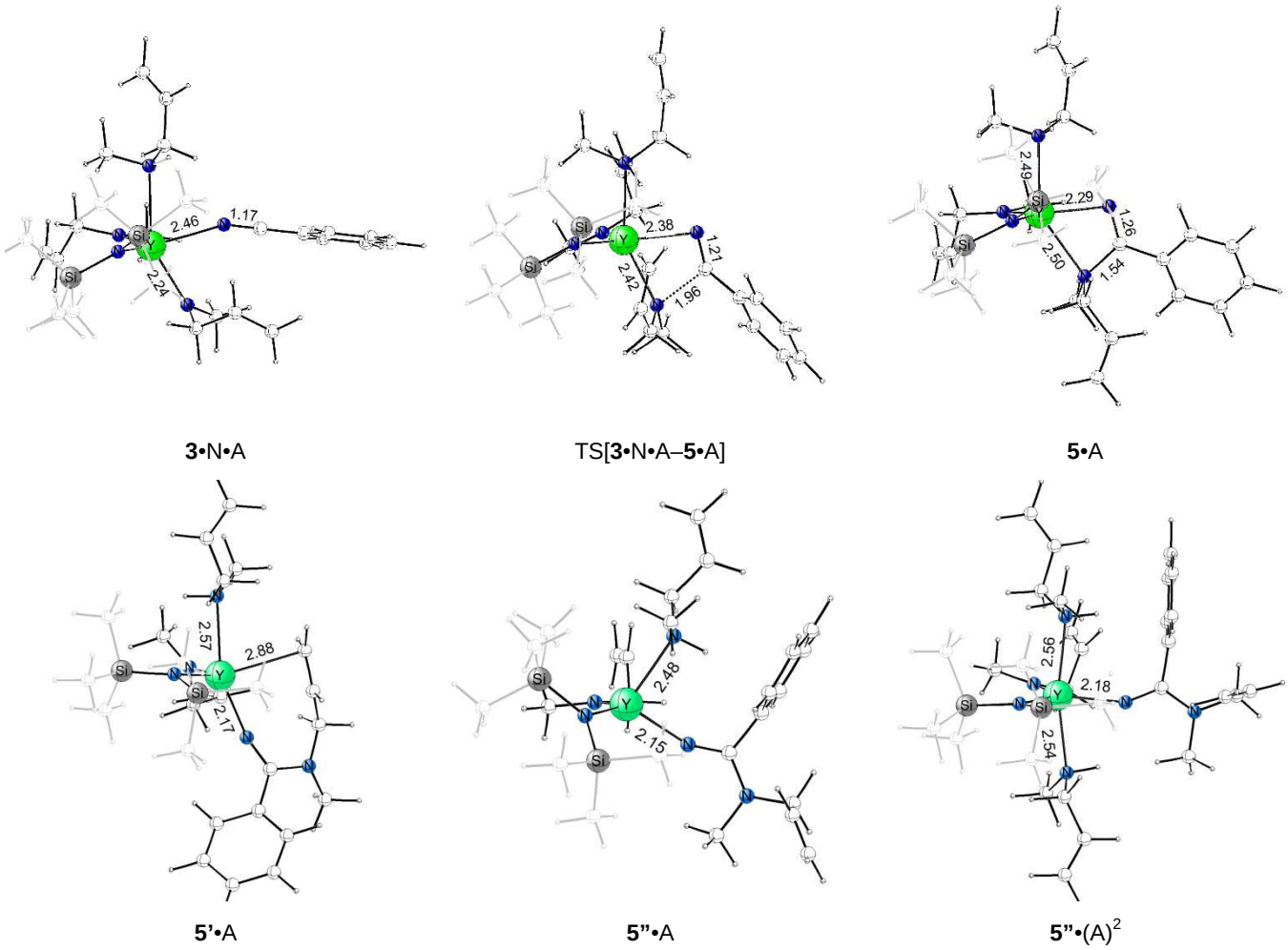


Fig.S5. Reagent association at [Y(NRR')$_3$] compound **4**.Free energies are given in kcal mol^{-1} relative to (**4**•(A)^2±*n*×A/N).

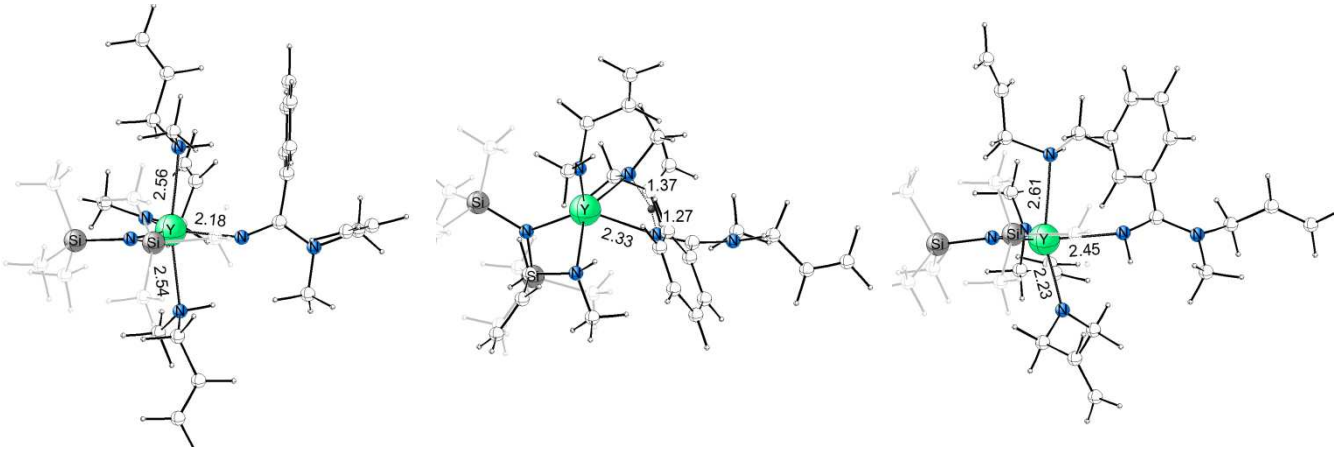


3•N•A TS[**3**•N•A–**5**•A] **5**•A

5'•A **5"**•A **5"**•$(A)^2$

Fig. S6. Selected structural parameter (angstroms) of the optimised structures of key stationary points for nitrile insertion into the Y–NRR'σ-bond at nitrile adduct **3**•N•A of the [Y{$N(SiMe_3)_2$}$(NRR')_2$] compound.

The silylamide ligand is greyed out to enhance the visualisation of crucial structural aspects.



5”•$(A)^2$ TS[**5”**•$(A)^2$–**3**•PP•A] **3**•PP•A

Fig. S7. Selected structural parameter (angstroms) of the optimised structures of key stationary points for Y–Nσ-bond aminolysis at amine adduct **5”**•$(A)^2$ of the yttrium amidinate.

The silylamide ligand is greyed out to enhance the visualisation of crucial structural aspects.

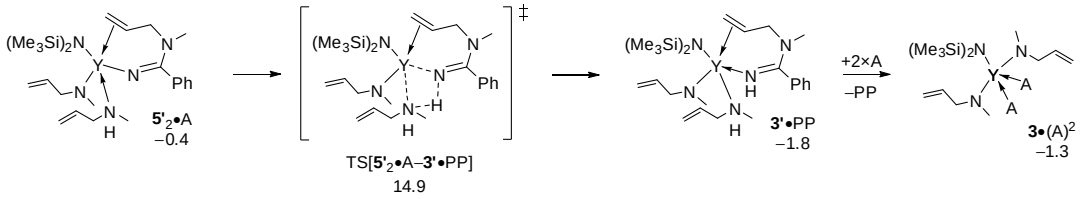
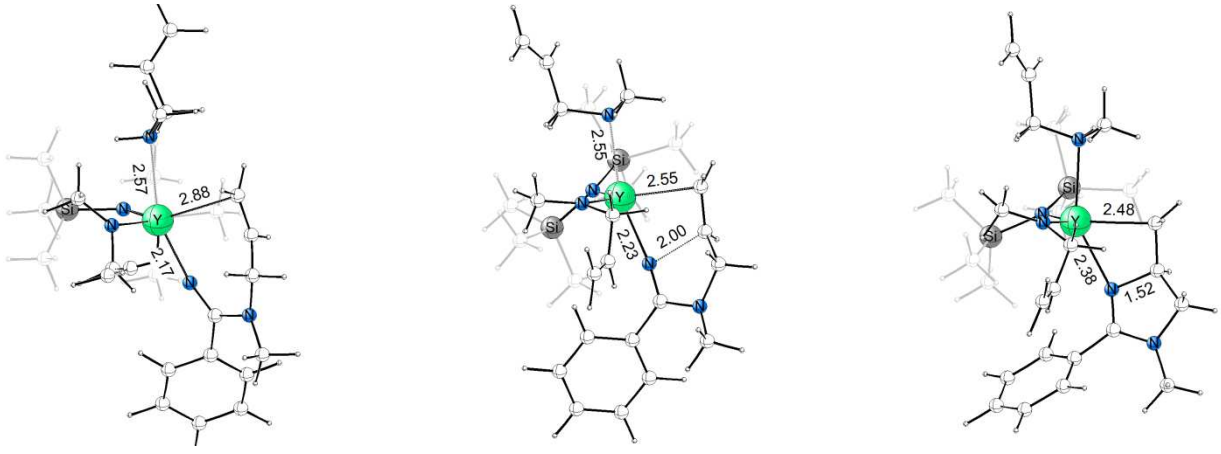


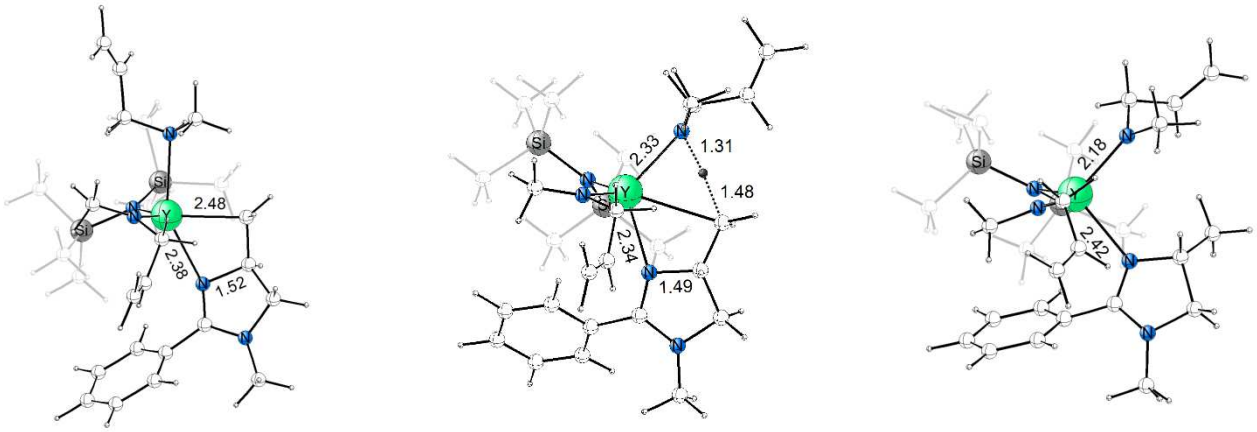
Fig.S8. Y–N bond aminolysis at amine adduct**5'**$_2$•A of the yttrium amidinate to involve species featuring a chelate Y–amidinate functionality. Free energies are given in kcal mol^{-1} relative to (**3**•$(A)^2$±*n*×A/N).



5'•A TS[**5'**•A–**6**•A] **6**•A

Fig. S9. Selected structural parameter (angstroms) of the optimised structures of key stationary points for migratory olefin insertion into the Y–N σ-bond at amine adduct **5'**•A of the yttrium amidinate.

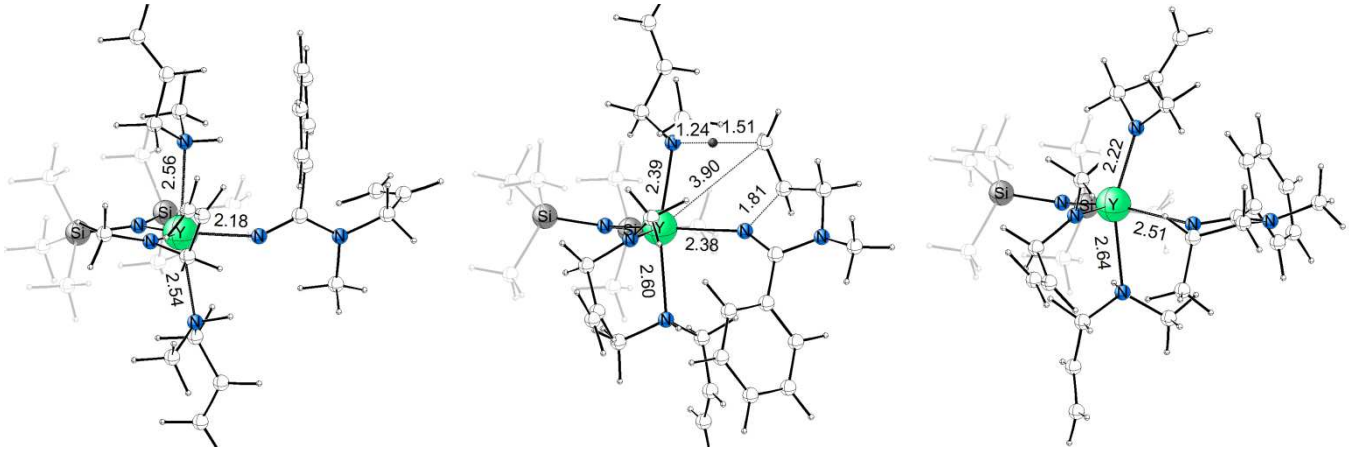
The silylamide ligand is greyed out to enhance the visualisation of crucial structural aspects.



6•A TS[**6**•A–**3**•P] **3**•P

Fig. S10. Selected structural parameter (angstroms) of the optimised structures of key stationary points for Y–C σ-bond azacycle tether aminolysis at amineadduct **6**•A of the yttrium 4-imidazolinylmethyl intermediate.

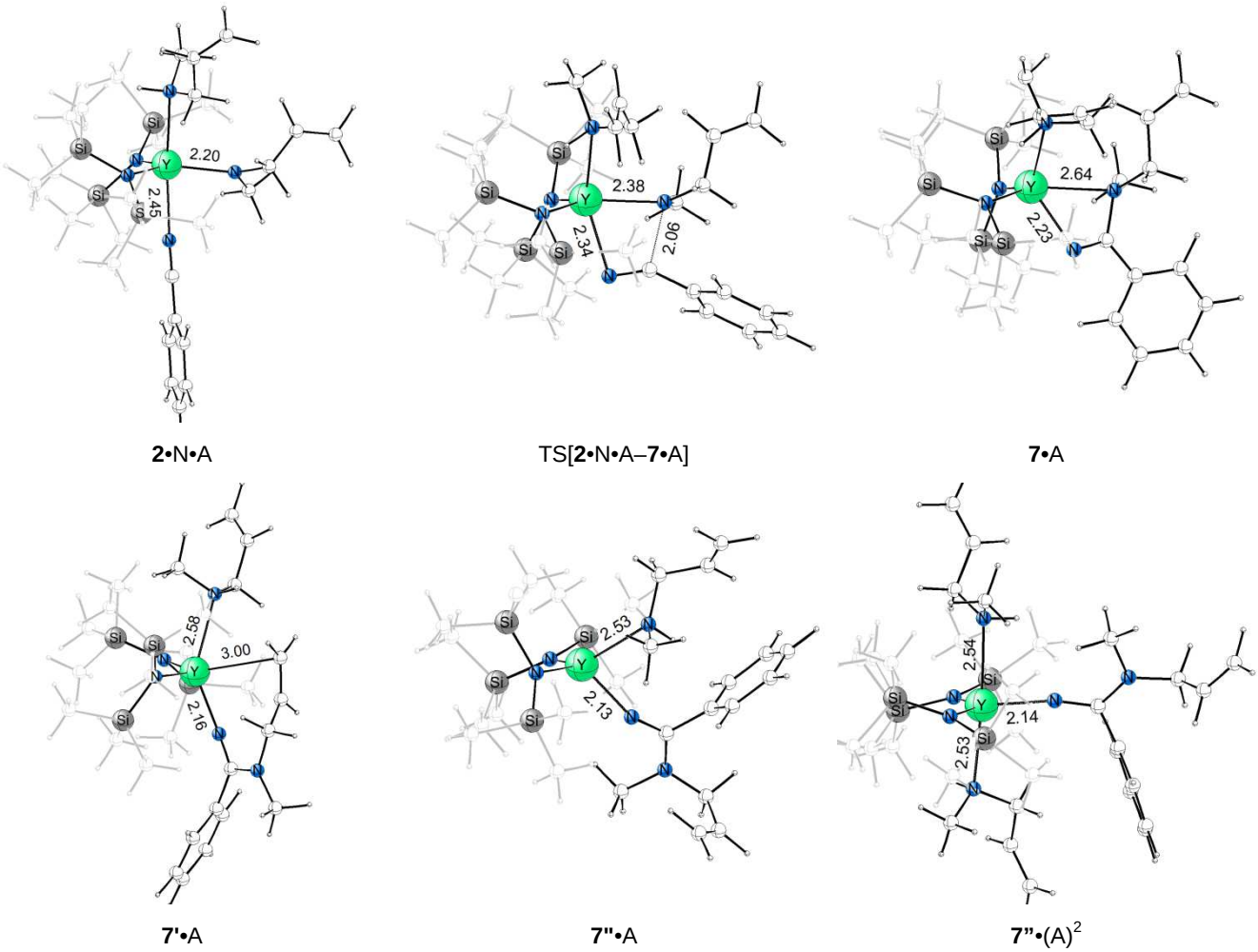
The silylamide ligand is greyed out to enhance the visualisation of crucial structural aspects.



5”•$(A)^2$ TS[**5”**•$(A)^2$–**3**•P•A] **3**•P•A

Fig. S11. Selected structural parameter (angstroms) of the optimised structures of key stationary points for non-insertive N–C ring closure with concurrent delivery of the amino proton to the olefin unit at amineadduct **5”**•$(A)^2$ of the yttrium amidinate.

The silylamide ligand is greyed out to enhance the visualisation of crucial structural aspects.



