Supporting Information

The Computational investigation on the role of disilene substituents towards N_2O activation

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Complete Reference of Gaussian 09

Gaussian 09, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

Choice of Functionals

In our previous report we have used BP86 functional because the calculations were more expensive due to large system. Unfortunately, there are few stationary point or transition geometries which are much difficult to converge at BP86 method. Thus, using of long-range dispersion corrected functional is a better choice. The long-range corrected hybrid density functional (LC-hybrid GGA), ωB97xD including empirical dispersion, provides a promising accuracy for the system in which non-covalent interaction is significant, as suggested by Head-Gordon et al. (Phys. Chem. Chem. Phys., 2008, 10, 6615–6620). In our mechanistic study this functional is seemed to be most suitable because of the presence of several loosely bound intermediates and transition states. To validate the thermochemical parameters at ωB97xD/TZVP another semiempirical functional, M06-2X, is used in addition to ωB97xD for single point calculations at higher basis set of quadruple-zeta quality: QZVP. No significant deviations in energetics were found between these two functional studies. Moreover, it is well known that the M06-2X functional is a preferred choice for the computation of main group

chemistry as reported by Truhlar et al. (Theor. Chem. Account 2008, 120, 215–241). There are several benchmark reports found in literature where M06-2X is considered as a very good functional for main group chemistry. Therefore, in order to incorporate long range dispersion we have undertaken hybrid GGA and meta-GGA type functionals, ωb97xD (in optimizations) and M06-2X (in single point calculations).

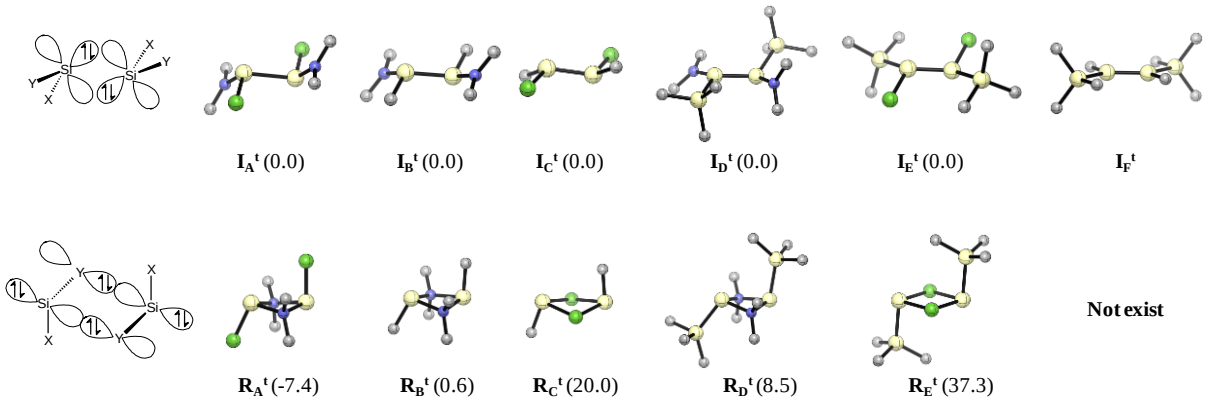

Figure S1. Hetero-bridged and trans-pyramidalized conformation of disilenes. Relative energy values in parenthesis are ΔG in kcal/mol at ωB97xD/TZVP level of theory.

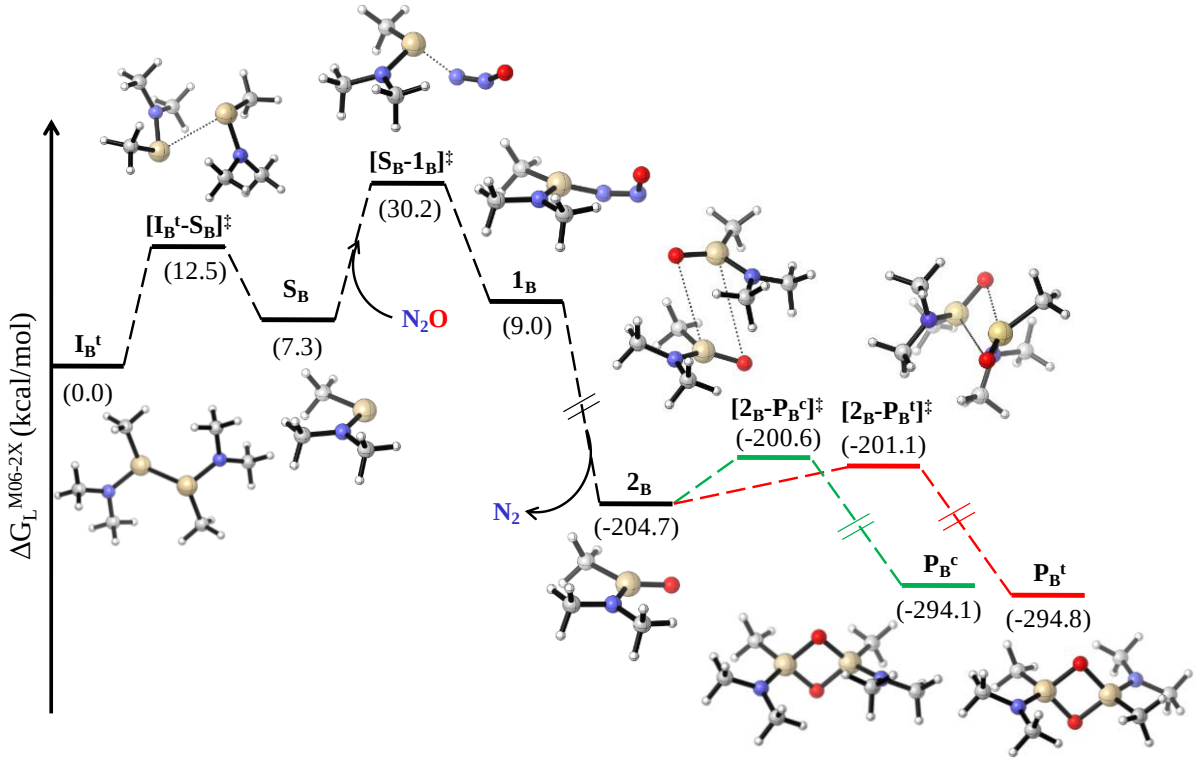

Figure S2. "Pathway I" energy profile for $\mathbf{I_B^t}$. Red line represents the *trans*-addition of silanone and green line represents *cis*-addition of silanone.