2•N•A TS[**2**•N•A–**7**•A] **7**•A

7'•A **7"**•A **7"**•$(A)^2$

Fig. S12. Selected structural parameter (angstroms) of the optimised structures of key stationary points for nitrile insertion into the Y–NRR' σ-bond at nitrile adduct **2**•N•A of the [Y{N(SiMe$_3$)$_2$}$_2$(NRR')] compound.

The silylamide ligands are greyed out to enhance the visualisation of crucial structural aspects.

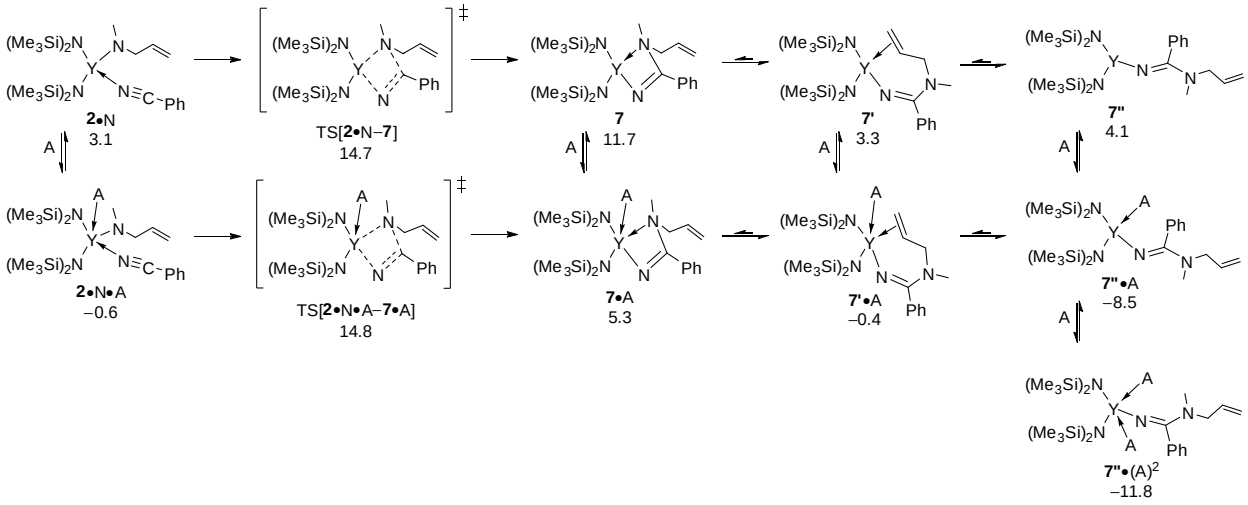
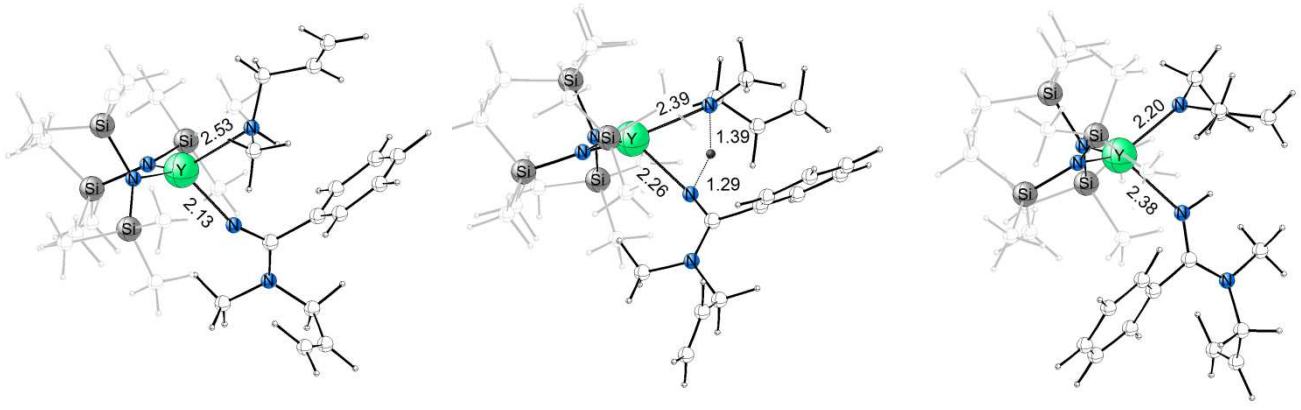


Fig.S13. Nitrile insertion into the Y–NRR' σ-bond at **2**.Free energies are given in kcal mol^{-1} relative to (**2**•A± *n*×A/N).



7”•A TS[**7”•**A–**2•**PP] **2•**PP

Fig. S14. Selected structural parameter (angstroms) of the optimised structures of key stationary points for Y–N bond aminolysis at amine adduct **7”•**A of the yttrium amidinate.

The silylamide ligands are greyed out to enhance the visualisation of crucial structural aspects.

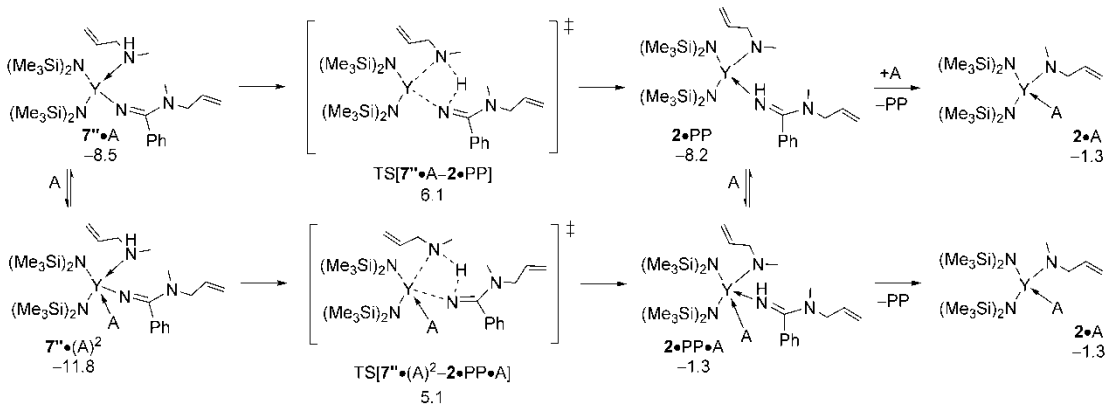
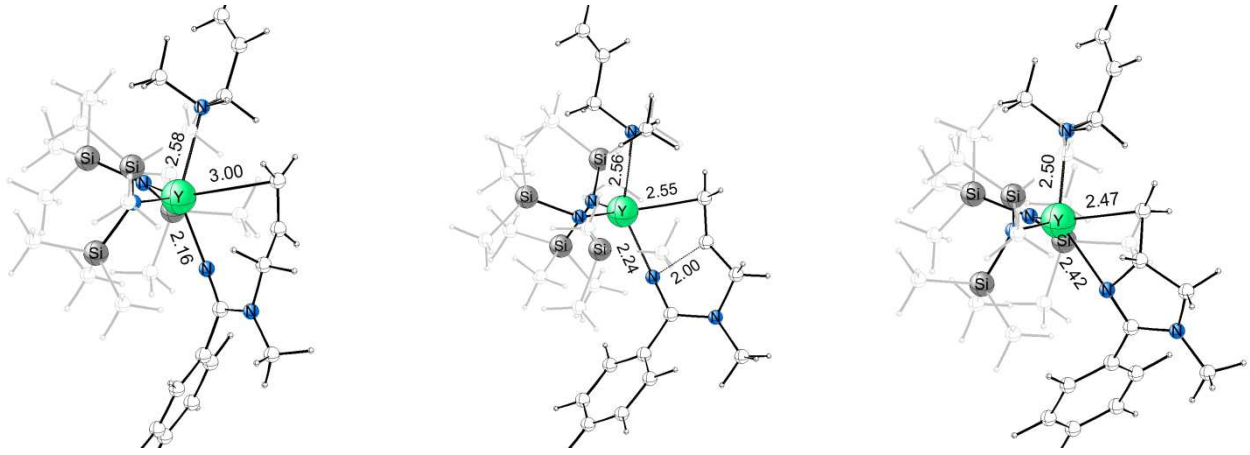


Fig.S15. Y–N bond aminolysis at amine adducts**7•**$(A)^n$ of the yttrium amidinate to involve species featuring a chelate Y–amidinate functionality.

Free energies are given in kcal mol^{-1} relative to (**2•**A±*n*×A/N).



7'•A TS[**7'•**A–**8•**A] **8•**A

Fig. S16. Selected structural parameter (angstroms) of the optimised structures of key stationary points for migratory olefin insertion into the Y–N σ-bond at amine adduct **7•**A of the yttrium amidinate.

The silylamide ligands are greyed out to enhance the visualisation of crucial structural aspects.

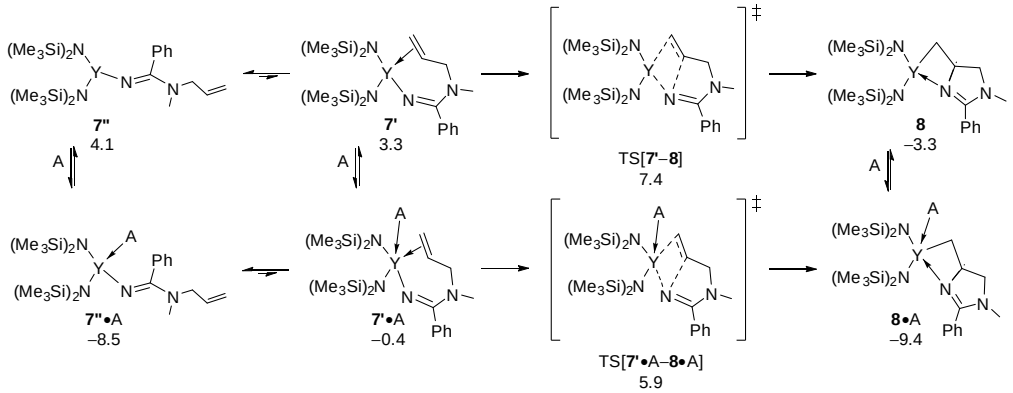
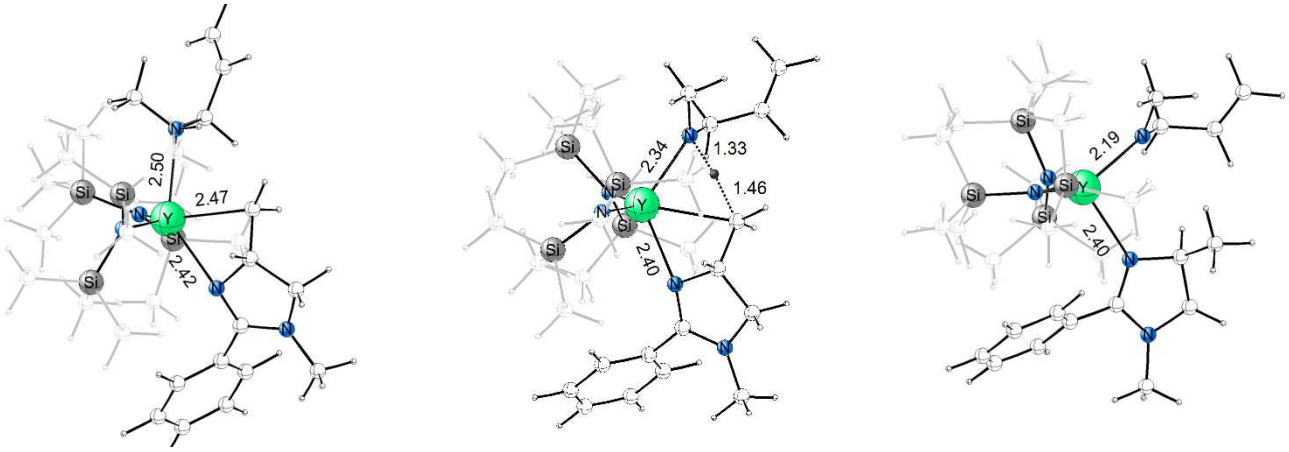


Fig. S17. Migratory C=C bond 1,2 insertion into the Y–N σ-bond at yttrium amidinate**7**. Free energies are given in kcal mol^{-1} relative to (**2**•A± *n*×A/N).



8•A TS[**8**•A–**2**•P] **2**•P

Fig. S18. Selected structural parameter (angstroms) of the optimised structures of key stationary points for Y–C σ-bond azacycle tether aminolysis at amineadduct **8**•A of the yttrium alkyl intermediate.

The silylamide ligands are greyed out to enhance the visualisation of crucial structural aspects.

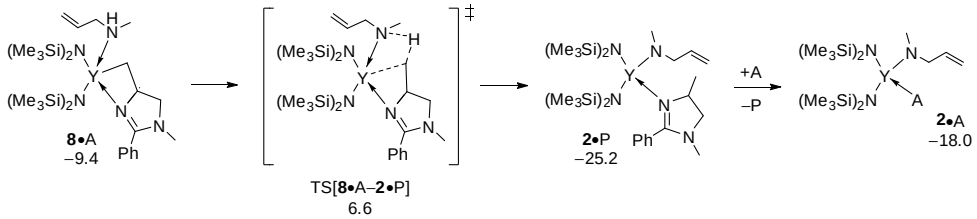
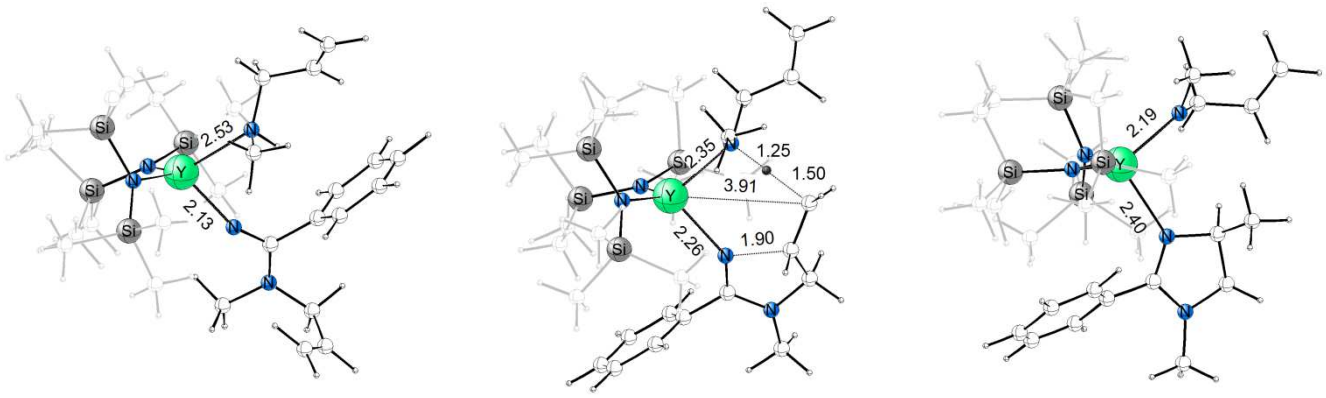


Fig.S19. Y–C σ-bond aminolysis at amine adduct **8**•A of the yttrium 4-imidazolinylmethyl intermediate.Free energies are given in kcal mol^{-1} relative to (**2**•A± *n*×A/N).



7”•A TS[**7”•**A–**2•**P] **2•**P

Fig. S20. Selected structural parameter (angstroms) of the optimised structures of key stationary points for non-insertive N–C ring closure with concurrent delivery of the amino proton to the olefin unit at amineadduct **7”•**A of the yttrium amidinate.

The silylamide ligands are greyed out to enhance the visualisation of crucial structural aspects.

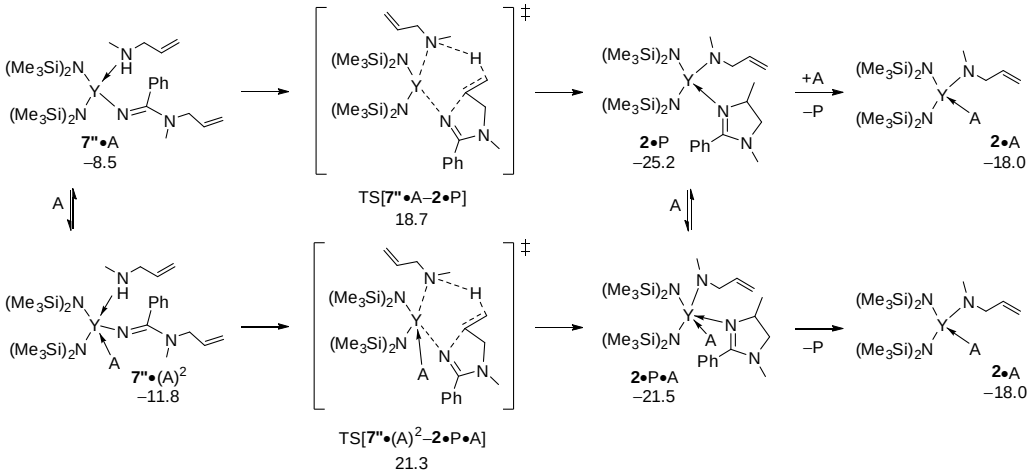


Fig.S21. N–C ring closure triggered by concomitant amino proton delivery onto the adjacent C=C linkage at amine adducts **7•**$(A)^n$ of the yttrium amidinate. Free energies are given in kcal mol^{-1} relative to (**2•**A± *n*×A/N).

Sensitivity of the predicted kinetic gap between crucial steps of the σ-insertive pathway upon the employed DFT method

Table 1. DFT assessed kinetic gap between preferable pathways for migratory C=C bond 1,2-insertion and Y–C σ-bond aminolysis traversed along the σ-insertive route

	PW6B96-D3	PWPB96-D3	M06-2X	TPSSh-D3	PBE0-D3
$\Delta\Delta G^{\ddagger}$	0.7	2.7	0.9	1.0	1.2

A positive value for the free-energy gap (given in kcal mol^{-1}) indicates that aminolysis is more demanding kinetically, hence slower than migratory 1,2-insertion.

Table 2. DFT assessed energetics (ΔG, $\Delta G^{\ddagger}$ in kcal mol^{-1}) for individual steps obtained at PW6B95-D3(SP)//BP86-D3(opt) and PW6B95-D3(SP)//PW6B95-D3(opt) levels.

nitrile insertion **3**•N →**5**	**3**•N	TS[**3**•N–**5**]	**5**	
PW6B95-D3(SP)//BP86-D3(opt)	0.0	12.1	8.2	
PW6B95-D3(SP)//PW6B95-D3(opt)	0.0	12.3	8.1	
olefin 1,2 insertion**5'**→**6**	**5"**	**5'**	TS[**5'**–**6**]	**6**
PW6B95-D3(SP)//BP86-D3(opt)	0.0	–1.0	1.7	–5.6
PW6B95-D3(SP)//PW6B95-D3(opt)	0.0	–1.1	1.9	–5.4

Cartesian coordinates (in Å) of located key structures

1•A
E = –2874.602164 a.u.
N_{imag} = 0

Y	-0.015838	0.078655	0.072792
N	-0.999624	-0.437001	1.997429
N	-1.236957	-0.115188	-1.798331
N	2.194995	-0.307921	0.191403
N	0.261611	2.502311	-0.354038
Si	2.322815	-2.000328	0.556485
Si	-2.087479	-1.775547	2.215309
Si	-0.599829	0.568334	3.347242
Si	-2.854491	0.510452	-1.814214
Si	-0.602373	-0.893869	-3.215227
C	3.436248	2.476039	0.312903
C	4.890355	0.142888	1.463647
C	4.514863	0.404645	-1.575844
C	0.755449	-2.862129	-0.090433
C	3.721721	-2.900512	-0.336968
C	2.430596	-2.335454	2.405845
C	0.966145	1.564554	2.953560
C	-1.956141	1.829875	3.729330
C	-0.231368	-0.369431	4.943801
C	-3.439331	0.935293	-0.060346
C	-3.027766	2.103077	-2.833063
C	-4.125201	-0.693316	-2.524358
C	1.290405	-0.842312	-3.201954
C	-1.184654	-2.686756	-3.339435
C	-1.093510	-0.050698	-4.837363
C	-2.721611	-2.449533	0.551639
C	-1.248843	-3.225787	3.090466
C	-3.609726	-1.314274	3.238079
H	3.327672	-1.879943	2.846728
H	1.550777	-1.906122	2.905320
H	2.452162	-3.413017	2.626993
H	4.787664	-0.641106	-1.772070
H	3.852270	0.726536	-2.392797
H	5.433194	1.009337	-1.627770
H	4.467478	0.358944	2.456138
H	5.176709	-0.917419	1.449182
H	5.812366	0.734535	1.357489
H	-2.302604	-1.952664	-0.335276
H	-2.498070	-3.522255	0.459394
H	-3.814047	-2.337234	0.491224
H	-3.348092	-1.034635	4.268689
H	-4.153597	-0.471153	2.788534
H	-4.299425	-2.170429	3.294663
H	-1.104313	-0.933146	5.301432
H	0.597318	-1.079741	4.813613
H	0.053086	0.338005	5.737688
H	-0.371907	-3.576035	2.528872
H	-0.910399	-2.961659	4.100988
H	-1.949228	-4.070816	3.179669
H	1.771795	0.930714	2.556504
H	0.790411	2.388635	2.247016
H	1.331242	2.034397	3.879129
H	-2.241516	2.397406	2.830826
H	-2.866281	1.339101	4.100039
H	-1.626266	2.550367	4.493465
H	1.641418	0.140090	-3.552975
H	1.754707	-1.012272	-2.220414
H	1.693517	-1.594984	-3.896377
H	-1.002847	-3.247024	-2.412366
H	-2.265778	-2.724188	-3.534207
H	-0.676934	-3.214094	-4.161367
H	-2.177360	-0.070021	-5.017856
H	-0.763222	0.998122	-4.863310
H	-0.610547	-0.569659	-5.679869
H	-2.447602	2.944388	-2.428120
H	-2.712304	1.953492	-3.874137
H	-4.083216	2.416932	-2.847583
H	-3.962676	-0.874719	-3.596523
H	-4.088085	-1.662659	-2.008983
H	-5.141814	-0.286924	-2.409335
H	-3.848524	0.046998	0.436594
H	-2.674263	1.335709	0.619740
H	-4.244087	1.683995	-0.118550
H	3.626394	-2.787316	-1.426374
H	4.717030	-2.538994	-0.045846
H	3.679105	-3.975697	-0.104972
H	2.998877	2.965058	-0.568314
H	2.863334	2.744219	1.213003
H	4.436049	2.919580	0.437579
H	-0.224925	-2.504551	0.260954
H	0.736945	-2.887795	-1.187635
H	0.788078	-3.906664	0.255075
Si	3.662881	0.602196	0.097614
C	0.586327	2.622512	-1.809721
H	-0.267632	2.228982	-2.373596
H	1.431511	1.939368	-1.994871
C	0.934492	4.012075	-2.252356
C	0.266808	4.671509	-3.201631
H	1.115856	2.746022	0.161228
C	-0.813224	3.420293	0.080214
H	1.792883	4.486081	-1.763388
H	-0.593275	4.222573	-3.703443
H	0.559478	5.672828	-3.518725
H	-0.971996	3.303122	1.159033
H	-1.742467	3.161331	-0.437278
H	-0.574515	4.471770	-0.138056

TS[**1**•A–**2**]
E = –2874.568805a.u.
N_{imag} = 1 (995i)

Y	-0.170945	0.215873	0.072016
N	2.043680	-0.824285	-0.298628
N	-1.245674	0.428256	-1.850010
N	-1.493738	0.042278	1.840079
N	1.605843	1.613539	0.574134
H	2.077933	0.364640	0.161587
Si	-1.567443	-0.784622	-3.048839
Si	-1.908275	2.020359	-1.995968
Si	2.995898	-0.6°80987	-1.784225
Si	2.413631	-2.1281°18	0.820827
C	-1.061458	2.792105	3.009847
C	-3.449189	1.169372	3.837611
C	-0.642655	0.291052	4.692964
C	-1.585012	-2.479986	0.383593
C	-2.680354	-2.427153	3.163904
C	-4.178359	-0.934451	0.911155
C	-1.722091	2.841922	-0.300295
C	-0.990424	3.087376	-3.251819
C	-3.747920	2.049157	-2.407980
C	2.099944	0.393992	-3.054926
C	4.640323	0.158421	-1.399484
C	3.383718	-2.356739	-2.552644
C	1.557385	-1.765071	2.463936
C	1.835904	-3.796547	0.152555
C	4.251918	-2.310692	1.206074
C	-0.267048	-2.166528	-2.957900
C	-3.272280	-1.564802	-2.820968
C	-1.503155	-0.098922	-4.808163
H	-4.760707	-0.323927	1.615240
H	-4.056162	-0.356070	-0.016007
H	-4.766404	-1.833892	0.675280
H	-0.927831	-0.750257	4.898503
H	0.433133	0.298347	4.465023
H	-0.791544	0.871644	5.616078
H	-4.069071	1.617512	3.047119
H	-3.902226	0.207726	4.114841
H	-3.507967	1.827423	4.718230
H	0.332869	-2.145130	-2.037362
H	-0.733231	-3.160219	-3.023220
H	0.439003	-2.073946	-3.794899
H	-2.288201	0.647602	-4.995688
H	-0.531261	0.370714	-5.016293
H	-1.645344	-0.915139	-5.533174
H	-3.951899	1.624145	-3.401130
H	-4.324380	1.472279	-1.670516
H	-4.130484	3.081118	-2.405054
H	-3.379535	-2.036772	-1.835281
H	-4.068883	-0.813652	-2.914640
H	-3.447788	-2.337734	-3.585168
H	-2.341627	2.340981	0.456980
H	-0.690169	2.900243	0.087671
H	-2.060029	3.886837	-0.362424
H	0.086501	3.119352	-3.031671
H	-1.106017	2.699280	-4.272761
H	-1.367064	4.121527	-3.239338
H	2.112535	-0.999727	3.024776
H	0.512886	-1.420656	2.397125
H	1.550942	-2.675615	3.081689
H	0.887677	-3.733149	-0.396110
H	2.581728	-4.221286	-0.532645
H	1.700244	-4.511680	0.978098
H	4.838067	-2.576598	0.315566
H	4.684384	-1.395444	1.633545
H	4.390226	-3.116855	1.943215
H	4.488871	1.137526	-0.922771
H	5.265639	-0.445188	-0.727886
H	5.207278	0.324465	-2.328449
H	4.041485	-2.962401	-1.914242
H	2.480858	-2.941827	-2.767474
H	3.913374	-2.191923	-3.503680
H	2.188420	-0.051858	-4.056351
H	1.027357	0.512324	-2.844705
H	2.547307	1.396482	-3.103757
H	-1.697136	-2.742570	3.542225
H	-3.200998	-1.905462	3.978014
H	-3.257607	-3.334153	2.927883
H	-0.144224	2.857405	2.412390
H	-1.826031	3.399560	2.507857
H	-0.855833	3.253548	3.987689
H	-1.351306	-2.045542	-0.601650
H	-0.662667	-2.888985	0.817617
H	-2.227214	-3.340613	0.143987
Si	-1.650937	1.015922	3.269250
C	2.165119	1.830895	1.917410
H	1.913627	2.843193	2.283701
H	1.687596	1.120320	2.612362
C	3.657385	1.646471	1.946442
C	4.539086	2.619892	2.184538
Si	-2.487883	-1.355788	1.622426
C	1.961804	2.690253	-0.346201
H	4.015602	0.642138	1.701714
H	4.209999	3.635680	2.417848
H	5.614814	2.441148	2.162979
H	1.541067	2.491483	-1.342491
H	1.556827	3.660860	-0.004143
H	3.053351	2.813479	-0.464771

2
E = –1999.567651a.u.
N_{imag} = 0

Y	0.736837	-0.213504	0.132279
N	-0.272448	0.045241	-1.815478
N	-0.700007	-0.295872	1.799918
N	2.074615	1.464076	0.511510
C	3.267861	1.475172	-0.329372
C	3.607326	0.037024	-0.636979
Si	-0.483024	1.529079	-2.675795
Si	-0.615173	-1.532944	-2.390752
Si	-2.200244	0.556311	1.960684
Si	0.103484	-1.154583	3.051624
C	1.992846	2.590361	1.419028
C	0.067903	-2.737755	-1.055046
C	0.258951	-1.957724	-4.007475
C	-2.440585	-1.948902	-2.571264
C	-3.194562	0.415073	0.367276
C	-1.870035	2.378878	2.324731
C	-3.274272	-0.121654	3.361258
C	1.778726	-1.743139	2.313521
C	-0.783274	-2.720213	3.610175
C	0.530346	-0.095316	4.549389
C	-0.627734	2.944961	-1.441316
C	-2.036838	1.504849	-3.749436
C	0.996027	1.883976	-3.798685
H	0.244467	2.959415	-0.770002
H	-1.531661	2.844928	-0.823768
H	-0.677701	3.918208	-1.951908
H	1.185866	1.047228	-4.487223
H	1.909300	2.047853	-3.206954
H	0.831613	2.786600	-4.406768
H	-2.914406	-1.311482	-3.330601
H	-2.974765	-1.788649	-1.625095
H	-2.581499	-2.997175	-2.875525
H	-2.930694	1.296813	-3.143589
H	-1.977321	0.737643	-4.536079
H	-2.184767	2.475498	-4.246536
H	-0.433899	-2.643399	-0.074267
H	1.165468	-2.697133	-0.916299
H	-0.130455	-3.768076	-1.384067
H	1.345535	-1.812960	-3.927373
H	-0.101560	-1.309286	-4.819984
H	0.073515	-2.999451	-4.309533
H	2.451157	-0.916396	2.016694
H	1.687503	-2.467908	1.483438
H	2.320536	-2.286212	3.101368
H	-1.023369	-3.360369	2.748583
H	-1.726517	-2.480580	4.119790
H	-0.163631	-3.304458	4.307296
H	-0.382197	0.287832	5.028933
H	1.134301	0.771638	4.244316
H	1.094674	-0.658043	5.308035
H	-1.284460	2.847159	1.520342
H	-1.299166	2.488931	3.258916
H	-2.805561	2.948499	2.432076
H	-2.774808	-0.056270	4.339102
H	-3.541378	-1.173852	3.186679
H	-4.210606	0.452539	3.432184
H	-3.578797	-0.608739	0.247664
H	-2.577639	0.638115	-0.514219
H	-4.056606	1.098597	0.370532
C	3.213906	-0.619637	-1.742864
H	2.877276	2.659097	2.085128
H	1.101489	2.494521	2.055135
H	1.916277	3.562303	0.888021
H	4.122782	1.930408	0.210053
H	3.142155	2.059109	-1.266063
H	4.138155	-0.505620	0.152595
H	2.689646	-0.104750	-2.550325
H	3.435141	-1.678466	-1.889877

2•A
E = –2212.497880a.u.
N_{imag} = 0

Y	0.215507	-0.114053	0.106272
N	2.320225	-0.608663	0.451981
N	1.030439	2.208390	-0.236035
N	-0.941288	-0.529051	1.971552
C	0.100153	3.225999	-0.772037
N	-0.703435	-0.050440	-1.942626
Si	-1.386399	-2.188155	1.896966
Si	-1.098594	0.508176	3.335395
Si	-2.397927	0.270669	-2.022028
Si	0.277778	-0.501939	-3.292193
C	4.217117	-1.418425	-0.951433
C	-1.505159	2.265260	2.760784
C	0.524712	0.586543	4.300481
C	-2.476440	-0.009059	4.518375
C	-2.967403	1.021470	-0.379740
C	-3.410826	-1.300794	-2.297581
C	-2.875889	1.525567	-3.354300
C	1.128105	-2.146851	-2.935920
C	1.610066	0.817846	-3.583656
C	-0.636466	-0.690066	-4.935290
C	-0.624460	-2.872973	0.284432
C	-3.247189	-2.462381	1.788497
C	-0.691790	-3.231290	3.307380
H	0.480267	-2.851116	0.261752
H	-1.001958	-2.402577	-0.641012
H	-0.897176	-3.934828	0.199376
H	-1.078824	-2.895927	4.280320
H	0.405128	-3.164617	3.344184
H	-0.962110	-4.291757	3.190524
H	-2.310310	-1.012640	4.935477
H	-3.450109	-0.013885	4.007202
H	-2.545213	0.692445	5.363661
H	-3.679211	-1.888813	0.955830
H	-3.744633	-2.133770	2.712192
H	-3.492720	-3.523862	1.633895
H	-2.511408	2.313603	2.321927
H	-0.799365	2.620021	1.995146
H	-1.461302	2.978578	3.597401
H	1.351037	0.927004	3.657581
H	0.799184	-0.408451	4.680720
H	0.462381	1.271903	5.159319
H	0.379477	-2.949132	-2.855136
H	1.699849	-2.121059	-1.996000
H	1.836208	-2.419566	-3.732630
H	2.309210	0.892988	-2.736044
H	1.149232	1.805202	-3.738907
H	2.220442	0.589556	-4.470407
H	-0.994519	0.272430	-5.324976
H	-1.499234	-1.366370	-4.854939
H	0.048943	-1.117191	-5.683436
H	-3.244803	-2.022889	-1.484500
H	-3.133856	-1.795539	-3.239640
H	-4.489453	-1.085512	-2.337072
H	-2.792805	1.108314	-4.366423
H	-2.237228	2.420557	-3.307930
H	-3.917553	1.852747	-3.213815
H	-2.553979	2.029448	-0.226669
H	-2.707082	0.415225	0.501554
H	-4.063348	1.123945	-0.390504
C	4.593404	-1.424244	-2.232083
H	3.048663	-2.319059	1.546068
H	1.690528	-1.445050	2.283488
H	3.323979	-0.745250	2.333770
H	4.267878	0.205115	0.441411
H	3.325808	0.506024	-1.029523
H	4.387862	-2.306974	-0.335866
H	4.427154	-0.557824	-2.877216
H	5.070206	-2.291872	-2.689611
C	3.539550	-0.262168	-0.263409
C	1.889292	2.715759	0.875864
H	1.226022	3.071147	1.676759
H	2.440390	1.840437	1.255675
C	2.833554	3.799908	0.452928
C	2.808123	5.050091	0.919988
H	3.583913	3.514114	-0.293256
H	2.073785	5.361008	1.666758
H	3.523604	5.802552	0.587267
C	2.611768	-1.311372	1.695744
H	1.660164	1.949635	-1.007918
H	-0.628951	3.490850	0.004237
H	-0.433635	2.785771	-1.622111
H	0.622250	4.141655	-1.088576

3•N•A
E = –1875.457346a.u.
N_{imag} = 0

Y	-0.586555	-0.165456	-0.358101
N	1.772643	0.516426	-0.519393
Si	-0.971289	0.149929	3.110584
N	0.593752	-2.065728	-0.449472
C	2.928066	0.387983	-0.631931
C	3.309309	-2.916089	1.396275
C	2.117786	-2.312035	1.459367
N	-0.642693	2.395921	-0.122761
N	-1.645908	-0.354714	1.613863
C	0.546690	1.262346	2.814420
C	-0.367846	-1.277930	4.190947
C	-2.179898	1.173634	4.146839
C	-3.091843	-2.256899	-0.082316
C	-4.594679	0.034935	1.297180
C	-3.553704	-2.332319	2.915644
H	-2.397240	-3.098291	0.054705
H	-2.774344	-1.727012	-0.997133
H	-4.089120	-2.670352	-0.296973
H	-4.466740	0.675093	0.411366
H	-4.658748	0.694591	2.175180
H	-5.558880	-0.485519	1.194199
H	-3.645291	-1.790965	3.868342
H	-2.775118	-3.099076	3.035665
H	-4.509266	-2.848242	2.735191
H	0.404193	-1.872164	3.681425
H	-1.190836	-1.956979	4.452064
H	0.065730	-0.900479	5.130113
H	-3.062545	0.581195	4.429681
H	-2.538014	2.053551	3.591661
H	-1.709848	1.530796	5.076033
H	1.204209	0.910554	2.004335
H	1.159685	1.296642	3.727769
H	0.253783	2.301129	2.596023
H	1.522655	-3.525701	-1.679248
H	1.245774	-1.937362	-2.438525
H	2.573938	-2.154307	-1.262946
H	0.002868	-2.676964	1.464134
H	0.964002	-3.890915	0.575923
H	2.036066	-1.338616	1.955946
H	3.423811	-3.884587	0.903080
H	4.206258	-2.482304	1.840455
C	1.516854	-2.431309	-1.492835
C	0.861696	-2.804747	0.785734
C	4.330920	0.236450	-0.728676
C	4.947860	0.076798	-1.986896
C	7.102109	-0.058219	-0.890603
C	5.110332	0.258240	0.447353
C	6.489596	0.107716	0.356025
H	7.092009	0.117374	1.264446
H	4.621530	0.380475	1.412724
C	6.328286	-0.070137	-2.057044
H	4.335723	0.056600	-2.887525
H	8.183647	-0.177977	-0.954078
H	6.805742	-0.199755	-3.028305
N	-1.610093	0.169565	-2.271260
C	-2.982906	0.464362	-2.642142
C	-0.715395	0.170435	-3.413834
C	-3.598360	-0.583681	-3.535468
C	-3.976677	-0.380096	-4.800013
H	-0.730810	1.137872	-3.965702
H	0.330046	0.019020	-3.083251
H	-0.931995	-0.620856	-4.157492
H	-3.585967	0.540624	-1.718608
H	-3.063739	1.451214	-3.155824
H	-3.672842	-1.585864	-3.100287
H	-3.892827	0.607595	-5.261582
H	-4.385160	-1.180930	-5.418246
Si	-3.155627	-1.179234	1.473141
C	-2.021646	2.784037	0.232452
C	-0.169343	3.057538	-1.365372
H	-0.844820	2.741474	-2.172704
H	0.826386	2.644588	-1.589587
C	-0.101785	4.554356	-1.273427
C	-0.839670	5.389082	-2.008863
H	0.601016	4.961760	-0.536754
H	-1.549746	5.011605	-2.748507
H	-0.758132	6.471953	-1.908585
H	-0.016771	2.655504	0.646062
H	-2.689813	2.459206	-0.576706
H	-2.313108	2.255931	1.147216
H	-2.142553	3.871047	0.364627