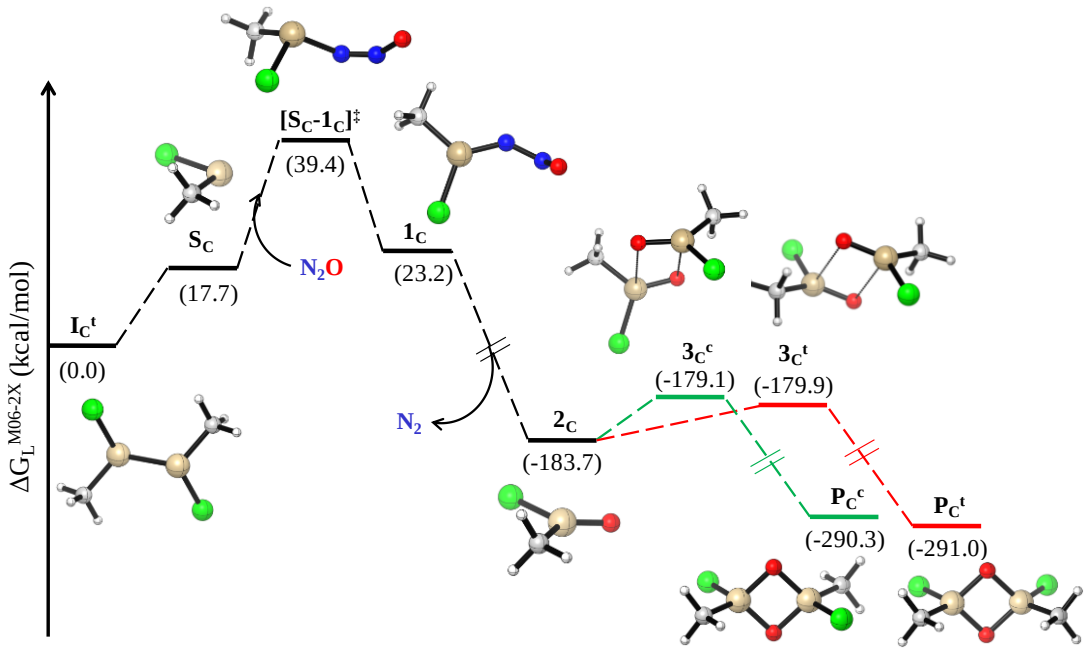

Figure S3. "Pathway I" energy profile for $\mathbf{I_C}^{\mathbf{t}}$. For color codes refer Figure S2.

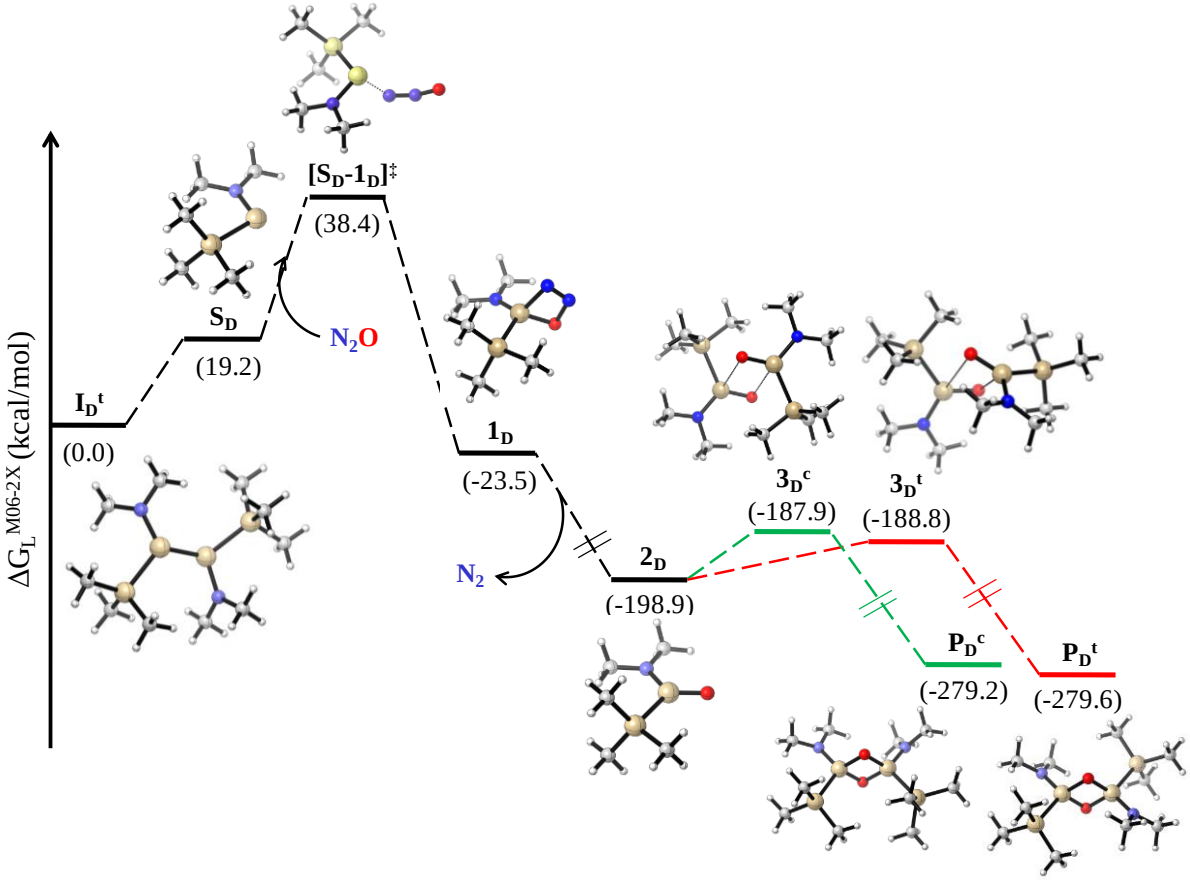

Figure S4. "Pathway I" energy profile for $\mathbf{I_D}^{\mathbf{t}}$. For color codes refer Figure S2.

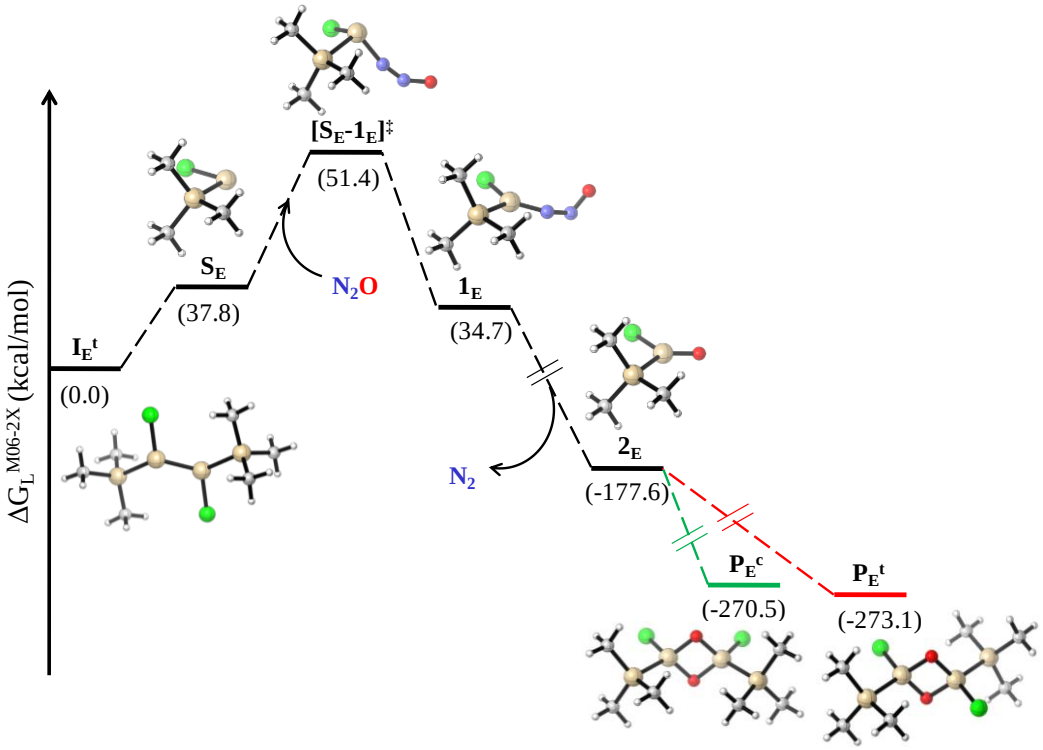

Figure S5. "Pathway I" energy profile for $\mathbf{I_E^t}$. For color codes refer Figure S2.

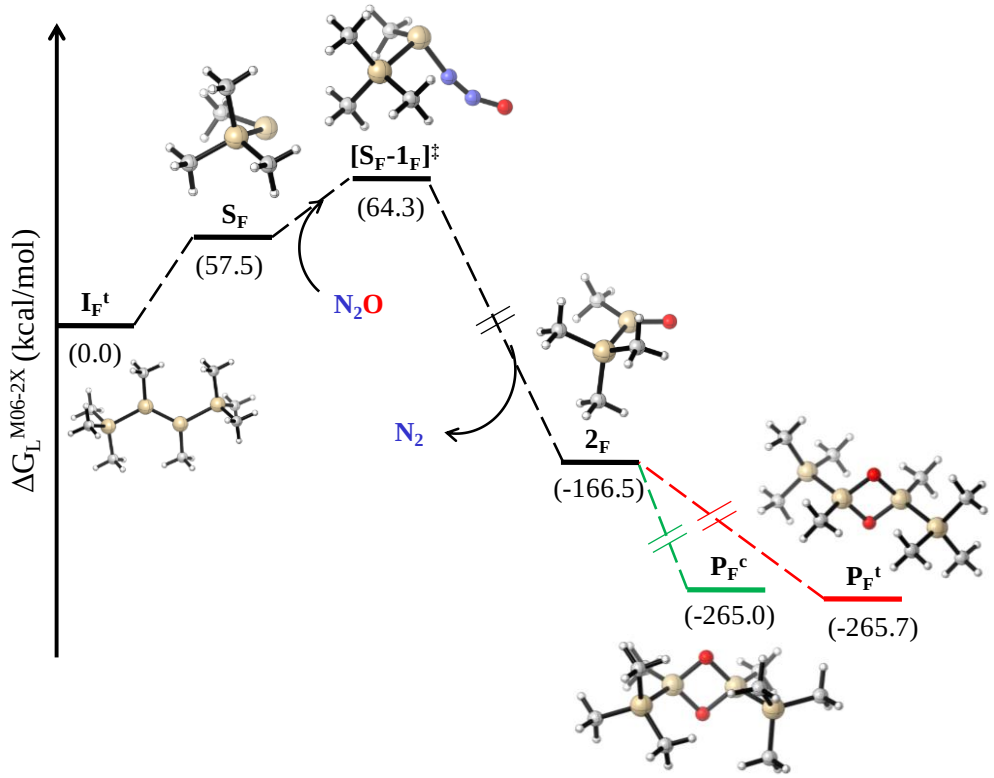

Figure S6. "Pathway I" energy profile for $\mathbf{I_F^t}$. For color codes refer Figure S2.

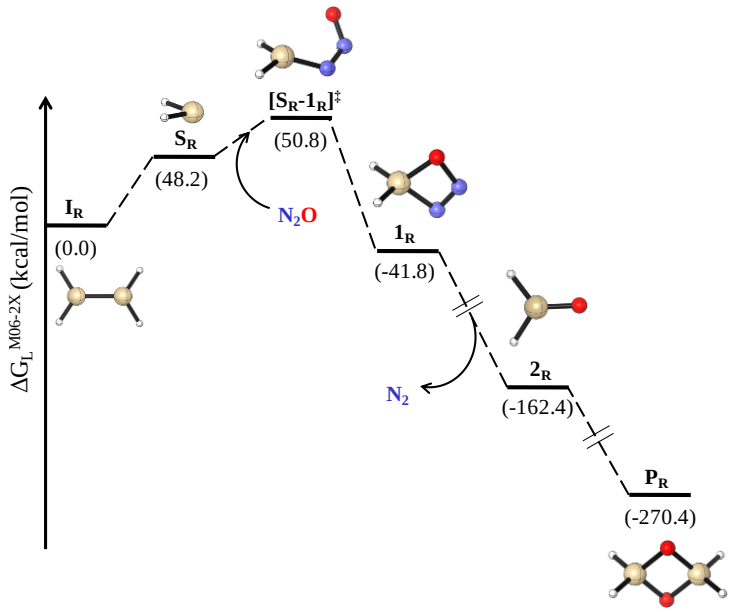

Figure S7. "Pathway I" energy profile for $\mathbf{I_R}$. For color codes refer Figure S2.

Table S1. Results of the EDA-NOCV calculations for transition states $\mathbf{[S_A\text{-}1_A]^‡}$, $\mathbf{[I_A{}^t\text{-}4_A{}^t]^‡}$ and $\mathbf{[I_F{}^t\text{-}4_F{}^t]^‡}$ at BP86/TZ2P level.

TS	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat} [a]	ΔE_{orb} [a]	ΔE_{σ} [b]	ΔE_{π} [b]
$\mathbf{[S_A\text{-}1_A]^‡}$	-14.6	111.6	-59.0	-67.1(53.2%)	-44.9(66.9%)	-15.6(23.2%)
$\mathbf{[I_A{}^t\text{-}4_A{}^t]^‡}$	-10.8	83.3	-50.1	-44.1(46.8%)	-27.2(58.1%)	-11.9(27.0%)
$\mathbf{[I_F{}^t\text{-}4_F{}^t]^‡}$	-6.2	46.9	-30.6	-22.5(42.3%)	-14.9(66.2%)	-5.1(22.7%)

[a] The value in parenthesis gives the percentage contribution to the total attractive interactions ΔE_{elstat} + ΔE_{orb}. [b] The value in parenthesis gives the percentage contribution to the total orbital interactions ΔE_{orb}.

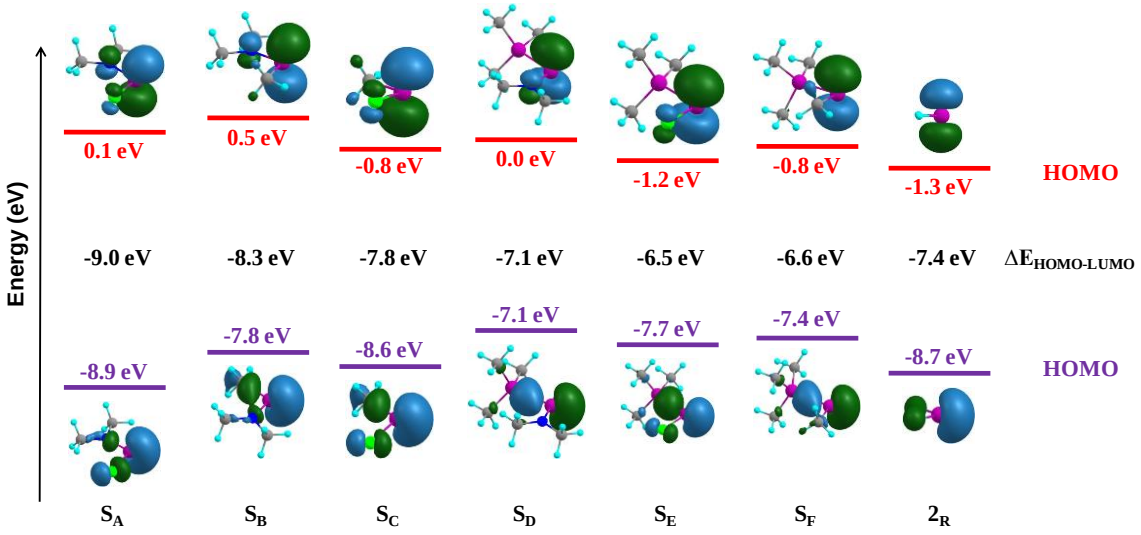

Figure S8. Frontier orbitals of silylene $\mathbf{S_{A\text{-}F,R}}$ at M06-2X/QZVP//ωB97xD/TZVP level of theory.