TS[**3**•N•A–**5**•A]
E = –1875.445023a.u.
N_{imag} = 1 (117i)

Y	-0.258845	0.209162	-0.380633
N	2.088889	0.461507	-0.046297
Si	-1.611111	0.622980	2.845083
N	0.800751	-1.881666	0.205489
C	2.364575	-0.709926	0.106270
C	0.548143	-0.707637	2.951570
C	0.282479	-1.983725	2.665611
N	-0.199467	2.685318	0.093368
N	-1.820956	0.098970	1.223865
C	0.134409	1.364063	3.098198
C	-1.775616	-0.758110	4.125155
C	-2.837959	1.979287	3.329898
C	-2.707298	-2.100885	-0.506048
C	-4.262002	0.567757	-0.415435
C	-4.397700	-1.405821	1.896823
H	-2.300711	-2.904753	0.125393
H	-1.942762	-1.865188	-1.264419
H	-3.567632	-2.510782	-1.056865
H	-3.651850	1.026579	-1.206904
H	-4.636361	1.377931	0.229026
H	-5.131016	0.089258	-0.891750
H	-4.755977	-0.657275	2.618079
H	-3.907445	-2.212718	2.458735
H	-5.281327	-1.832255	1.397545
H	-1.109658	-1.601857	3.895635
H	-2.801831	-1.145864	4.170441
H	-1.515599	-0.386068	5.128139
H	-3.874714	1.625100	3.229533
H	-2.730799	2.866598	2.688552
H	-2.695708	2.300941	4.372986
H	0.910613	0.981890	2.416555
H	0.476744	1.135229	4.118780
H	0.135434	2.463851	3.023362
H	0.082589	-3.377803	-1.113979
H	1.173193	-2.190993	-1.853113
H	1.840636	-3.462416	-0.798293
H	-0.225430	-3.413005	1.185979
H	1.487286	-3.354611	1.572281
H	-0.210982	-2.602330	3.422369
H	1.061844	-0.044587	2.255361
H	0.269739	-0.273143	3.912167
C	0.987665	-2.770572	-0.939894
C	0.600997	-2.701643	1.391031
C	3.461956	-1.626148	0.394074
C	4.009098	-1.657407	1.687872
C	5.388091	-3.545770	1.060548
C	3.902576	-2.546781	-0.569051
C	4.866279	-3.496199	-0.234739
H	5.199652	-4.209885	-0.988680
H	3.479198	-2.515369	-1.572644
C	4.964225	-2.619449	2.016673
H	3.674713	-0.930406	2.428242
H	6.122314	-4.307131	1.324508
H	5.373916	-2.649737	3.026865
N	-0.949442	0.452880	-2.430163
C	0.121508	1.138603	-3.141913
C	-1.981524	-0.012097	-3.333635
C	-0.306369	2.431348	-3.788462
C	-0.184300	2.710450	-5.088159
H	-1.579408	-0.722261	-4.087789
H	-2.769648	-0.533918	-2.776767
H	-2.463530	0.809750	-3.896782
H	0.949048	1.366134	-2.429207
H	0.581527	0.496506	-3.925941
H	-0.798374	3.151864	-3.127011
H	0.277222	1.997817	-5.776290
H	-0.535520	3.651947	-5.512205
Si	-3.245088	-0.655451	0.603261
C	-1.538497	3.263327	-0.147031
C	0.906471	3.508767	-0.472714
H	0.716543	3.638906	-1.547064
H	1.827707	2.917519	-0.361863
C	1.045045	4.843201	0.199025
C	0.875750	6.022412	-0.403347
H	1.297905	4.814651	1.265654
H	0.626729	6.085700	-1.465208
H	0.993383	6.964392	0.133578
H	-0.054387	2.647846	1.108455
H	-1.761746	3.206331	-1.219282
H	-2.277541	2.651829	0.382502
H	-1.611104	4.311278	0.183798

5•A
E = –1875.458676a.u.
N_{imag} = 0

Y	-0.457570	0.376313	-0.435618
N	1.798954	0.595013	-0.726198
Si	-0.495660	0.752118	2.982097
N	1.001342	-1.649952	-0.488463
C	2.128867	-0.611755	-0.598958
C	1.414866	-4.900801	0.753249
C	1.868046	-3.647405	0.840623
N	-0.486636	2.855719	-0.205528
N	-1.325842	0.116342	1.618866
C	1.286528	1.219512	2.519900
C	-0.314535	-0.465315	4.415739
C	-1.341460	2.309889	3.648871
C	-2.859735	-1.922422	0.188004
C	-4.258818	0.584219	1.260638
C	-3.320977	-1.586721	3.172632
H	-2.268469	-2.806306	0.470502
H	-2.449967	-1.540752	-0.763718
H	-3.880791	-2.265453	-0.036863
H	-4.120467	1.096230	0.296436
H	-4.286724	1.357522	2.043300
H	-5.244219	0.094729	1.236361
H	-3.456345	-0.907983	4.026973
H	-2.549363	-2.320640	3.443648
H	-4.268573	-2.127861	3.027187
H	0.078910	-1.429424	4.060626
H	-1.269197	-0.661894	4.921188
H	0.388161	-0.073123	5.166837
H	-2.377741	2.089833	3.946890
H	-1.386260	3.106455	2.890172
H	-0.820184	2.716922	4.528575
H	1.909595	0.321443	2.392827
H	1.726055	1.801620	3.344610
H	1.416339	1.808342	1.599902
H	-0.321514	-2.802568	-1.661011
H	0.837299	-1.811588	-2.578811
H	1.372229	-3.330398	-1.792509
H	1.209189	-1.741722	1.586992
H	-0.071590	-2.759905	0.926438
H	2.937371	-3.465431	0.964256
H	0.349342	-5.111784	0.628539
H	2.084022	-5.760190	0.811193
C	0.720248	-2.447450	-1.692202
C	0.971790	-2.442297	0.773074
C	3.533153	-1.099717	-0.460026
C	4.022762	-2.257923	-1.082841
C	6.227837	-1.848603	-0.170704
C	4.416316	-0.316380	0.300644
C	5.747973	-0.694678	0.457751
H	6.417170	-0.086669	1.068238
H	4.028349	0.594024	0.758198
C	5.363966	-2.621993	-0.949217
H	3.361001	-2.875624	-1.687225
H	7.272479	-2.141044	-0.057363
H	5.734434	-3.515163	-1.454208
N	-1.606825	0.412934	-2.291303
C	-3.008772	0.335057	-2.673842
C	-0.734669	0.620612	-3.438536
C	-3.322231	-0.903449	-3.474307
C	-3.669507	-0.913178	-4.764074
H	-0.980038	1.553373	-3.992264
H	0.318187	0.714358	-3.111299
H	-0.770967	-0.203569	-4.177857
H	-3.624143	0.337463	-1.757407
H	-3.314596	1.226621	-3.265191
H	-3.185536	-1.851836	-2.943147
H	-3.797030	0.018996	-5.320800
H	-3.845389	-1.841607	-5.309509
Si	-2.865729	-0.650350	1.599679
C	-1.889458	3.317729	-0.188363
C	0.327290	3.481229	-1.286804
H	-0.168905	3.247686	-2.240492
H	1.301473	2.967013	-1.281017
C	0.492565	4.963116	-1.127448
C	0.002457	5.875822	-1.969458
H	1.053773	5.290044	-0.244160
H	-0.557933	5.580567	-2.859786
H	0.153150	6.944385	-1.812441
H	-0.055362	3.085798	0.696230
H	-2.373504	2.981808	-1.115473
H	-2.403535	2.852486	0.661306
H	-1.975261	4.413369	-0.116665

5'•A
E = –1875.467259a.u.
N_{imag} = 0

Y	0.119096	0.689807	-0.404471
N	2.970056	-2.213329	-1.241759
N	0.979301	-1.301606	-0.410985
C	1.723163	-2.315951	-0.599266
Si	-3.039321	0.832011	1.007661
C	3.098840	0.188439	-0.700367
C	2.827744	1.490635	-0.955561
N	0.015868	3.241398	-0.095073
C	-3.479264	2.565208	0.371551
C	-4.117686	0.545092	2.535333
C	-3.560442	-0.416784	-0.310103
C	-1.058521	1.097090	4.292391
C	1.282280	0.307952	2.529867
C	-0.925154	-1.708690	3.025736
H	-2.114848	0.960157	4.560705
H	-0.885566	2.175600	4.158334
H	-0.451201	0.764614	5.148380
H	1.604086	1.332405	2.279262
H	1.670911	-0.392059	1.773714
H	1.777691	0.050366	3.477831
H	-0.582879	-2.280314	2.150269
H	-1.996941	-1.912356	3.164613
H	-0.394217	-2.088215	3.911956
H	-3.977907	1.335794	3.286052
H	-3.901557	-0.419538	3.016701
H	-5.180610	0.541287	2.248937
H	-3.343455	-1.440690	0.029441
H	-2.994342	-0.244604	-1.238574
H	-4.633817	-0.354796	-0.544996
H	-3.024248	2.769952	-0.609863
H	-3.147122	3.336552	1.083560
H	-4.565815	2.682690	0.241649
H	3.170366	-3.166983	-3.133288
H	3.098561	-4.254175	-1.725117
H	4.581448	-3.318653	-2.043896
H	2.697400	-0.630140	-2.644656
H	4.346697	-0.894452	-2.032799
H	3.373156	-0.106168	0.317213
H	2.615785	1.845873	-1.967060
H	2.903728	2.239245	-0.166236
N	-1.347698	0.729174	1.304847
C	3.283104	-0.877987	-1.736403
C	1.347009	-3.652708	-0.038853
C	3.482193	-3.293537	-2.079869
C	2.263521	-4.447268	0.666228
C	0.509470	-6.026527	1.203346
C	0.005556	-4.055106	-0.106331
C	-0.408273	-5.239525	0.499666
H	-1.453024	-5.545702	0.433934
H	-0.704696	-3.410169	-0.624464
C	1.843721	-5.623129	1.291490
H	3.302519	-4.124276	0.746166
H	0.182918	-6.946875	1.688891
H	2.560009	-6.223006	1.854739
C	-1.701597	1.956652	-2.959346
N	-0.859689	0.958717	-2.335258
C	-0.738489	-0.237362	-3.177671
C	0.128044	0.009470	-4.383447
C	-0.300659	0.048232	-5.648354
H	-1.749141	2.869494	-2.345429
H	-2.747201	1.602895	-3.088212
H	-1.342374	2.259723	-3.962816
H	-1.735129	-0.601665	-3.507297
H	-0.290969	-1.050932	-2.575171
H	1.176928	0.241075	-4.161261
H	-1.344549	-0.160653	-5.895620
H	0.366670	0.281152	-6.479668
Si	-0.604821	0.125682	2.734126
C	0.624718	4.109943	-1.120374
C	0.235922	3.728504	1.292441
H	1.318050	3.702291	1.495153
H	-0.256716	2.991459	1.945814
C	-0.309540	5.100973	1.552036
C	0.423648	6.154780	1.917534
H	-1.392900	5.211082	1.427425
H	1.505288	6.074182	2.050540
H	-0.025738	7.129388	2.110155
H	-1.002681	3.233791	-0.239372
H	1.708311	4.154945	-0.950745
H	0.445161	3.671434	-2.109375
H	0.234095	5.139225	-1.096309

5"•A
E = –1875.467521 a.u.
N_{imag} = 0

Y	-0.898680	-0.024104	-0.641087
N	2.615272	-2.693137	-0.006963
N	0.899045	-1.194735	-0.636505
C	2.099908	-1.437299	-0.278733
Si	-3.436515	0.723774	1.298354
C	3.949455	-3.247536	1.986275
C	4.403824	-4.388642	2.507696
N	0.489744	1.976175	-0.158888
C	-3.574350	1.649809	2.939454
C	-5.085746	-0.124146	0.945384
C	-3.197251	2.074748	-0.028773
C	-2.831246	-1.767545	3.791682
C	0.064672	-1.503407	2.874206
C	-1.869196	-3.291332	1.321317
H	-3.896101	-1.821012	3.522082
H	-2.693075	-0.901221	4.454002
H	-2.590979	-2.671940	4.371367
H	0.201744	-0.574418	3.448572
H	0.752444	-1.487624	2.016619
H	0.350143	-2.346416	3.521632
H	-1.231953	-3.271777	0.424001
H	-2.906477	-3.453425	0.992433
H	-1.564401	-4.156855	1.929123
H	-5.281917	-0.917072	1.682098
H	-5.072824	-0.595358	-0.048780
H	-5.930731	0.580277	0.977072
H	-2.938683	1.722318	-1.043858
H	-2.441020	2.812917	0.279443
H	-4.142221	2.626973	-0.143457
H	-2.609701	2.101420	3.215256
H	-3.875007	0.980384	3.757038
H	-4.320963	2.456331	2.876436
H	1.392390	-4.162581	0.922329
H	0.860674	-3.564251	-0.674756
H	2.262092	-4.687479	-0.547883
H	4.429836	-3.743862	-0.045228
H	4.550341	-2.012704	0.334251
H	3.510013	-2.484955	2.637475
H	4.830173	-5.170655	1.874388
H	4.372296	-4.584249	3.579882
N	-2.102053	-0.350099	1.211093
C	3.957461	-2.919984	0.517394
C	3.033370	-0.263645	-0.123829
C	1.733778	-3.845819	-0.075831
C	3.257781	0.313795	1.137630
C	4.483484	2.137868	0.117770
C	3.544468	0.380577	-1.263440
C	4.267653	1.568074	-1.142372
H	4.663884	2.052818	-2.035876
H	3.357435	-0.055394	-2.245692
C	3.971823	1.508359	1.255526
H	2.849230	-0.169494	2.026682
H	5.046048	3.067201	0.211260
H	4.129026	1.948746	2.241055
C	-3.167910	-0.081074	-3.134012
N	-1.820453	0.045928	-2.615423
C	-0.811608	0.095634	-3.669335
C	-0.886086	1.356374	-4.492475
C	-1.170578	1.406371	-5.796471
H	-3.885889	-0.146453	-2.301901
H	-3.292777	-0.997941	-3.747985
H	-3.475064	0.771192	-3.771930
H	-0.878519	-0.782376	-4.348610
H	0.194346	0.031801	-3.197884
H	-0.760972	2.290598	-3.932247
H	-1.329585	0.491628	-6.373122
H	-1.254682	2.351369	-6.335164
Si	-1.721390	-1.661479	2.264678
C	0.380710	2.367260	1.262389
C	0.413814	3.124353	-1.099599
H	-0.597043	3.553317	-1.033841
H	0.527373	2.708562	-2.113273
C	1.452564	4.180080	-0.857080
C	1.176410	5.451214	-0.559425
H	2.492784	3.845466	-0.926759
H	0.145663	5.804346	-0.476092
H	1.964296	6.187685	-0.398122
H	1.401821	1.515411	-0.286199
H	-0.596677	2.834924	1.435905
H	0.441606	1.465388	1.883416
H	1.169443	3.072846	1.563495

5”•(A)^2
E = –2088.411896a.u.
N_{imag} = 0

Y	-0.632239	-0.339569	-0.529396
N	3.762998	-0.874856	0.233371
N	1.538088	-0.566444	-0.475924
C	2.692110	-0.103533	-0.196651
Si	-1.155642	-0.734814	2.922392
C	5.533020	-0.212626	1.855597
C	4.737776	-0.384548	2.913252
N	-0.346185	-2.825948	-0.976174
N	-0.386757	2.185477	-0.194444
C	-1.757213	0.610849	4.112111
C	0.734011	-0.581191	2.824521
C	-3.877755	-1.734913	-0.477033
C	-4.225559	1.065696	0.709538
C	-4.614504	-1.410992	2.439363
H	-3.695404	-2.793515	-0.237318
H	-3.237895	-1.474757	-1.335934
H	-4.921103	-1.644552	-0.815200
H	-5.304753	1.060474	0.494171
H	-3.720512	1.519234	-0.157272
H	-4.055060	1.725533	1.573515
H	-4.507478	-0.868502	3.389370
H	-4.357103	-2.463853	2.621275
H	-5.676691	-1.371042	2.152697
H	-2.849770	0.571934	4.232912
H	-1.501406	1.616616	3.750680
H	-1.309900	0.489124	5.110588
H	1.077256	0.346140	2.345524
H	1.189516	-1.410225	2.264548
H	1.146039	-0.600341	3.845243
H	-1.169745	-3.240163	3.139004
H	-2.532894	-2.529113	4.024678
H	-0.898971	-2.464480	4.713619
H	2.563755	-2.493382	0.785332
H	3.642736	-2.831643	-0.588169
H	4.319144	-2.707126	1.068993
H	5.826235	-1.009181	-0.111592
H	5.175191	0.623565	-0.079692
H	6.583658	0.060162	2.000292
H	3.687174	-0.656977	2.794653
H	5.110369	-0.255865	3.929241
N	-1.860777	-0.619770	1.358613
C	5.105829	-0.357047	0.417253
C	2.927105	1.382539	-0.287612
C	3.565850	-2.305525	0.380324
C	3.007299	2.182322	0.863663
C	2.988820	4.188432	-0.496513
C	2.893424	2.007387	-1.546009
C	2.932451	3.397781	-1.650495
H	2.912305	3.867001	-2.635261
H	2.823024	1.386826	-2.440043
C	3.023737	3.575526	0.758078
H	3.048912	1.706669	1.843877
H	3.004289	5.275687	-0.576288
H	3.063933	4.184705	1.662046
C	-2.648560	0.464882	-3.136473
N	-1.398534	0.020545	-2.561606
C	-0.361078	-0.171099	-3.575607
C	0.130666	1.144250	-4.123697
C	-0.213310	1.661538	-5.307426
H	-3.401210	0.608005	-2.346561
H	-3.066185	-0.270354	-3.858684
H	-2.564453	1.426590	-3.684684
H	-0.721186	-0.808651	-4.414161
H	0.497635	-0.701283	-3.116875
H	0.741930	1.736140	-3.433647
H	-0.830539	1.097306	-6.011217
H	0.106999	2.656778	-5.619814
Si	-3.555808	-0.671153	1.059261
C	-1.009888	-3.482578	-2.112979
C	-0.418841	-3.601185	0.284087
H	-1.476588	-3.684260	0.571903
H	0.071796	-2.990710	1.058445
C	0.225813	-4.954568	0.214685
C	-0.415612	-6.109082	0.408088
H	1.297406	-4.962398	-0.016988
H	-1.483469	-6.129925	0.638304
H	0.097204	-7.070079	0.355353
H	0.647447	-2.653199	-1.182945
H	-2.080876	-3.578029	-1.892853
H	-0.904256	-2.847980	-3.000287
H	-0.606589	-4.486601	-2.324053
C	-1.471406	-2.395949	3.775557
C	-0.544474	2.665016	1.191268
C	-1.168976	3.007829	-1.158839
H	-2.229135	2.939706	-0.872649
H	-1.066040	2.525109	-2.141004
C	-0.736152	4.441552	-1.219746
C	-1.513197	5.484422	-0.917754
H	0.300406	4.608170	-1.531527
H	-2.547954	5.345254	-0.595236
H	-1.153288	6.511422	-0.991899
H	0.606807	2.267019	-0.447885
H	-1.573856	2.470630	1.516509
H	0.132324	2.105419	1.844938
H	-0.328011	3.740434	1.292348

TS[**5”**•(A)^2–**3**•PP•A]
E = –2088.383771a.u.
N_{imag} = 1 (1021i)

Y	-0.764544	-0.250321	-0.334356
N	-2.056631	-0.439875	1.507560
N	1.530903	0.131787	-0.419324
N	3.786543	0.238749	-1.090262
C	2.478475	0.681533	-1.091117
C	6.005752	1.153731	-1.646559
C	7.215187	0.623099	-1.839535
N	-0.931155	2.262697	-0.250480
N	0.628830	-2.209965	-0.162113
H	1.425733	-1.092821	-0.118692
C	-1.422105	-1.400728	4.329973
C	-3.896805	-1.771700	-0.370002
C	-4.935290	0.471501	1.404031
C	-4.248137	-2.228664	2.608424
H	-3.258183	-2.663609	-0.470273
H	-3.648636	-1.081965	-1.191737
H	-4.937487	-2.099388	-0.512835
H	-4.361958	-1.785354	3.607574
H	-3.531611	-3.058272	2.688918
H	-5.224090	-2.649368	2.321128
H	-1.086568	-2.367911	3.928233
H	-2.437056	-1.538845	4.724914
H	-0.765575	-1.146209	5.176649
H	-4.811371	1.168762	0.563473
H	-4.821727	1.047861	2.333877
H	-5.968839	0.093844	1.370484
H	-3.153574	1.338766	4.037017
H	-2.041656	2.380819	3.134632
H	-1.582395	1.772787	4.739930
H	0.829769	0.826313	1.893317
H	1.074081	-0.693664	2.755629
H	0.909715	0.818172	3.657475
Si	-1.331923	-0.041670	3.018170
H	3.836129	-1.859468	-0.715089
H	3.614588	-0.814715	0.707916
H	5.216216	-0.904209	-0.090181
H	4.231354	1.268892	-2.843000
H	4.947576	-0.351267	-2.750491
H	5.898401	2.078103	-1.070225
H	7.343305	-0.303774	-2.404032
H	8.118768	1.094198	-1.451934
C	4.727858	0.560584	-2.165651
C	2.189434	1.946813	-1.845030
C	4.131333	-0.901377	-0.254770
C	2.824565	3.150708	-1.503669
C	1.388242	4.367453	-3.025393
C	1.160297	1.964534	-2.799674
C	0.768768	3.166999	-3.390983
H	-0.026400	3.164262	-4.137337
H	0.640246	1.035868	-3.043927
C	2.417441	4.355140	-2.080800
H	3.619115	3.142154	-0.755847
H	1.072162	5.307624	-3.478437
H	2.901509	5.287519	-1.787435
C	-2.232295	0.901862	-3.229402
N	-1.614795	-0.070144	-2.356519
C	-1.607241	-1.404698	-2.958759
C	-0.659579	-1.491483	-4.125800
C	-1.031565	-1.600106	-5.404423
H	-2.171594	1.911032	-2.795178
H	-3.308985	0.688797	-3.409662
H	-1.754697	0.952946	-4.228919
H	-2.623221	-1.719896	-3.281325
H	-1.294760	-2.147993	-2.193493
H	0.401380	-1.373770	-3.879719
H	-2.084626	-1.705480	-5.677479
H	-0.307016	-1.597304	-6.220095
Si	-3.694503	-0.957182	1.323934
C	-0.080230	3.059788	0.652821
C	-2.372509	2.605523	-0.119289
H	-2.663436	2.411062	0.920930
H	-2.934737	1.893644	-0.744672
C	-2.696759	4.013647	-0.520188
C	-3.209379	4.930826	0.302891
H	-2.478270	4.278964	-1.561217
H	-3.434910	4.691390	1.344620
H	-3.433542	5.944164	-0.032024
H	-0.631455	2.465090	-1.213602
H	-0.382559	2.866919	1.689010
H	0.960052	2.743726	0.524211
H	-0.160258	4.140488	0.458573
C	-2.092233	1.507471	3.801074
C	1.155206	-2.968329	-1.290154
C	0.511863	-3.040687	1.047603
H	-0.010250	-3.989303	0.814722
H	-0.123601	-2.508218	1.773120
C	1.851210	-3.340291	1.661394
C	2.439994	-4.539423	1.675799
H	2.383254	-2.475503	2.073856
H	1.936523	-5.419786	1.268226
H	3.432592	-4.691751	2.102483
C	0.529896	0.261328	2.787018
H	0.430786	-3.711754	-1.673791
H	1.393836	-2.281608	-2.116598
H	2.083165	-3.517918	-1.038211

3•PP•A
E = –2088.407519 a.u.
N_{imag} = 0

Y	-0.603737	-0.459297	0.007670
N	-2.196900	-0.405578	1.611360
N	1.832857	-0.258210	0.106011
N	4.099878	-0.306665	-0.532891
C	2.841937	0.219979	-0.566793
C	6.374258	0.560079	-0.925641
C	7.577698	-0.004546	-1.044254
N	-0.408203	2.137212	0.170744
N	-0.039609	-2.615520	0.075864
H	2.047285	-1.141106	0.584229
C	-1.951647	-1.753660	4.335738
C	-4.014280	-1.353790	-0.509487
C	-4.824039	1.024755	1.225420
C	-4.785137	-1.764574	2.401750
H	-3.539077	-2.345892	-0.556749
H	-3.530841	-0.721895	-1.270083
H	-5.071736	-1.476489	-0.788627
H	-4.891056	-1.328188	3.405489
H	-4.270036	-2.730016	2.506861
H	-5.798621	-1.961924	2.019549
H	-1.697189	-2.710317	3.857143
H	-3.013912	-1.791089	4.609921
H	-1.368125	-1.678624	5.266620
H	-4.507994	1.693346	0.412172
H	-4.683337	1.564099	2.174238
H	-5.903067	0.844170	1.101965
H	-3.179039	1.288908	4.245235
H	-1.825980	2.183136	3.532618
H	-1.621270	1.359298	5.095740
H	0.778451	0.547354	2.522388
H	0.722230	-1.226337	2.652074
H	0.759126	-0.225073	4.107965
Si	-1.554774	-0.298244	3.197847
H	3.879028	-2.370905	-0.055073
H	4.013185	-1.265063	1.345104
H	5.450712	-1.616265	0.360451
H	4.687302	0.734451	-2.240658
H	5.351251	-0.905017	-2.116893
H	6.253974	1.482326	-0.349035
H	7.717773	-0.927873	-1.611622
H	8.466277	0.436727	-0.592698
C	5.122013	0.008271	-1.541641
C	2.622221	1.466013	-1.357864
C	4.367585	-1.456776	0.322680
C	3.268270	2.652961	-0.980662
C	2.077635	3.857704	-2.705562
C	1.706617	1.478254	-2.418666
C	1.445388	2.674003	-3.094293
H	0.737215	2.673468	-3.922277
H	1.169000	0.567165	-2.688002
C	2.989784	3.846390	-1.646165
H	3.969196	2.641216	-0.144748
H	1.861528	4.789723	-3.228861
H	3.480467	4.768706	-1.334297
C	-1.629818	0.978670	-2.896132
N	-1.200191	-0.161648	-2.118155
C	-1.346529	-1.394581	-2.908593
C	-0.263039	-1.484067	-3.949013
C	-0.416416	-1.209597	-5.249589
H	-1.421307	1.924498	-2.374491
H	-2.721392	0.959754	-3.113004
H	-1.122903	1.044762	-3.882436
H	-2.342617	-1.440559	-3.398484
H	-1.283227	-2.261921	-2.230502
H	0.737156	-1.712579	-3.563589
H	-1.401872	-0.984308	-5.665209
H	0.422984	-1.218546	-5.947306
Si	-3.863969	-0.610117	1.219388
C	0.453380	2.793166	1.168872
C	-1.798626	2.661618	0.207290
H	-2.194110	2.472606	1.213494
H	-2.398321	2.048689	-0.482970
C	-1.910331	4.110763	-0.161500
C	-2.364846	5.063588	0.655468
H	-1.583296	4.374643	-1.174467
H	-2.699410	4.825832	1.667856
H	-2.434973	6.106070	0.342787
H	-0.013206	2.324752	-0.759419
H	0.018106	2.641179	2.164754
H	1.444759	2.327470	1.145789
H	0.556431	3.876820	0.998665
C	-2.087951	1.278712	4.102058
C	0.912613	-3.226927	-0.827428
C	-0.644796	-3.605559	0.966128
H	-1.030987	-4.476621	0.391956
H	-1.507547	-3.137532	1.467891
C	0.338668	-4.094411	1.997273
C	0.964322	-5.276331	1.963374
H	0.602403	-3.372523	2.778091
H	0.724869	-6.017999	1.196688
H	1.719703	-5.554695	2.700566
C	0.345827	-0.287745	3.089861
H	0.443506	-3.992819	-1.483859
H	1.353918	-2.465494	-1.491689
H	1.753793	-3.741537	-0.310714

TS[**5'**•A–**6**• A]
E = –1875.460146a.u.
N_{imag} = 1 (157i)

Y	0.025708	0.542822	-0.062031
N	-0.808304	0.752801	-2.145566
N	0.923680	-1.491018	-0.174640
N	2.467161	-2.811236	0.920154
C	1.259505	-2.651375	0.254761
C	2.634048	-0.507867	0.178132
C	2.499564	0.870869	0.475999
N	-0.309977	3.068279	0.091422
C	0.255115	0.766096	-4.983550
C	1.729640	2.187036	-2.787471
C	-0.942290	3.287095	-3.738131
C	-3.031987	-0.783675	-0.965405
C	-1.346716	-2.012055	-3.188478
C	-3.310243	0.287633	-3.772245
H	-3.648941	0.075106	-0.661801
H	-2.406423	-1.059010	-0.102026
H	-3.710579	-1.629602	-1.151818
H	-2.859524	0.516556	-4.748442
H	-3.771337	1.211412	-3.391961
H	-4.115547	-0.443106	-3.944122
H	-1.026270	3.935219	-2.852292
H	-1.965208	3.070386	-4.078363
H	-0.439311	3.868925	-4.525538
H	-0.609268	-2.405662	-2.473925
H	-0.840303	-1.871872	-4.153993
H	-2.131634	-2.771616	-3.323548
H	-0.690553	0.459707	-5.451810
H	0.855994	-0.140876	-4.822845
H	0.790955	1.403840	-5.703241
H	2.361112	1.304928	-2.603330
H	1.756698	2.807264	-1.879246
H	2.212337	2.771896	-3.585400
Si	-0.013521	1.681819	-3.350855
H	2.429140	-3.525686	2.914122
H	2.100164	-4.744077	1.652489
H	3.762842	-4.150162	1.898047
H	2.724352	-1.167722	2.228197
H	4.150067	-1.593279	1.244308
H	2.995501	-0.752300	-0.826187
H	2.586433	1.183021	1.520350
H	2.862522	1.590177	-0.258705
C	3.052040	-1.506546	1.224818
C	0.399372	-3.834514	-0.024748
C	2.701487	-3.863486	1.897267
C	0.917890	-4.995195	-0.616966
C	-1.305400	-5.947389	-0.713520
C	-0.977906	-3.738711	0.215431
C	-1.824437	-4.793248	-0.119904
H	-2.894176	-4.709258	0.073803
H	-1.373376	-2.824304	0.657064
C	0.065489	-6.043878	-0.965424
H	1.985620	-5.060114	-0.830756
H	-1.969431	-6.768010	-0.987246
H	0.472235	-6.935816	-1.443477
C	-2.491493	0.447087	2.289480
N	-1.134482	0.355014	1.796418
C	-0.199263	0.001362	2.861985
C	-0.346600	-1.425471	3.324034
C	-0.766173	-1.802995	4.534868
H	-3.175383	0.726210	1.475997
H	-2.591627	1.213770	3.090029
H	-2.869956	-0.501697	2.719984
H	-0.294157	0.681333	3.738362
H	0.836638	0.141928	2.490050
H	-0.153903	-2.182605	2.557420
H	-0.987755	-1.065687	5.310938
H	-0.904895	-2.853071	4.796966
Si	-2.047861	-0.387730	-2.533869
C	0.255310	3.641854	1.326409
C	-1.785974	3.249228	-0.006104
H	-2.227764	2.765187	0.876183
H	-2.105662	2.686910	-0.899090
C	-2.218315	4.681991	-0.096175
C	-2.947910	5.310456	0.828797
H	-1.895988	5.226386	-0.991447
H	-3.286750	4.792236	1.729081
H	-3.244816	6.353847	0.716952
H	0.118361	3.524004	-0.720602
H	-0.134310	3.066832	2.177549
H	1.346333	3.532561	1.304450
H	-0.004392	4.703833	1.464994

6•A
E = –1875.476412a.u.
N_{imag} = 0

Y	0.404801	0.706535	0.267476
N	-0.615078	0.935334	-1.748722
N	1.512607	-1.388354	0.099058
N	2.820465	-3.038376	0.880888
C	1.576312	-2.633068	0.486231
C	2.913938	-0.796326	0.159852
C	2.855983	0.648708	0.617367
N	0.511890	3.211963	0.380342
C	-0.081443	0.985376	-4.742031
C	2.080721	1.659012	-2.727369
C	-0.255086	3.565397	-3.179115
C	-2.745836	-0.483968	-0.264932
C	-2.274169	-1.162393	-3.182856
C	-3.483018	1.524926	-2.428666
H	-2.961133	0.288199	0.485110
H	-2.025151	-1.185019	0.183352
H	-3.677033	-1.049828	-0.423052
H	-3.251687	1.954265	-3.415134
H	-3.524375	2.354890	-1.707213
H	-4.488804	1.081517	-2.487969
H	0.113797	4.171039	-2.337871
H	-1.346696	3.692279	-3.218949
H	0.168317	4.002739	-4.096380
H	-1.454347	-1.881534	-3.044496
H	-2.211489	-0.792292	-4.214819
H	-3.225643	-1.707328	-3.082001
H	-1.123201	1.109619	-5.071657
H	0.150830	-0.088782	-4.757617
H	0.561313	1.482506	-5.484855
H	2.445634	0.623469	-2.803991
H	2.385826	2.028738	-1.736100
H	2.614684	2.257058	-3.481543
Si	0.213182	1.730818	-3.029625
H	3.234078	-4.326380	2.518200
H	2.533782	-5.100778	1.064235
H	4.230386	-4.564140	1.057661
H	3.729990	-1.533951	2.071223
H	4.686302	-2.041788	0.644268
H	3.284749	-0.841311	-0.880872
H	3.080955	0.726921	1.695862
H	3.583149	1.271952	0.079618
C	3.669947	-1.843243	1.009867
C	0.380576	-3.497358	0.466058
C	3.218759	-4.320043	1.413079
C	0.041777	-4.351280	1.527639
C	-2.016713	-4.946580	0.400783
C	-0.496211	-3.373148	-0.622631
C	-1.685785	-4.096178	-0.657351
H	-2.359193	-3.983386	-1.507042
H	-0.232972	-2.688449	-1.428192
C	-1.154120	-5.068523	1.493287
H	0.686448	-4.418300	2.403184
H	-2.951726	-5.507340	0.379691
H	-1.419744	-5.714442	2.330576
C	-1.852363	1.052491	2.811910
N	-0.588306	0.667068	2.223846
C	0.265595	-0.016925	3.191143
C	-0.265445	-1.374636	3.573090
C	-0.590809	-1.764795	4.808502
H	-2.466275	1.600383	2.080536
H	-1.716023	1.721776	3.690494
H	-2.458936	0.194520	3.164740
H	0.421455	0.588579	4.112334
H	1.272240	-0.148930	2.745426
H	-0.445082	-2.046891	2.727644
H	-0.451597	-1.102850	5.667253
H	-1.009869	-2.752291	5.009664
Si	-2.184027	0.246465	-1.917801
C	1.288655	3.660211	1.552634
C	-0.892892	3.705274	0.390530
H	-1.354315	3.339882	1.318879
H	-1.401412	3.217193	-0.456809
C	-1.020217	5.196417	0.294559
C	-1.516901	5.974526	1.259100
H	-0.671210	5.649096	-0.640361
H	-1.875473	5.549964	2.199867
H	-1.595241	7.056031	1.142748
H	0.966656	3.551278	-0.473505
H	0.846083	3.202407	2.447759
H	2.316032	3.292567	1.452401
H	1.288004	4.755938	1.668832

TS[**6**•A–**3**• P]
E = –1875.455411 a.u.
N_{imag} = 1 (1053i)