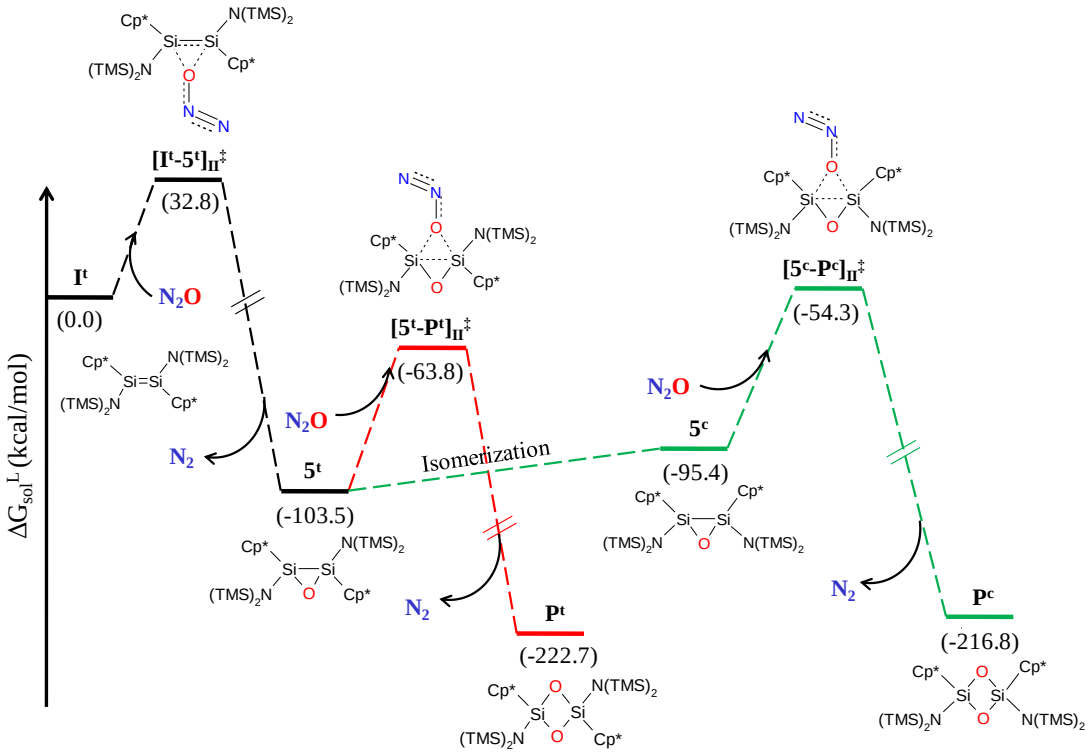

Figure S9. "Pathway IIa" energy profile diagram for $\mathbf{I}^{t}$. The energy values were calculated at BP86(SMD)/TZVP//BP86/SVP level.

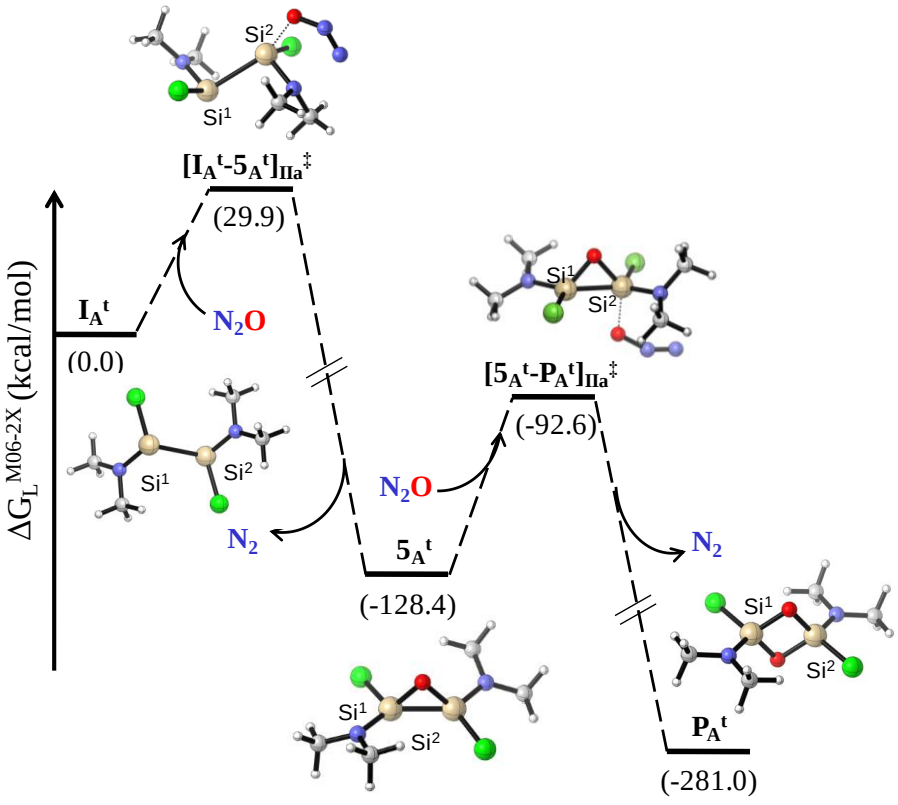

Figure S10. "Pathway IIa" energy profile diagram for $\mathbf{I}_{\mathbf{A}}^{t}$.

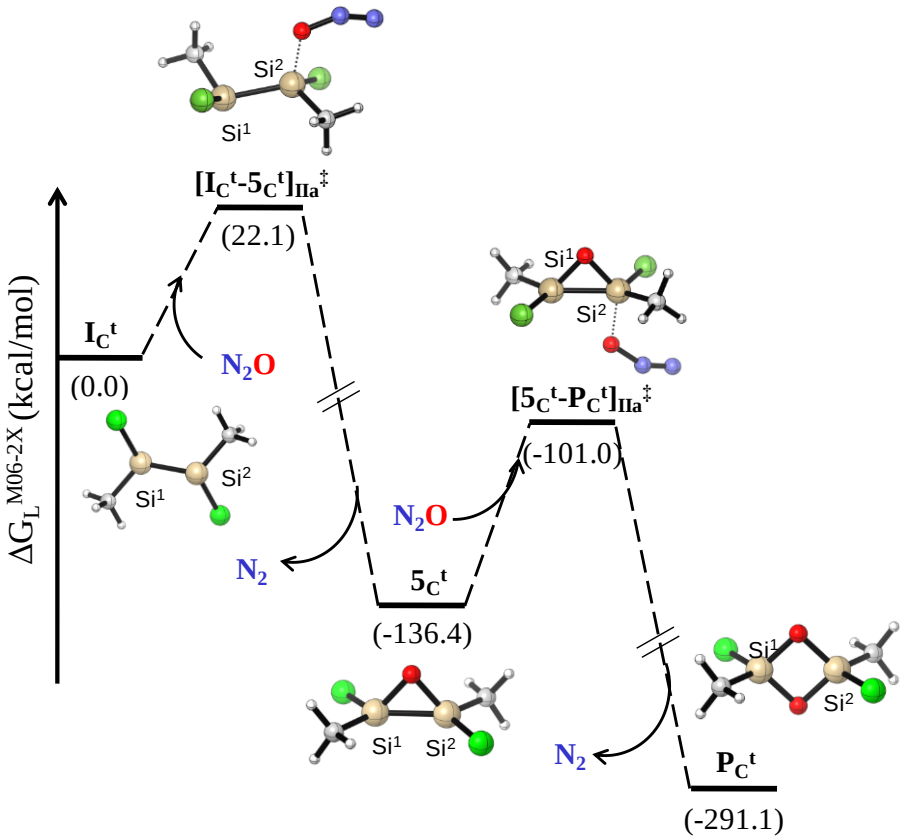

Figure S11. "Pathway IIa" energy profile diagram for $\mathbf{I_C^t}$.

Table S2. Energies ($\Delta G_L^{M06\text{-}2X}$ in kcal/mol) for all the steps involved in "Pathway IIa".

Steps: (X = A, C and E)	$\mathbf{I_A^t}$	$\mathbf{I_B^t}$	$\mathbf{I_C^t}$	$\mathbf{I_D^t}$	$\mathbf{I_E^t}$	$\mathbf{I_F^t}$
$\mathbf{I_X^t + N_2O \rightarrow [I_X^t\text{-}5_X^t]_{IIa}^{\ddagger}}$	29.9	–	22.8	–	27.0	–
$\mathbf{[I_X^t\text{-}5_X^t]_{IIa}^{\ddagger} \rightarrow 5_X^t + N_2}$	-158.3	–	-158.5	–	-152.4	–
$\mathbf{5_X^t + N_2O \rightarrow [5_X^t\text{-}P_X^t]_{IIa}^{\ddagger}}$	35.8	34.2	35.4	33.5	36.2	35.5
$\mathbf{[5_X^t\text{-}P_X^t]_{IIa}^{\ddagger} \rightarrow P_X^t + N_2}$	-188.4	-193.1	-104.2	-279.6	-183.9	-182.9

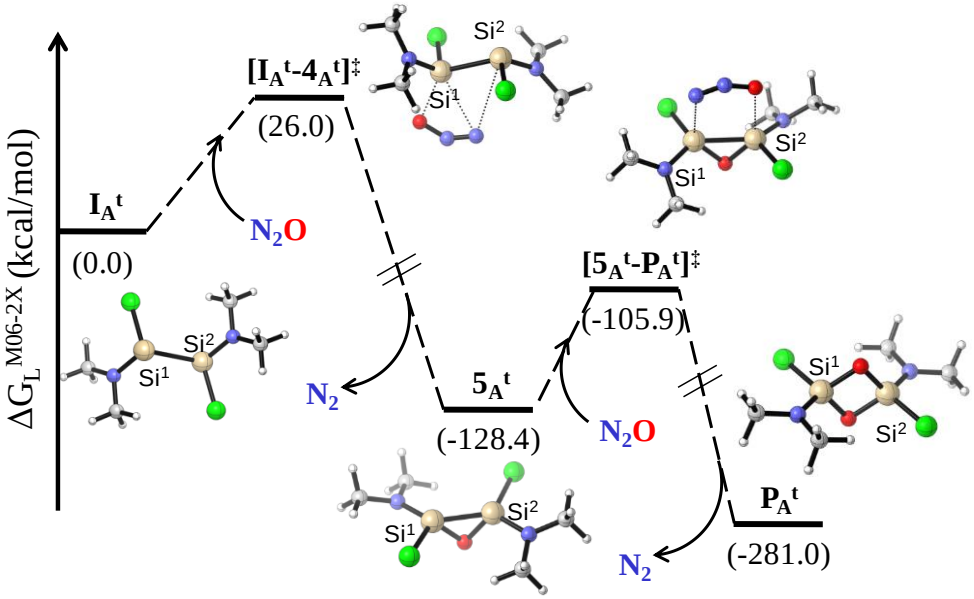

Figure S12. "Pathway IIb" energy profile diagram for $\mathbf{I_A}^{\mathbf{t}}$.

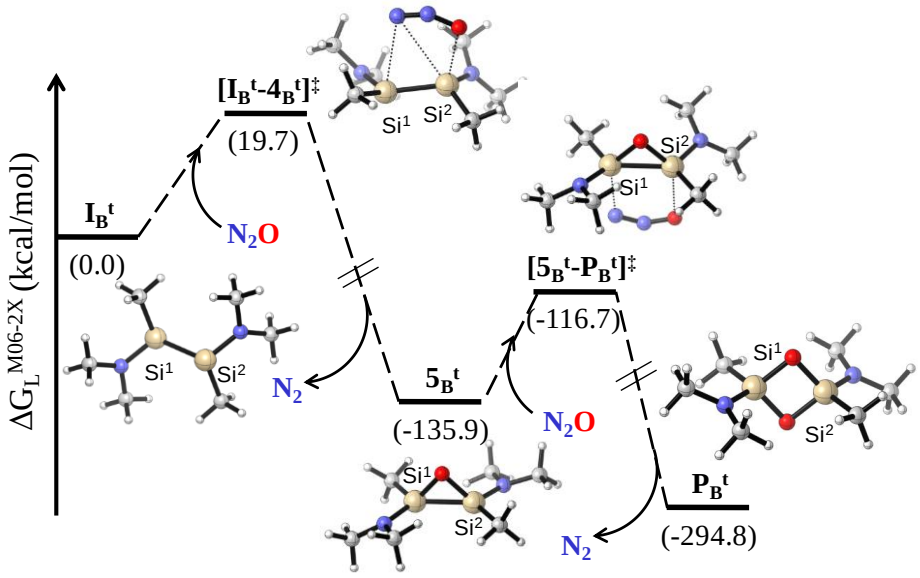

Figure S13. "Pathway IIb" energy profile diagram for $\mathbf{I_B}^{\mathbf{t}}$.

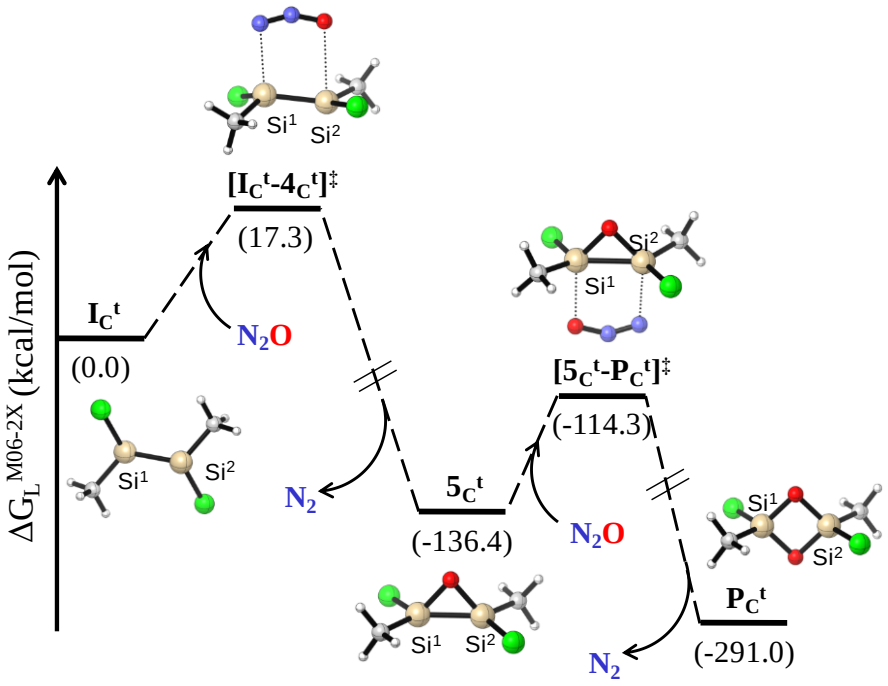

Figure S14. "Pathway IIb" energy profile diagram for $\mathbf{I_C^t}$.