Y	0.038393	0.628859	0.668514
N	-1.004263	0.960421	-1.262801
N	0.704949	-1.615320	0.800707
N	1.499732	-3.652722	0.328680
C	0.430188	-2.805871	0.337343
C	2.135593	-1.557222	1.211128
C	2.742871	-0.225417	0.783699
N	1.613759	2.322210	0.929069
H	2.211551	1.152381	0.931829
C	0.944022	-0.892817	-2.560203
C	0.038903	1.570787	-4.017891
C	-2.008093	3.190775	0.352242
C	-3.927127	0.994482	-0.670726
C	-2.777630	3.071046	-2.573597
H	-1.212251	3.890599	0.055928
H	-1.693905	2.710623	1.294510
H	-2.902714	3.784959	0.593175
H	-3.042190	2.470184	-3.455531
H	-1.930652	3.716924	-2.844185
H	-3.637691	3.719204	-2.344838
H	0.843792	2.187804	-3.590654
H	-0.772669	2.246186	-4.317956
H	0.431916	1.092536	-4.928394
H	-3.769839	0.373690	0.222826
H	-4.163753	0.314143	-1.502139
H	-4.804196	1.634505	-0.491083
H	-2.795670	-0.090148	-3.794455
H	-2.289001	-1.500857	-2.843279
H	-1.618939	-1.234667	-4.472257
H	0.691155	-1.796208	-1.992831
H	1.794412	-0.405410	-2.060572
H	1.292130	-1.208737	-3.555588
Si	-0.536725	0.270016	-2.771439
H	1.947930	-5.129627	-1.131710
H	0.571419	-5.488427	-0.044193
H	2.238697	-5.586498	0.567478
H	3.279790	-2.686669	-0.311320
H	3.363475	-3.411713	1.324064
H	2.151659	-1.624498	2.315341
H	3.041964	-0.281749	-0.278032
H	3.659281	-0.027396	1.362479
C	2.715021	-2.871121	0.621256
C	-0.925737	-3.121236	-0.147954
C	1.564728	-5.030439	-0.100236
C	-2.012467	-2.495631	0.488608
C	-3.532642	-3.489492	-1.108057
C	-1.157496	-3.917468	-1.280891
C	-2.456147	-4.099312	-1.755917
H	-2.624708	-4.702206	-2.648336
H	-0.322650	-4.356337	-1.824820
C	-3.306596	-2.684384	0.011570
H	-1.826488	-1.850395	1.350194
H	-4.545750	-3.627534	-1.486706
H	-4.141217	-2.191529	0.509340
C	-2.479201	0.746647	2.998872
N	-1.138491	0.540405	2.495693
C	-0.212015	0.118381	3.543629
C	-0.474182	-1.285943	4.022309
C	-0.966836	-1.600996	5.223370
H	-3.132600	1.108701	2.193474
H	-2.506335	1.501872	3.813177
H	-2.936447	-0.175184	3.410829
H	-0.229759	0.816065	4.408966
H	0.830549	0.162873	3.151765
H	-0.307059	-2.069130	3.275508
H	-1.156212	-0.830603	5.975341
H	-1.197234	-2.630344	5.502430
Si	-2.375264	1.995193	-1.074659
C	1.868117	3.071443	2.151160
C	1.954424	3.049167	-0.299431
H	1.398505	4.004897	-0.352488
H	1.605826	2.446278	-1.158638
C	3.429749	3.312156	-0.442643
C	3.987161	4.524958	-0.468974
H	4.065065	2.420850	-0.488849
H	3.374646	5.428461	-0.411648
H	5.065690	4.664210	-0.555502
C	-1.937541	-0.732342	-3.546117
H	1.184295	3.934469	2.248089
H	1.699318	2.420256	3.021867
H	2.902944	3.455825	2.211230

3•P
E = –1875.506757 a.u.
N_{imag} = 0

Y	0.070653	0.737916	0.287740
N	-1.069843	0.898575	-1.644667
N	1.592579	-1.117377	0.609020
N	2.096693	-3.127726	1.509303
C	1.166438	-2.316007	0.919324
C	3.006785	-1.002493	1.052980
C	3.902599	-0.345554	0.015937
N	1.518803	2.367329	0.393402
H	4.928858	-0.254046	0.398659
C	-2.593085	2.719299	0.065404
C	-4.005505	0.366857	-1.332433
C	1.408737	-0.269738	-2.751955
C	0.053307	1.955003	-4.249833
C	-1.282661	-0.790834	-4.115890
H	1.382471	-1.251470	-2.258793
H	2.017433	0.395744	-2.120202
H	1.957354	-0.396281	-3.697755
H	-2.278366	-0.397410	-4.370585
H	-1.431740	-1.720037	-3.546044
H	-0.777433	-1.053436	-5.057848
H	-3.837806	-0.305694	-0.479312
H	-4.061296	-0.253877	-2.239530
H	-4.985092	0.849178	-1.194101
H	0.628489	2.727889	-3.718990
H	-0.869504	2.421342	-4.618943
H	0.643641	1.640926	-5.124513
H	-3.170893	2.219989	-3.879245
H	-2.344382	3.572230	-3.072921
H	-4.060023	3.245968	-2.736952
H	-1.907864	3.570557	-0.068948
H	-2.284305	2.184008	0.980141
H	-3.594034	3.130063	0.267084
Si	-2.617325	1.641328	-1.493045
H	2.679122	-5.002532	0.733462
H	1.021916	-4.921677	1.397995
H	2.422846	-4.951768	2.501787
H	4.009088	-2.925284	0.631735
H	3.948307	-2.525762	2.373329
H	3.001809	-0.377456	1.963652
H	3.921979	-0.937628	-0.909508
H	3.528379	0.660897	-0.216928
C	3.399535	-2.451555	1.424994
C	-0.237597	-2.718665	0.716608
C	2.051682	-4.578202	1.537187
C	-0.870517	-2.426279	-0.501724
C	-2.943676	-3.332533	0.346775
C	-0.971521	-3.320622	1.751159
C	-2.317708	-3.624823	1.562491
H	-2.887706	-4.069886	2.378145
H	-0.501453	-3.492895	2.718451
C	-2.219361	-2.729250	-0.682252
H	-0.304955	-1.965544	-1.310117
H	-4.000781	-3.560212	0.208422
H	-2.701950	-2.479014	-1.625951
C	-2.307422	-0.143669	2.375857
N	-0.963828	0.359382	2.186638
C	-0.269750	0.557445	3.454844
C	0.163293	-0.760763	4.045431
C	-0.436715	-1.379329	5.068141
H	-2.780428	-0.344426	1.402070
H	-2.957700	0.579060	2.915469
H	-2.340300	-1.092083	2.948403
H	-0.903991	1.101363	4.187675
H	0.619890	1.192089	3.287391
H	0.978616	-1.267570	3.516787
H	-1.258416	-0.904683	5.610199
H	-0.127690	-2.368785	5.411147
Si	-0.297271	0.481933	-3.119875
C	2.427744	2.689034	1.474330
C	1.569893	3.366005	-0.678129
H	1.469178	4.393708	-0.267700
H	0.708208	3.203411	-1.349644
C	2.845978	3.271974	-1.473350
C	3.875082	4.119079	-1.373256
H	2.935104	2.393201	-2.121236
H	3.816873	5.003033	-0.732866
H	4.802849	3.971774	-1.928573
C	-3.085306	2.772794	-2.932218
H	2.204887	3.675619	1.933079
H	2.350675	1.936904	2.277720
H	3.491433	2.719825	1.159655

2•N•A
E = –2537.561352 a.u.
N_{imag} = 0

Y	0.285521	0.441475	-0.087274
N	-0.683546	0.590056	-2.112254
N	0.366640	-1.985444	-0.378080
N	2.472961	0.203062	-0.170452
C	0.461138	-3.140591	-0.468161
C	4.458805	1.534839	0.342004
C	5.709290	1.422198	-0.114737
N	0.384863	2.802594	0.902225
Si	-2.468687	0.953213	1.937352
Si	-1.904205	-0.543429	-2.582282
C	0.030349	1.167349	-5.011996
C	1.608599	2.397272	-2.773958
C	-1.301568	3.275502	-3.257045
C	1.343961	-1.430122	2.836416
C	-1.415104	-2.754392	2.610959
C	-0.873418	-0.646810	4.719229
C	-3.949154	-0.172536	2.272513
C	-2.830950	1.974535	0.366457
C	-2.461735	2.227085	3.343287
C	-2.776198	-1.298486	-1.080587
C	-1.155202	-1.951348	-3.608293
C	-3.303751	0.223061	-3.600623
H	-3.570953	-0.624006	-0.733721
H	-2.126040	-1.503041	-0.220165
H	-3.254732	-2.247362	-1.367948
H	-2.962757	0.638439	-4.558677
H	-3.790277	1.032194	-3.036311
H	-4.069735	-0.536441	-3.822013
H	-1.477610	3.667844	-2.244242
H	-2.282901	2.989481	-3.661812
H	-0.906207	4.095099	-3.876436
H	-0.246567	-2.330910	-3.119931
H	-0.865539	-1.599558	-4.608377
H	-1.862091	-2.785902	-3.734413
H	-0.927393	0.854999	-5.449961
H	0.720896	0.312599	-5.062246
H	0.441590	1.965935	-5.649056
H	1.903417	2.238749	-1.725561
H	1.713424	3.469962	-2.993474
H	2.354133	1.862096	-3.378762
H	-3.859556	-0.657907	3.255526
H	-4.038712	-0.962211	1.514898
H	-4.884770	0.407422	2.276208
H	-2.347712	1.608358	-0.552895
H	-2.554790	3.034899	0.484360
H	-3.914845	1.966025	0.175296
H	-1.665200	2.975907	3.220310
H	-2.316279	1.756418	4.324684
H	-3.418489	2.771936	3.367565
H	-1.318256	-3.083982	1.568018
H	-2.489874	-2.655439	2.818328
H	-1.023973	-3.551290	3.262804
H	-1.949243	-0.534217	4.916676
H	-0.381365	0.298423	4.992115
H	-0.494906	-1.428349	5.396212
H	1.597608	-2.324824	3.426053
H	1.900785	-0.589394	3.276916
H	1.728115	-1.578296	1.816945
Si	-0.131825	1.786961	-3.230862
H	3.690227	0.239446	-1.939603
H	2.078852	-0.487144	-2.127099
H	3.361020	-1.386429	-1.281180
H	4.197993	-0.535544	0.835138
H	3.176522	0.570015	1.766393
H	3.977646	2.520127	0.350882
H	6.206921	0.450133	-0.158642
H	6.281297	2.286228	-0.456274
N	-0.972203	0.108281	1.783804
C	3.578104	0.383806	0.756472
C	0.550292	-4.553400	-0.543337
C	2.924671	-0.374832	-1.427669
C	0.349944	-5.208875	-1.773189
C	0.698561	-7.329953	-0.662382
C	0.821919	-5.287573	0.627714
C	0.893439	-6.675275	0.558110
H	1.101123	-7.249766	1.460670
H	0.965870	-4.760572	1.569819
C	0.427629	-6.597260	-1.822636
H	0.131008	-4.623708	-2.665723
H	0.756078	-8.417683	-0.709248
H	0.273094	-7.111370	-2.771142
Si	-0.520986	-1.112610	2.917912
C	1.194283	2.681504	2.147399
H	2.232509	2.484790	1.848787
H	0.808430	1.790559	2.670039
C	1.141424	3.878427	3.049187
C	2.207625	4.606119	3.389360
H	0.156029	4.143003	3.448329
H	3.202861	4.363396	3.009033
H	2.130716	5.457492	4.066319
C	0.758242	3.982919	0.099363
H	-0.595648	2.907560	1.186406
H	1.800970	3.878382	-0.223987
H	0.125639	4.027114	-0.794010
H	0.661920	4.922997	0.664233

TS[**2**•N•A–**7**•A]
E = –2537.539206a.u.
N_{imag} = 1 (121i)

Y	-0.005189	0.350545	0.112539
N	-1.275336	-0.062009	1.954572
N	0.681240	-1.890548	0.063522
N	2.306341	0.274412	-0.428743
C	1.861698	-1.701364	-0.078987
C	3.744593	2.209173	0.061201
C	4.929522	2.659787	-0.357076
N	0.194151	2.455664	1.694742
Si	-0.787958	1.710568	-2.860916
Si	-1.762117	-1.122089	-2.419610
N	-1.013195	0.337883	-1.842262
C	-3.307142	1.464281	0.406284
C	-3.093906	1.859493	3.383363
C	-4.208571	-0.762118	2.287916
C	0.333460	2.962924	-1.968912
C	-2.384316	2.647215	-3.230939
C	0.032641	1.289294	-4.510833
C	-0.478859	-2.254542	-3.220937
C	-3.120287	-0.791356	-3.694111
C	-2.579694	-2.052462	-0.998860
C	-1.189907	-2.977868	2.670443
C	-1.375387	-0.877959	4.873509
C	1.173632	-1.142205	3.309096
H	-0.715589	-3.262895	1.721114
H	-2.278020	-3.077409	2.550533
H	-0.867767	-3.689681	3.446020
H	1.479267	-0.436708	4.094296
H	1.700180	-0.863935	2.386247
H	1.551606	-2.135353	3.595304
H	-4.098725	-1.248092	3.267943
H	-4.146060	-1.544208	1.519121
H	-5.216479	-0.321983	2.247452
H	-2.464812	-1.003851	4.947325
H	-1.132697	0.142054	5.204671
H	-0.914919	-1.582184	5.583924
H	-4.311682	1.905441	0.498171
H	-3.297569	0.810806	-0.473963
H	-2.622123	2.299081	0.188290
H	-2.936639	1.428420	4.381046
H	-4.106965	2.290037	3.357952
H	-2.382764	2.693037	3.274086
H	0.246600	-2.590628	-2.466588
H	0.067155	-1.732445	-4.020152
H	-0.946796	-3.149153	-3.658971
H	-2.741306	-0.309257	-4.606495
H	-3.908964	-0.149575	-3.275638
H	-3.586977	-1.742397	-3.993455
H	-3.479134	-1.524990	-0.652254
H	-1.910876	-2.188623	-0.138652
H	-2.890729	-3.053135	-1.335537
H	-2.928419	2.869351	-2.300996
H	-3.056308	2.067808	-3.878701
H	-2.169324	3.601183	-3.737177
H	0.153266	2.192965	-5.127887
H	-0.570410	0.573543	-5.087650
H	1.027497	0.845460	-4.365808
H	-0.246959	3.623819	-1.315603
H	0.817963	3.605965	-2.718379
H	1.149994	2.520493	-1.376176
Si	-0.724440	-1.211444	3.126735
H	2.785700	1.267633	-2.257178
H	1.805861	-0.209440	-2.413832
H	3.556569	-0.320413	-2.058358
H	4.343266	0.161535	0.189247
H	3.179220	0.661172	1.431423
H	2.907661	2.907849	0.163803
H	5.775791	1.982656	-0.494585
H	5.099286	3.715040	-0.574011
C	2.631337	0.252644	-1.855185
C	3.431628	0.768203	0.362156
C	3.163788	-2.332060	-0.195758
C	4.050884	-2.355882	0.891841
C	5.678415	-3.525618	-0.465951
C	3.540874	-2.908501	-1.419763
C	4.796370	-3.501714	-1.549014
H	5.083792	-3.951667	-2.499720
H	2.840953	-2.898312	-2.254837
C	5.300838	-2.957284	0.753818
H	3.748718	-1.918798	1.842913
H	6.658413	-3.992081	-0.570347
H	5.982507	-2.984053	1.604438
Si	-2.889341	0.559227	2.017481
C	1.327500	2.486455	2.657660
H	2.167335	3.005609	2.171856
H	1.636799	1.447980	2.835847
C	0.997094	3.135747	3.973536
C	0.866764	2.463988	5.119661
H	0.852454	4.220169	3.972805
H	1.007164	1.382253	5.164961
H	0.614120	2.966296	6.053905
C	-0.284123	3.800998	1.339996
H	-0.559565	1.936930	2.178478
H	0.508244	4.344907	0.808379
H	-1.150410	3.717882	0.672840
H	-0.592231	4.391771	2.217290

7•A
E = –2537.557383 a.u.
N_{imag} = 0

Y	-0.145946	0.363315	0.142629
N	-1.470048	-0.111138	1.929240
N	1.111710	-1.478033	0.242578
N	2.277115	0.257268	-0.900913
C	2.048454	-1.204333	-0.555085
C	3.252494	2.390225	-0.162798
C	4.270677	3.183871	-0.500380
N	0.275086	2.231340	1.874445
Si	-1.149138	1.763085	-2.795376
Si	-1.609594	-1.223361	-2.479317
N	-1.074666	0.310831	-1.873415
C	-3.450797	1.405967	0.323568
C	-3.482073	1.655802	3.319732
C	-4.382720	-0.950707	1.979071
C	-0.236772	3.108865	-1.810263
C	-2.884738	2.444683	-3.094875
C	-0.352300	1.627149	-4.504636
C	-0.346139	-1.996310	-3.652230
C	-3.252794	-1.103134	-3.405262
C	-1.849317	-2.403685	-1.030811
C	-1.247178	-3.057506	2.501064
C	-1.830502	-1.100796	4.774889
C	0.883324	-1.132467	3.492992
H	-0.589838	-3.265386	1.645561
H	-2.286462	-3.216827	2.181631
H	-1.017971	-3.785175	3.294598
H	1.105596	-0.202473	4.034197
H	1.494812	-1.197456	2.581604
H	1.185282	-1.967452	4.143844
H	-4.291864	-1.553606	2.893209
H	-4.262936	-1.629770	1.122518
H	-5.405512	-0.545614	1.946017
H	-2.922059	-1.210255	4.712709
H	-1.612736	-0.123968	5.230681
H	-1.461516	-1.875260	5.465021
H	-4.476626	1.804435	0.352921
H	-3.350717	0.784102	-0.574970
H	-2.785056	2.274476	0.189795
H	-3.329709	1.206173	4.309744
H	-4.525725	2.002257	3.265634
H	-2.842167	2.549681	3.253222
H	0.614520	-2.169222	-3.145845
H	-0.157399	-1.352575	-4.523316
H	-0.698239	-2.969807	-4.026851
H	-3.164187	-0.508199	-4.326030
H	-4.030636	-0.640859	-2.780379
H	-3.603143	-2.106044	-3.693265
H	-2.584613	-2.024428	-0.307089
H	-0.910739	-2.583153	-0.484601
H	-2.210260	-3.378754	-1.391274
H	-3.426511	2.613694	-2.155138
H	-3.486037	1.758743	-3.707043
H	-2.825302	3.404363	-3.631832
H	-0.373892	2.600982	-5.017646
H	-0.909355	0.915777	-5.132367
H	0.690594	1.287567	-4.465207
H	-0.108028	4.010608	-2.427209
H	0.771763	2.811795	-1.483042
H	-0.813078	3.419049	-0.926782
Si	-0.958834	-1.297017	3.102690
H	2.274177	1.592898	-2.534214
H	1.699107	-0.050871	-2.891558
H	3.451307	0.268211	-2.710358
H	4.341895	0.569549	-0.372189
H	3.169012	0.557010	0.958925
H	2.275092	2.829087	0.059678
H	5.253414	2.774719	-0.745047
H	4.162525	4.267922	-0.540447
C	2.446735	0.527134	-2.338770
C	3.327363	0.896537	-0.078389
C	2.894566	-2.231660	-1.233091
C	4.219798	-2.025257	-1.647096
C	4.362468	-4.308218	-2.437422
C	2.320520	-3.499984	-1.426402
C	3.042036	-4.525403	-2.030063
H	2.575524	-5.499279	-2.183433
H	1.297811	-3.652300	-1.082141
C	4.950771	-3.058243	-2.236571
H	4.702203	-1.061844	-1.493453
H	4.931443	-5.111631	-2.906824
H	5.984277	-2.885101	-2.539311
Si	-3.108646	0.441529	1.913907
C	1.494139	2.251595	2.702626
H	2.184350	3.002762	2.288918
H	2.005730	1.279727	2.594785
C	1.287648	2.502426	4.173573
C	0.128778	2.417281	4.828754
H	2.202087	2.735580	4.728081
H	-0.810743	2.172349	4.329509
H	0.076103	2.580343	5.904634
C	-0.312125	3.574983	1.722706
H	-0.421541	1.610316	2.339354
H	0.310305	4.177833	1.047753
H	-1.313190	3.487855	1.282454
H	-0.403083	4.100595	2.685594