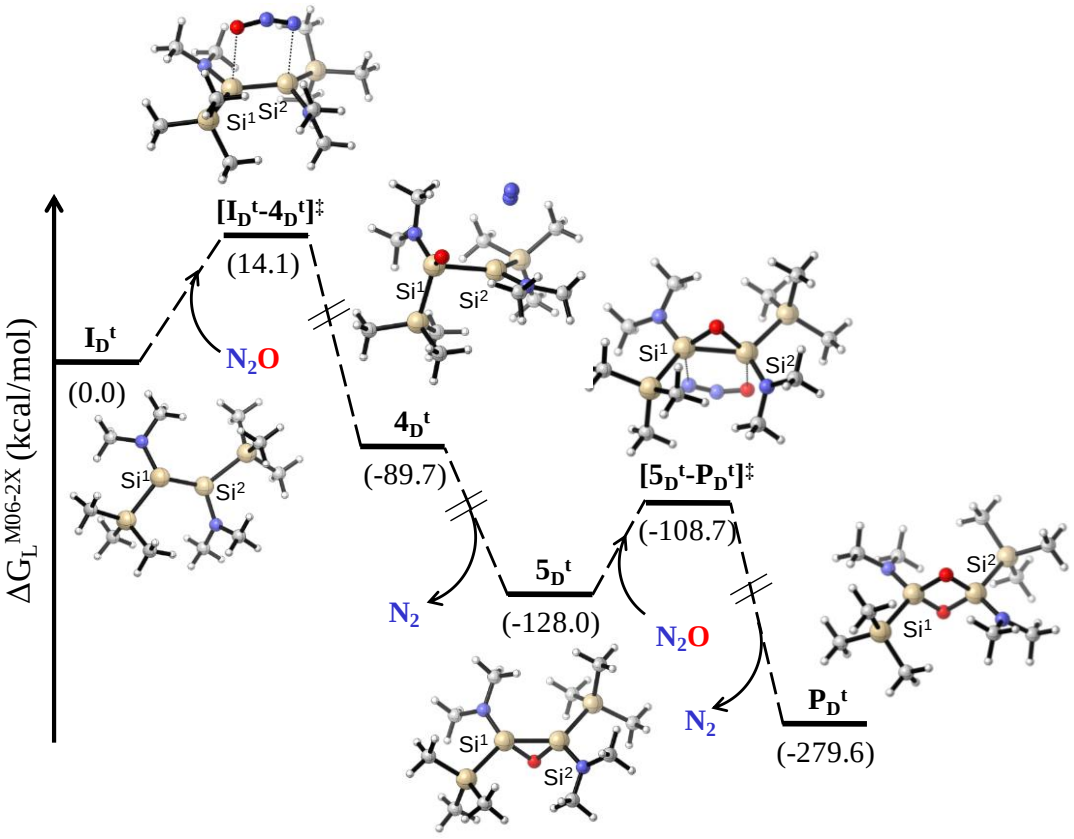

Figure S15. "Pathway IIb" energy profile diagram for $\mathbf{I_D^t}$.

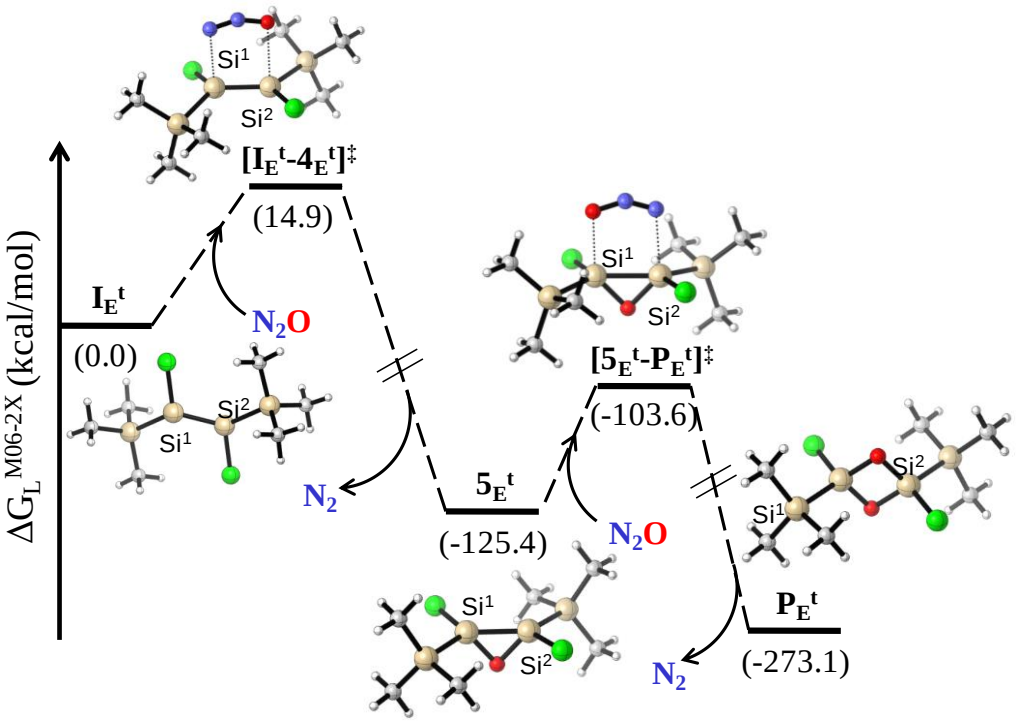

Figure S16. "Pathway IIb" energy profile diagram for $\mathbf{I_E^t}$.

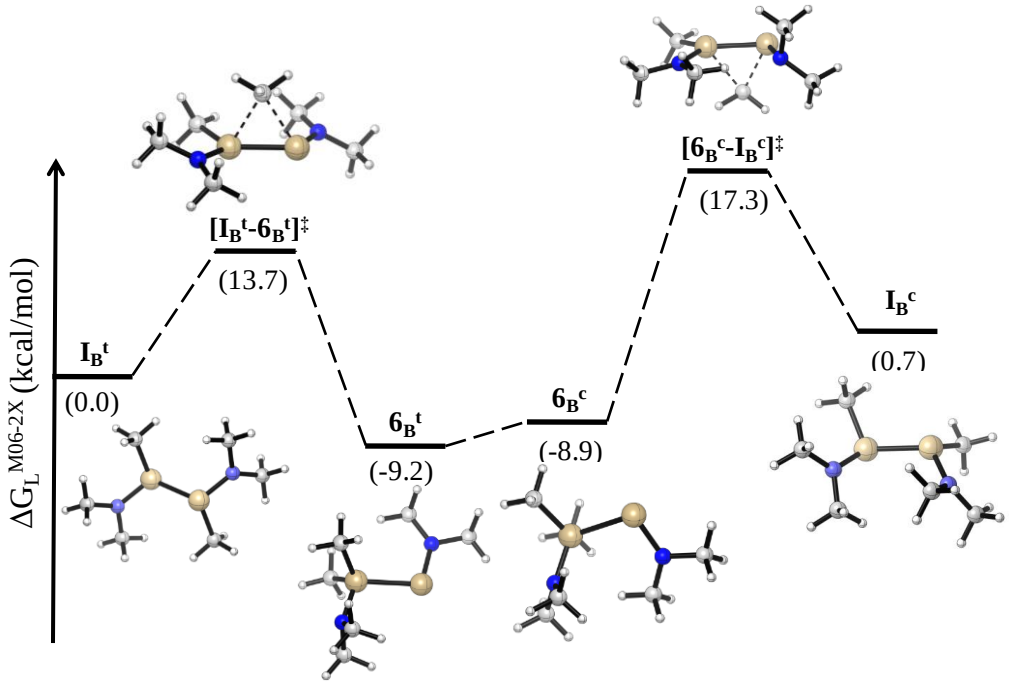

Figure S17. Energy profile for the isomerization of $\mathbf{I_B^t}$ to $\mathbf{I_B^c}$ *via* disilene-(silyl)silylene rearrangement.

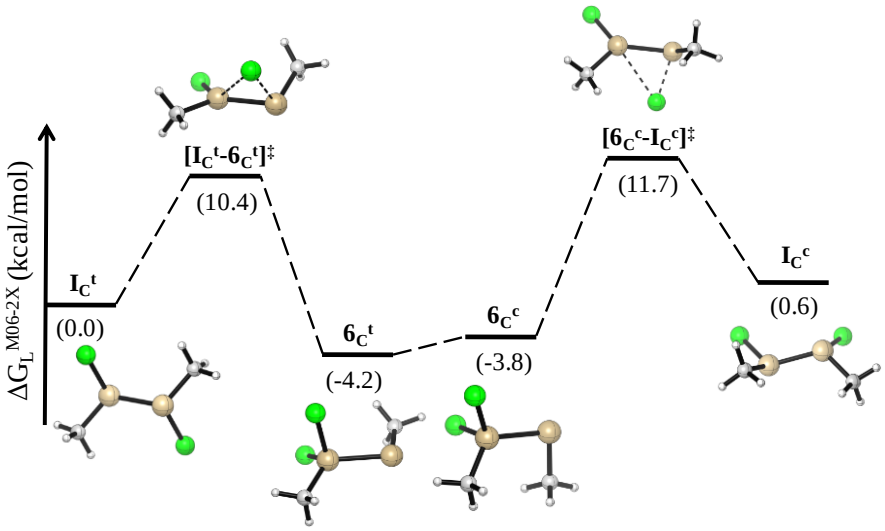

Figure S18. Energy profile for the isomerization of $\mathbf{I_C^t}$ to $\mathbf{I_C^c}$ *via* disilene-(silyl)silylene rearrangement.

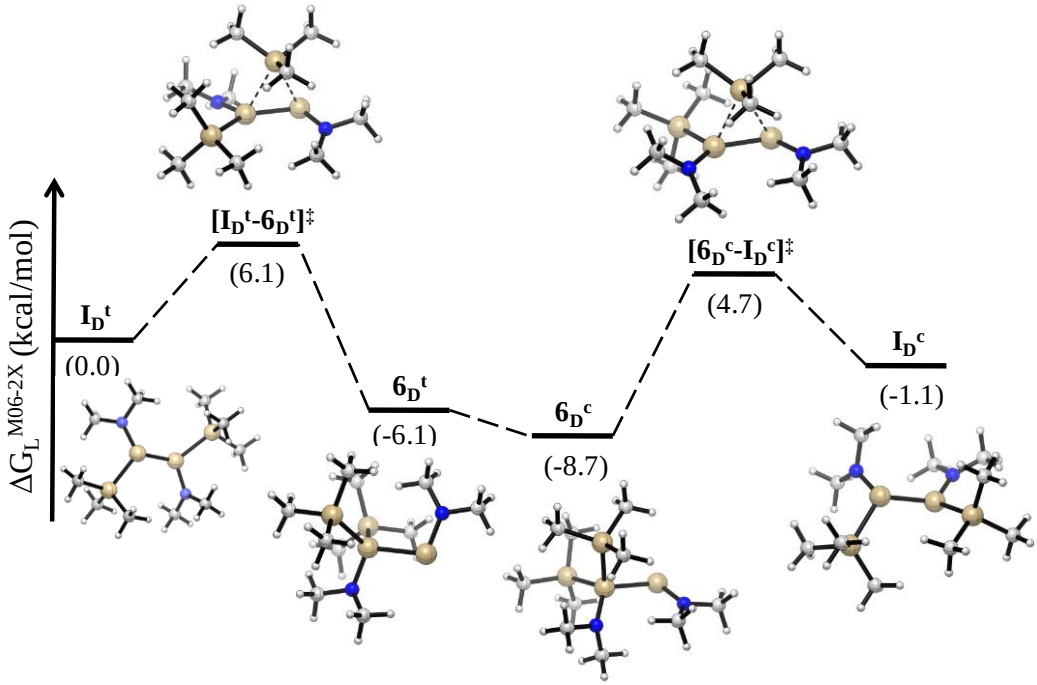

Figure S19. Energy profile for the isomerization of $\mathbf{I_D^t}$ to $\mathbf{I_D^c}$ *via* disilene-(silyl)silylene rearrangement.

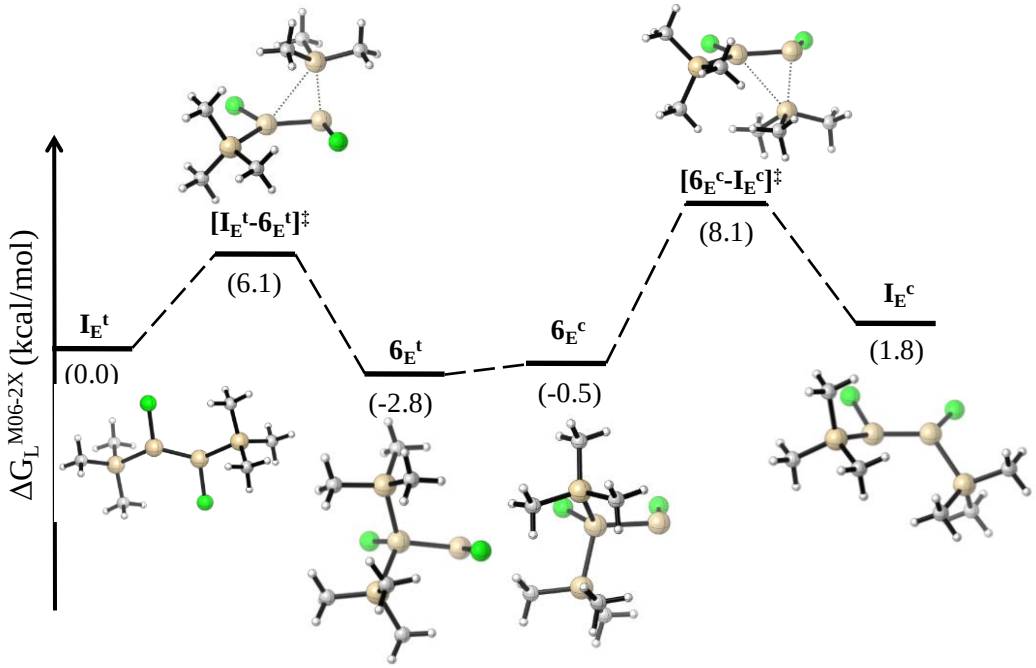

Figure S20. Energy profile for the isomerization of $\mathbf{I_E^t}$ to $\mathbf{I_E^c}$ *via* disilene-(silyl)silylene rearrangement.