7'•A
E = –2537.567632 a.u.
N_{imag} = 0

Y	0.386267	0.595034	0.126846
N	-0.879241	0.435764	1.958820
N	1.168764	-1.408851	-0.043299
N	2.401306	-2.587441	1.534348
C	1.552792	-2.528366	0.437341
C	3.162162	-0.297401	1.067750
C	3.139917	1.047252	1.232340
N	1.035017	3.088581	0.036107
Si	0.233344	0.222852	-3.187327
Si	-0.905541	1.428471	3.370022
C	-1.172001	-2.386568	2.922796
C	-2.134870	-1.588033	0.138807
C	-3.656467	-0.632444	2.552539
C	-3.022208	1.984944	-0.429382
C	-3.311763	0.584182	-3.117102
C	-2.080858	3.340497	-3.003306
C	-0.403368	-1.518258	-3.524673
C	2.094165	0.091780	-2.823762
C	0.121523	1.209201	-4.800934
C	0.694099	2.431938	3.581235
C	-1.019639	0.459405	4.992522
C	-2.339490	2.662064	3.359817
H	0.969548	3.052105	2.718085
H	1.541849	1.772016	3.816127
H	0.572099	3.115888	4.435078
H	-3.301764	2.131449	3.367548
H	-2.337220	3.301614	2.465700
H	-2.307235	3.316947	4.244031
H	-4.134771	0.169218	1.971688
H	-3.676766	-0.339842	3.611514
H	-4.274769	-1.537398	2.447962
H	-0.180980	-0.244857	5.092803
H	-1.951522	-0.115018	5.081102
H	-0.978103	1.154556	5.845317
H	-1.195391	-2.169181	3.998997
H	-0.123361	-2.546438	2.634534
H	-1.722047	-3.324624	2.754347
H	-1.191101	-1.828946	-0.370721
H	-2.686769	-0.869985	-0.481286
H	-2.725840	-2.516292	0.175860
H	-1.444642	-1.498973	-3.874657
H	-0.368654	-2.115732	-2.603902
H	0.200448	-2.031444	-4.288895
H	2.301353	-0.450031	-1.888393
H	2.587435	1.074118	-2.794754
H	2.572516	-0.482018	-3.632890
H	0.507465	2.231966	-4.677385
H	-0.909001	1.282258	-5.176168
H	0.722270	0.718001	-5.582064
H	-3.421000	-0.412466	-2.665580
H	-2.950258	0.446087	-4.146193
H	-4.311997	1.040731	-3.175108
H	-1.684880	3.220308	-4.021058
H	-1.449677	4.080934	-2.490056
H	-3.090242	3.772954	-3.085701
H	-3.356813	3.029304	-0.340894
H	-2.402889	1.756043	0.449941
H	-3.917710	1.351179	-0.350303
Si	-1.909955	-0.970796	1.909095
H	2.559986	-4.029386	3.091592
H	2.783634	-4.638488	1.432601
H	4.072020	-3.683007	2.204254
H	1.923402	-0.891522	2.723038
H	3.602555	-1.473867	2.797404
H	3.668108	-0.719078	0.195498
H	2.745913	1.505233	2.140878
H	3.620544	1.701315	0.503954
N	-0.587233	0.980451	-1.861211
C	2.753911	-1.299305	2.116117
C	1.078357	-3.811785	-0.172528
C	2.980847	-3.793289	2.099031
C	0.335764	-4.753128	0.555164
C	-0.001903	-6.064005	-1.451961
C	1.271527	-4.009193	-1.546932
C	0.744815	-5.133296	-2.180714
H	0.904441	-5.276394	-3.250005
H	1.822907	-3.257945	-2.112063
C	-0.209211	-5.867704	-0.084583
H	0.160810	-4.597322	1.619621
H	-0.427258	-6.935806	-1.950372
H	-0.802816	-6.582546	0.486969
Si	-2.152463	1.674522	-2.093105
C	-0.158239	3.924307	0.286020
C	1.663332	3.388133	-1.281862
H	0.942075	3.080229	-2.051368
H	2.539527	2.726516	-1.373591
C	2.077057	4.818446	-1.462128
C	1.578009	5.621499	-2.404508
H	2.834998	5.201410	-0.768350
H	0.820758	5.264402	-3.106247
H	1.910100	6.654169	-2.515744
H	1.724962	3.284196	0.768181
H	-0.910295	3.698280	-0.476159
H	-0.576660	3.677025	1.267392
H	0.063952	5.001571	0.246872

7"•A
E = –2537.581632 a.u.
N_{imag} = 0

Y	-0.512508	0.333542	0.146559
N	-1.453436	0.496346	-1.874341
N	0.940611	-1.193207	-0.146462
N	1.923110	-2.741848	-1.626428
C	1.957785	-1.665979	-0.754628
C	3.492994	-4.510029	-0.821749
C	2.914775	-4.592137	0.378029
N	1.431346	1.514113	1.256788
Si	-2.711918	1.571245	2.099710
Si	-2.998564	-0.181227	-2.229406
C	-1.203486	2.371750	-4.220809
C	0.512424	-0.173457	-4.065408
C	0.966076	2.103901	-2.109360
C	-3.761829	-1.705261	3.367183
C	-1.021179	-1.079395	4.534145
C	-1.241326	-2.792796	2.019330
C	-4.566715	1.445357	1.791984
C	-2.023865	2.791216	0.795723
C	-2.442001	2.376676	3.786816
C	-3.457410	-1.436964	-0.895025
C	-3.030653	-1.100495	-3.882860
C	-4.332844	1.155568	-2.284397
H	-3.450030	-0.995486	0.112220
H	-2.748925	-2.279620	-0.893202
H	-4.461854	-1.848642	-1.075346
H	-4.128333	1.872866	-3.092860
H	-4.364115	1.721531	-1.341953
H	-5.334073	0.731192	-2.453890
H	1.587633	1.461042	-1.464420
H	0.532394	2.918028	-1.507529
H	1.665319	2.570324	-2.818938
H	-2.296871	-1.919854	-3.890503
H	-2.802263	-0.437551	-4.730216
H	-4.024294	-1.537938	-4.064370
H	-1.679002	3.187795	-3.657153
H	-1.984770	1.886423	-4.823799
H	-0.475175	2.815831	-4.916359
H	-0.194272	-0.749078	-4.679548
H	1.030738	-0.883170	-3.403373
H	1.257113	0.273812	-4.742072
H	-5.054239	0.831981	2.562386
H	-4.773147	0.978138	0.818891
H	-5.042840	2.437607	1.799963
H	-2.157154	2.459074	-0.249829
H	-0.963327	3.050524	0.955519
H	-2.575546	3.738997	0.878770
H	-1.370478	2.511122	3.996877
H	-2.859090	1.751646	4.590155
H	-2.927166	3.362690	3.847455
H	-1.347018	-0.176110	5.070040
H	0.060653	-0.991081	4.359131
H	-1.178811	-1.940379	5.201837
H	-0.242579	-2.578308	1.608923
H	-1.878149	-3.099220	1.176812
H	-1.156733	-3.648985	2.705753
H	-4.384081	-1.807562	2.466545
H	-4.207916	-0.921659	3.997620
H	-3.818001	-2.651324	3.926951
Si	-0.381709	1.141915	-3.047230
H	0.680893	-3.946259	-2.794842
H	-0.130102	-2.587989	-1.944959
H	0.332283	-4.047446	-1.041007
H	3.967667	-2.834560	-2.056126
H	2.979097	-4.050505	-2.856417
H	4.320060	-5.182099	-1.075369
H	2.087715	-3.938955	0.662050
H	3.248387	-5.319714	1.117582
N	-1.856713	0.096165	1.902487
C	3.121060	-3.522810	-1.898838
C	3.270542	-0.944464	-0.607982
C	0.630384	-3.373024	-1.860054
C	3.893658	-0.870141	0.647562
C	5.498505	0.724662	-0.216871
C	3.786308	-0.184193	-1.670353
C	4.885116	0.654894	-1.470687
H	5.263989	1.255964	-2.298501
H	3.304104	-0.237857	-2.647586
C	5.003420	-0.047302	0.840235
H	3.491237	-1.461026	1.470766
H	6.360696	1.374697	-0.063995
H	5.481733	-0.003153	1.819516
Si	-1.973096	-1.299984	2.912201
C	1.494082	0.878318	2.590971
C	1.747627	2.965101	1.310303
H	1.058332	3.435829	2.027090
H	1.536999	3.383929	0.314927
C	3.174576	3.238780	1.686086
C	3.558954	3.883637	2.789477
H	3.925872	2.846974	0.991366
H	2.829677	4.276058	3.502317
H	4.611782	4.052949	3.017780
H	2.145307	1.047992	0.678986
H	0.669867	1.253367	3.209326
H	1.366916	-0.203969	2.463189
H	2.452005	1.070197	3.099138

TS[**7”**•A–**2**•PP]
E = –2537.550307 a.u.
N_{imag} = 1 (1163i)

Y	-0.449184	0.570011	-0.210619
N	-1.816470	0.197000	1.505250
N	1.181686	-0.973984	0.010767
N	1.208781	-2.838810	1.419818
C	1.785867	-1.719658	0.877567
C	1.508595	-4.244566	3.424831
C	1.057908	-5.444561	3.796504
N	1.721502	1.499414	-0.583595
H	1.749200	0.145006	-0.275774
Si	-1.108595	0.591622	3.028278
C	-3.710206	-1.282858	-0.239980
C	-4.660062	1.108464	1.423964
C	-3.932754	-1.532642	2.772516
C	-1.616917	3.099259	-0.677395
C	-4.026473	2.209363	-2.351337
C	-1.483922	3.214735	-3.722618
C	-3.063217	-0.785893	-4.282393
C	-0.875867	-2.224362	-2.680220
C	-0.120935	-0.125407	-4.751015
C	0.500679	1.528906	2.684316
C	-0.611468	-0.925970	4.035906
C	-2.191610	1.705569	4.100030
H	0.373567	2.425329	2.056174
H	1.263464	0.885452	2.221020
H	0.936039	1.876967	3.632976
H	-3.128313	1.208052	4.389176
H	-2.456029	2.628772	3.564051
H	-1.667329	1.989106	5.025413
H	-3.878565	-1.057340	3.762551
H	-3.273609	-2.413062	2.786293
H	-4.964902	-1.889272	2.634130
H	0.049561	-1.572062	3.440399
H	-1.481375	-1.526808	4.333448
H	-0.072710	-0.634878	4.950995
H	-3.112733	-2.206827	-0.258770
H	-3.418879	-0.677944	-1.109723
H	-4.766007	-1.569393	-0.357812
H	-4.408279	1.858108	0.660241
H	-4.628130	1.611228	2.401107
H	-5.696577	0.784377	1.245452
H	-3.360014	0.129102	-4.816649
H	-3.853608	-1.021968	-3.555521
H	-3.026179	-1.601349	-5.020555
H	-1.645444	-2.608278	-1.995145
H	0.063896	-2.130625	-2.114662
H	-0.723997	-2.975973	-3.469355
H	0.898558	-0.089732	-4.340233
H	-0.330240	0.855937	-5.199792
H	-0.125408	-0.871456	-5.560467
H	-4.459172	1.596627	-1.549085
H	-4.380915	1.798564	-3.307414
H	-4.425402	3.230490	-2.255980
H	-1.789602	2.777999	-4.684799
H	-0.385664	3.256670	-3.709565
H	-1.867756	4.245612	-3.690237
H	-0.519662	3.211241	-0.573350
H	-2.031780	2.663424	0.250671
H	-2.009249	4.125278	-0.715725
Si	-3.456758	-0.347334	1.376471
H	-0.528202	-3.948656	1.716965
H	-0.800325	-2.269214	1.178105
H	-0.236405	-3.490812	0.003392
H	1.937085	-4.816055	1.402715
H	3.037782	-3.593382	2.067998
H	1.531888	-3.422201	4.145901
H	1.012980	-6.277344	3.090250
H	0.724948	-5.642471	4.815498
N	-1.464230	0.617119	-2.172724
C	1.988283	-3.916158	2.041190
C	3.124947	-1.298182	1.398317
C	-0.165919	-3.156917	1.050718
C	4.151249	-0.975367	0.499823
C	5.519582	-0.172258	2.326347
C	3.308553	-1.050007	2.767548
C	4.497410	-0.482735	3.226909
H	4.622338	-0.274982	4.290265
H	2.501086	-1.272628	3.466113
C	5.344788	-0.424334	0.962641
H	3.996499	-1.140065	-0.565979
H	6.448176	0.272047	2.685955
H	6.135310	-0.176439	0.253867
Si	-2.145347	2.191033	-2.285082
C	2.738718	2.230324	0.161748
C	1.884890	1.706288	-2.037629
H	2.018334	2.782690	-2.263077
H	0.959381	1.391697	-2.549854
C	3.039853	0.918305	-2.590195
C	4.192429	1.440190	-3.020404
H	2.908740	-0.169854	-2.575907
H	4.349043	2.522012	-3.043411
H	5.012841	0.815400	-3.377034
Si	-1.393788	-0.570684	-3.426776
H	2.564464	3.323804	0.128981
H	2.739866	1.923539	1.214815
H	3.754901	2.045661	-0.231841

2•PP
E = –2537.579323 a.u.
N_{imag} = 0

Y	0.042550	0.928112	0.218449
N	-1.117375	0.722998	2.136713
N	1.793196	-0.681497	0.092479
N	3.044957	-2.558433	-0.553536
C	1.989009	-1.975309	0.072459
C	3.295699	-4.828784	-1.545944
C	2.676198	-4.490804	-2.678211
N	1.732324	2.329288	0.215189
H	2.565521	-0.140595	-0.314937
Si	-2.588962	-0.157382	1.966481
C	0.023711	3.233424	3.261073
C	0.809934	0.488024	4.383574
C	-1.950572	1.647372	4.913544
C	-1.606562	3.475527	-0.050546
C	-3.750246	2.371839	-1.927268
C	-1.377536	3.904522	-3.057057
C	-2.571069	-0.471874	-3.700265
C	0.135542	-1.398485	-2.722487
C	-0.035490	0.950004	-4.624314
C	-2.458374	-1.207595	0.392999
C	-4.093780	0.967183	1.761001
C	-2.991125	-1.312792	3.418371
H	-1.640627	-1.941401	0.452711
H	-2.315217	-0.590730	-0.509923
H	-3.387887	-1.775500	0.237701
H	-3.679209	-0.826970	4.124409
H	-2.089519	-1.597021	3.975164
H	-3.473112	-2.236320	3.064067
H	-2.293653	0.674717	5.290869
H	-2.825601	2.187340	4.523282
H	-1.564486	2.220733	5.770365
H	-3.985242	1.640899	0.900306
H	-4.234178	1.591681	2.655485
H	-5.015114	0.382000	1.615001
H	-0.820110	3.891635	3.006017
H	0.731914	3.275173	2.420773
H	0.520061	3.651389	4.150237
H	1.654717	0.369224	3.687242
H	0.461547	-0.518488	4.661753
H	1.198143	0.970947	5.293098
H	-3.192605	0.345720	-4.091227
H	-3.120831	-0.937961	-2.869647
H	-2.465283	-1.220693	-4.500333
H	-0.262428	-1.933912	-1.848568
H	1.188890	-1.155454	-2.526675
H	0.101984	-2.088306	-3.579436
H	0.943480	1.372203	-4.354584
H	-0.639988	1.768876	-5.038510
H	0.121949	0.213763	-5.427726
H	-4.094092	1.531420	-1.308567
H	-4.014285	2.143635	-2.969567
H	-4.317669	3.266791	-1.629819
H	-1.655739	3.561970	-4.063960
H	-0.291367	4.073948	-3.052450
H	-1.873252	4.872790	-2.888408
H	-0.555974	3.756864	0.130408
H	-1.946176	2.868987	0.804997
H	-2.190728	4.407067	-0.015362
Si	-0.600540	1.483362	3.598526
H	4.624226	-2.375299	-1.903063
H	4.586696	-1.091397	-0.653763
H	3.421227	-1.069849	-2.003078
H	2.866373	-4.355851	0.500603
H	4.502359	-3.953438	-0.007718
H	3.740921	-5.822681	-1.440495
H	2.219038	-3.508256	-2.811367
H	2.599294	-5.190945	-3.509377
N	-0.966383	1.194299	-1.766264
C	3.447846	-3.946204	-0.337637
C	0.993110	-2.834457	0.764378
C	3.970802	-1.724656	-1.313471
C	0.341350	-3.888250	0.106530
C	-0.919485	-4.360229	2.116738
C	0.671634	-2.539341	2.096528
C	-0.266197	-3.316031	2.773751
H	-0.496980	-3.095818	3.814687
H	1.159912	-1.702918	2.594247
C	-0.621039	-4.639183	0.780262
H	0.577063	-4.106264	-0.934469
H	-1.669000	-4.950973	2.643871
H	-1.143016	-5.440860	0.257494
Si	-1.891550	2.653663	-1.738155
C	2.821976	2.170993	1.153674
C	2.145173	3.065369	-0.980871
H	2.801450	3.921249	-0.722363
H	1.255068	3.476548	-1.482900
C	2.859000	2.118764	-1.909928
C	4.188678	1.982451	-2.006729
H	2.201321	1.435285	-2.460656
H	4.866470	2.661619	-1.484433
H	4.648498	1.217738	-2.635867
Si	-0.878629	0.150249	-3.132545
H	3.182418	3.141658	1.553392
H	2.503895	1.566820	2.018896
H	3.711160	1.661078	0.714677

TS[**7’**•A–**8**•A]
E = –2537.561796 a.u.
N_{imag} = 1 (201i)

Y	0.572271	0.495000	-0.115846
N	-0.352429	0.805133	-2.123870
N	1.501016	-1.517197	-0.447791
N	3.419300	-2.749199	-0.162764
C	2.048780	-2.661506	-0.222523
C	3.139032	-0.438657	-0.813518
C	3.080214	0.900357	-0.354901
N	0.870606	2.928562	0.633141
Si	-2.362420	0.931840	1.807320
Si	-1.311644	-0.565668	-2.605650
C	0.247054	1.478998	-5.015555
C	1.408343	3.153476	-2.838275
C	-1.585125	3.258745	-3.357115
C	-0.767552	-2.441836	2.884059
C	-0.491033	-0.022667	4.717594
C	1.774188	-0.766176	2.874319
C	-3.625795	-0.388464	2.301730
C	-2.949666	1.660406	0.147908
C	-2.555001	2.312951	3.098802
C	-1.951566	-1.513545	-1.097821
C	-0.300751	-1.762309	-3.665260
C	-2.868697	-0.095591	-3.571543
H	-2.723811	-0.940346	-0.570501
H	-1.186079	-1.802046	-0.365214
H	-2.418960	-2.446326	-1.449653
H	-2.648044	0.392369	-4.531069
H	-3.500068	0.585299	-2.982742
H	-3.460195	-0.998484	-3.788737
H	-1.864634	3.665597	-2.374676
H	-2.468661	2.737062	-3.749927
H	-1.370916	4.108225	-4.023663
H	0.645138	-1.999366	-3.156819
H	-0.053436	-1.321722	-4.640648
H	-0.843239	-2.702070	-3.852229
H	-0.589933	0.908635	-5.440999
H	1.138054	0.834629	-5.039355
H	0.433657	2.336388	-5.680420
H	2.334649	2.562274	-2.824304
H	1.329291	3.698417	-1.888150
H	1.520735	3.915558	-3.624601
H	-3.458336	-0.752039	3.325976
H	-3.581666	-1.255488	1.627321
H	-4.645906	0.023831	2.260068
H	-3.809933	1.088577	-0.230013
H	-2.191833	1.646938	-0.649047
H	-3.285769	2.700411	0.271908
H	-1.828588	3.127696	2.966190
H	-2.425712	1.929767	4.120020
H	-3.562547	2.752685	3.032266
H	-1.567402	-0.029861	4.940274
H	-0.127753	1.006443	4.854121
H	0.004464	-0.657101	5.468814
H	2.154655	-1.237240	3.793664
H	2.248514	0.223023	2.798926
H	2.117816	-1.375049	2.027940
H	-0.654169	-2.842810	1.867905
H	-1.834915	-2.487556	3.140443
H	-0.226839	-3.109589	3.571814
Si	-0.103734	2.085349	-3.256738
H	4.657688	-4.030256	0.994160
H	3.605734	-4.828749	-0.206511
H	5.047406	-3.929579	-0.744554
H	4.255396	-1.119397	0.899236
H	5.009327	-1.481677	-0.676139
H	3.045938	-0.586938	-1.894586
H	3.576234	1.135468	0.590859
H	3.092174	1.694987	-1.102192
N	-0.745977	0.325721	1.711309
C	4.047921	-1.436188	-0.140491
C	1.225472	-3.875229	0.033185
C	4.221297	-3.943852	-0.016469
C	1.403111	-4.626289	1.205055
C	-0.475756	-6.025608	0.607283
C	0.187410	-4.208018	-0.846226
C	-0.654153	-5.282296	-0.562697
H	-1.458888	-5.534848	-1.253878
H	0.043907	-3.609884	-1.743874
C	0.552621	-5.693027	1.492119
H	2.185196	-4.348007	1.912213
H	-1.143021	-6.857769	0.833896
H	0.683295	-6.256275	2.416594
Si	-0.122447	-0.670978	2.977161
C	1.299019	2.998271	2.044921
C	-0.303514	3.798304	0.357509
H	-1.115569	3.473280	1.017779
H	-0.625387	3.594947	-0.673991
C	-0.035518	5.262846	0.537212
C	-0.647563	6.033336	1.439407
H	0.718032	5.700579	-0.128142
H	-1.404274	5.622946	2.112144
H	-0.427739	7.097451	1.532016
H	1.649789	3.244163	0.046554
H	0.528960	2.519750	2.662086
H	2.233077	2.434979	2.159431
H	1.457781	4.033103	2.387035

8•A
E = –2537.584213 a.u.
N_{imag} = 0

Y	0.201637	0.539048	0.335072
N	-1.057450	0.261376	2.160297
N	1.559578	-1.400453	0.812855
N	3.510793	-2.532470	0.850565
C	2.229898	-2.433978	0.385326
C	2.478435	-0.570056	1.687937
C	2.556541	0.804485	1.048291
N	0.426763	3.030033	0.322103
Si	-2.175916	1.275060	-2.073616
Si	-1.061783	1.209574	3.598939
C	-1.057647	-2.627003	2.995763
C	-2.081376	-1.778774	0.258326
C	-3.702809	-1.105784	2.712116
C	2.176107	-0.109344	-2.520939
C	0.334968	0.986437	-4.643379
C	-0.196949	-1.776667	-3.474692
C	-2.148934	2.930795	-3.000632
C	-3.125458	1.570884	-0.447299
C	-3.251485	0.121683	-3.119964
C	0.412861	2.402467	3.666758
C	-0.934954	0.168251	5.174597
C	-2.628949	2.258958	3.744954
H	0.267339	3.298158	3.046265
H	1.353555	1.919036	3.366530
H	0.538969	2.759690	4.700097
H	-3.515751	1.622625	3.875168
H	-2.796416	2.861012	2.839500
H	-2.577147	2.946030	4.603471
H	-4.251802	-0.311455	2.186236
H	-3.732854	-0.879415	3.787694
H	-4.243206	-2.052335	2.557894
H	-0.014397	-0.433653	5.179510
H	-1.784866	-0.520124	5.285681
H	-0.918475	0.818118	6.062951
H	-1.071858	-2.464085	4.081880
H	-0.005400	-2.680369	2.680225
H	-1.531536	-3.601492	2.799148
H	-1.146162	-1.829760	-0.318751
H	-2.772273	-1.137864	-0.302741
H	-2.497572	-2.798151	0.244635
H	-1.715377	2.818641	-4.003902
H	-1.564420	3.700401	-2.476330
H	-3.172596	3.318919	-3.119852
H	-3.629616	2.548406	-0.470266
H	-2.520101	1.534286	0.471217
H	-3.908814	0.809278	-0.321442
H	-3.314650	-0.879014	-2.668693
H	-2.853110	0.004680	-4.138397
H	-4.274323	0.519670	-3.208079
H	0.652364	2.024600	-4.467110
H	-0.664968	1.013507	-5.099923
H	1.022414	0.545720	-5.381991
H	-1.213739	-1.775394	-3.891356
H	-0.210335	-2.414748	-2.580489
H	0.471299	-2.245730	-4.212077
H	2.337700	-0.646493	-1.576674
H	2.614593	0.893108	-2.411589
H	2.749384	-0.637663	-3.298293
Si	-1.930894	-1.227799	2.068850
H	5.365862	-3.428330	0.422123
H	3.934075	-4.461872	0.164469
H	4.499812	-4.116443	1.823326
H	4.667415	-0.877069	1.508097
H	3.922602	-1.856604	2.806999
H	1.996215	-0.494294	2.676734
H	3.287222	0.786990	0.220716
H	2.890642	1.564201	1.773708
N	-0.594853	0.653927	-1.773385
C	3.767130	-1.442105	1.795524
C	1.681362	-3.416753	-0.570932
C	4.370931	-3.694082	0.811618
C	2.360201	-3.718657	-1.761313
C	0.603818	-5.262687	-2.376443
C	0.459891	-4.043229	-0.291837
C	-0.074811	-4.963836	-1.193064
H	-1.027728	-5.444906	-0.971781
H	-0.059384	-3.803832	0.634291
C	1.820351	-4.636792	-2.660182
H	3.296367	-3.209245	-1.990719
H	0.179483	-5.975297	-3.084092
H	2.342534	-4.852958	-3.592433
Si	0.355667	-0.024557	-3.043324
C	-0.736223	3.916918	0.504011
C	1.226156	3.354553	-0.891333
H	0.597230	3.147765	-1.767424
H	2.058962	2.632875	-0.904495
C	1.755789	4.756972	-0.919247
C	1.443340	5.656314	-1.855283
H	2.441010	5.032076	-0.108940
H	0.762008	5.406965	-2.672193
H	1.860570	6.663860	-1.848503
H	1.048996	3.106785	1.134767
H	-1.410988	3.800287	-0.350852
H	-1.278246	3.620082	1.408704
H	-0.452235	4.978115	0.580315

TS[**8**•A–**2**•P]
E = –2537.557664 a.u.
N_{imag} = 1 (1082i)

Y	0.265688	0.474998	0.413398
N	-0.855288	0.271782	2.328394
N	1.183752	-1.732733	0.614575
N	2.575628	-3.501616	0.582744
C	1.393964	-2.950222	0.190353
C	2.370373	-1.307895	1.433744
C	2.903952	0.011646	0.888373
N	1.589449	2.402180	0.413455
H	2.271949	1.327956	0.788240
Si	-2.221065	-0.779477	2.240075
C	-1.199635	2.748696	3.946856
C	1.476626	1.193624	3.960224
C	-0.905878	0.078737	5.365595
C	-2.092000	2.716934	0.148079
C	-3.473399	1.556579	-2.343631
C	-1.255960	3.613705	-2.594670
C	-1.393137	-1.551926	-3.242529
C	1.548299	-0.760888	-2.810467
C	-0.220699	0.907357	-4.587779
C	-2.633142	-1.143338	0.427850
C	-3.800034	-0.033929	2.963907
C	-1.888443	-2.434958	3.097695
H	-1.795041	-1.484500	-0.195466
H	-3.062383	-0.265011	-0.070537
H	-3.389939	-1.942251	0.390161
H	-1.903866	-2.328330	4.190971
H	-0.892106	-2.810978	2.820369
H	-2.636979	-3.195844	2.827829
H	-0.433630	-0.913854	5.390068
H	-1.991574	-0.060024	5.459040
H	-0.566887	0.630035	6.256562
H	-4.051652	0.906602	2.451821
H	-3.703680	0.186787	4.036038
H	-4.651641	-0.720696	2.840888
H	-2.294443	2.647149	3.987738
H	-0.968930	3.379941	3.077549
H	-0.874954	3.282328	4.852999
H	1.989399	1.528074	3.050167
H	1.906475	0.219582	4.239336
H	1.734880	1.904888	4.759713
H	-2.419881	-1.186798	-3.391617
H	-1.407626	-2.215593	-2.368037
H	-1.115381	-2.155918	-4.119132
H	1.722477	-1.275971	-1.856374
H	2.284680	0.052683	-2.890730
H	1.762035	-1.477891	-3.617758
H	0.461012	1.767273	-4.522398
H	-1.221134	1.287121	-4.840140
H	0.112898	0.275669	-5.425746
H	-3.891914	0.687781	-1.816577
H	-3.364004	1.277078	-3.402333
H	-4.209741	2.373035	-2.291876
H	-1.097628	3.392269	-3.658113
H	-0.316039	4.017832	-2.192933
H	-2.017143	4.406338	-2.526207
H	-1.174318	3.153717	0.573937
H	-2.455947	1.959487	0.855369
H	-2.838259	3.525574	0.123343
Si	-0.407849	1.038937	3.811161
H	3.960654	-4.885910	-0.198976
H	2.265640	-5.442303	-0.120801
H	3.238705	-5.329984	1.372352
H	4.286281	-2.284300	0.886911
H	3.553182	-2.949305	2.375000
H	2.012534	-1.162781	2.465897
H	3.371839	-0.170813	-0.095532
H	3.694231	0.386913	1.559252
N	-0.649025	0.813727	-1.585794
C	3.331074	-2.532797	1.379656
C	0.451224	-3.700126	-0.666194
C	3.034027	-4.858924	0.397205
C	0.844887	-4.153030	-1.934319
C	-1.340677	-5.132649	-2.265736
C	-0.842660	-3.969297	-0.203794
C	-1.733917	-4.685961	-1.002828
H	-2.741183	-4.888256	-0.638614
H	-1.141608	-3.618040	0.781803
C	-0.051338	-4.862339	-2.731617
H	1.845667	-3.925228	-2.301456
H	-2.042543	-5.682502	-2.893133
H	0.252857	-5.194044	-3.724465
Si	-1.809901	2.092145	-1.619613
C	1.554471	3.569694	1.285031
C	2.150622	2.714074	-0.909629
H	1.561290	3.512276	-1.395271
H	2.034448	1.823292	-1.551122
C	3.601886	3.109098	-0.864161
C	4.076620	4.298156	-1.242611
H	4.286678	2.354358	-0.461847
H	3.411614	5.071332	-1.635791
H	5.137845	4.543394	-1.181897
Si	-0.220708	-0.097180	-2.985539
H	0.951976	4.379973	0.831832
H	1.092728	3.315729	2.245944
H	2.557490	3.986399	1.489125

2•P
E = –2537.608487 a.u.
N_{imag} = 0

Y	0.339404	0.584214	0.155089
N	-0.988550	0.453831	1.976096
N	1.653255	-1.412872	-0.038068
N	2.161129	-3.510001	-0.681158
C	1.270260	-2.667675	-0.099224
C	3.055809	-1.342804	-0.550958
C	4.018661	-0.983318	0.573736
N	1.994350	2.021230	0.150162
H	3.765265	0.003217	0.980379
Si	-2.714568	0.372454	1.849957
C	-0.284665	2.404138	4.135344
C	1.702809	0.257228	3.162088
C	-0.623278	-0.531711	4.857214
C	-0.984242	3.335444	-0.271795
C	-3.197189	2.389754	-2.188480
C	-0.586121	3.577094	-3.224841
C	-2.172230	-1.456155	-3.023948
C	0.841031	-1.285187	-3.346456
C	-0.938181	0.606999	-4.864410
C	-3.157611	-0.560170	0.275564
C	-3.544286	2.073160	1.783919
C	-3.577169	-0.502945	3.291780
H	-2.835410	-1.608683	0.336335
H	-2.674740	-0.114454	-0.605366
H	-4.243822	-0.553841	0.098684
H	-3.562439	0.106745	4.206394
H	-3.137066	-1.478906	3.529246
H	-4.632805	-0.665867	3.023922
H	-0.624091	-1.580330	4.526190
H	-1.615185	-0.311994	5.271378
H	0.108298	-0.444915	5.675779
H	-3.362182	2.599956	0.839252
H	-3.185399	2.718917	2.599177
H	-4.633983	1.964408	1.898160
H	-1.328592	2.615100	4.413179
H	0.005818	3.145793	3.377069
H	0.337992	2.564894	5.028356
H	2.159853	0.758171	2.295372
H	1.860958	-0.824135	3.034649
H	2.285357	0.569242	4.042344
H	-3.136592	-0.927496	-3.033156
H	-2.124320	-2.020436	-2.082678
H	-2.173712	-2.175478	-3.858027
H	0.921006	-2.036199	-2.550295
H	1.743064	-0.655717	-3.321332
H	0.836496	-1.822190	-4.307216
H	-0.085023	1.259092	-5.098159
H	-1.852009	1.215405	-4.918322
H	-1.004903	-0.157371	-5.654088
H	-3.709684	1.826440	-1.396978
H	-3.438301	1.906209	-3.147004
H	-3.621602	3.405052	-2.213311
H	-0.922377	3.329703	-4.239865
H	0.511895	3.526521	-3.208827
H	-0.876850	4.619411	-3.020729
H	0.025641	3.765848	-0.263027
H	-1.118975	2.759463	0.659419
H	-1.699600	4.168870	-0.194028
Si	-0.132741	0.647102	3.458823
H	3.013255	-5.395504	-0.348151
H	1.232142	-5.326791	-0.240145
H	2.033222	-5.270348	-1.835950
H	4.250562	-3.194199	-0.788219
H	3.340780	-2.741674	-2.260446
H	3.099818	-0.572572	-1.332368
H	3.963845	-1.726828	1.382092
H	5.051171	-0.952075	0.195780
N	-0.632290	0.851485	-1.854284
C	3.316148	-2.745146	-1.159076
C	-0.030471	-3.144106	0.408386
C	2.104810	-4.951063	-0.783831
C	-0.376565	-2.905314	1.745239
C	-2.457392	-4.092251	1.415431
C	-0.915788	-3.839932	-0.429460
C	-2.131806	-4.301029	0.072037
H	-2.829064	-4.816147	-0.588405
H	-0.659920	-3.994986	-1.477765
C	-1.579221	-3.397311	2.248440
H	0.304452	-2.346489	2.384473
H	-3.405799	-4.458169	1.809158
H	-1.835010	-3.224683	3.292884
Si	-1.328139	2.435737	-1.913650
C	2.375436	3.068101	1.078638
C	2.506205	2.297243	-1.192157
H	2.191050	3.306224	-1.542871
H	2.049820	1.578663	-1.901623
C	4.006663	2.212867	-1.293646
C	4.809210	3.243057	-1.574008
H	4.449102	1.237440	-1.066931
H	4.399130	4.234401	-1.782787
H	5.894832	3.139474	-1.608231
Si	-0.734062	-0.239608	-3.184665
H	2.042879	4.070679	0.729204
H	1.913312	2.900329	2.061443
H	3.469829	3.140270	1.232149