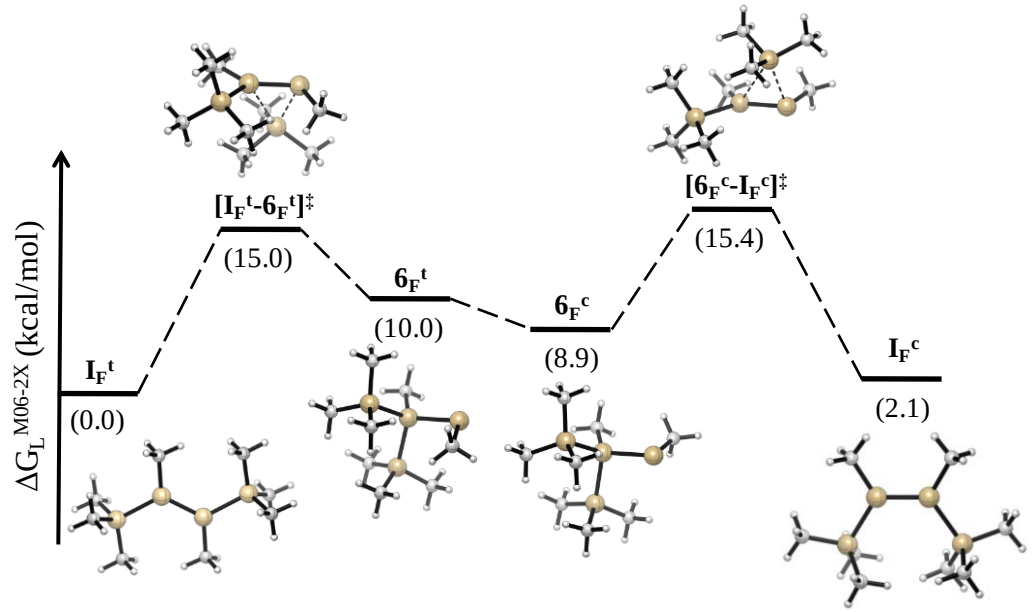

Figure S21. Energy profile for the isomerization of $\mathbf{I_F^t}$ to $\mathbf{I_F^c}$ *via* disilene-(silyl)silylene rearrangement.

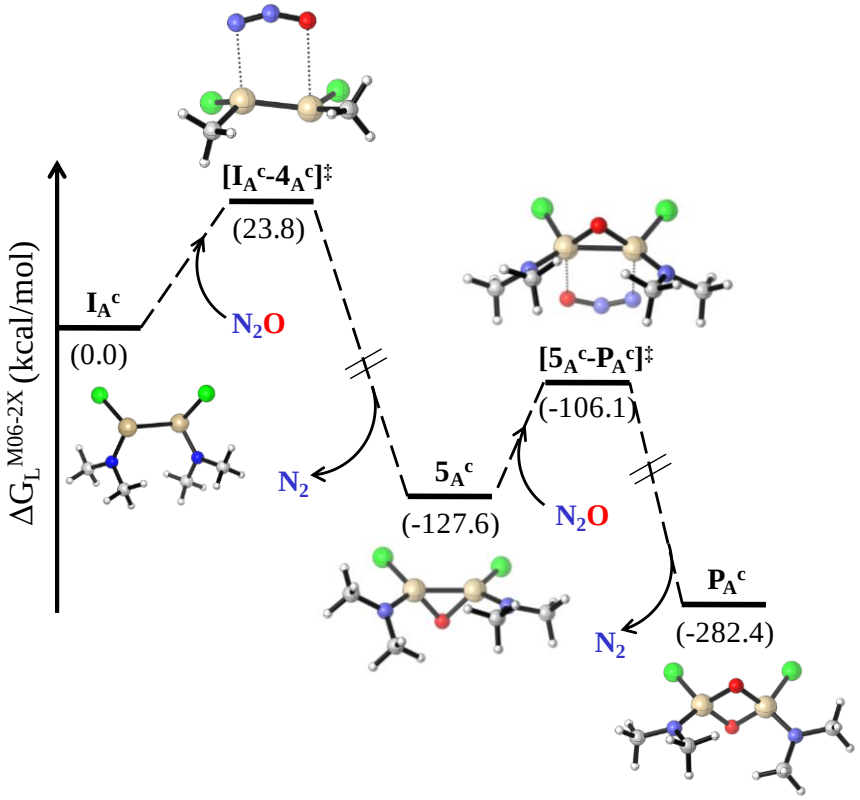

Figure S22. "Pathway IIb" energy profile diagram for $\mathbf{I_A^c}$.

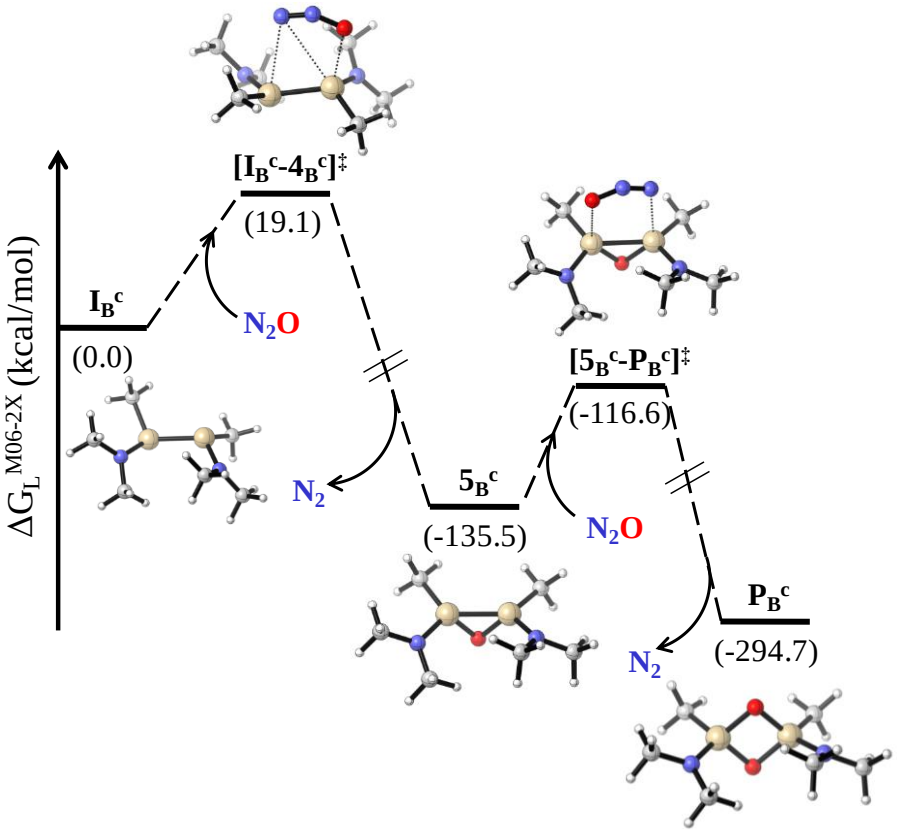

Figure S23. "Pathway IIb" energy profile diagram for $\mathbf{I_B^c}$.

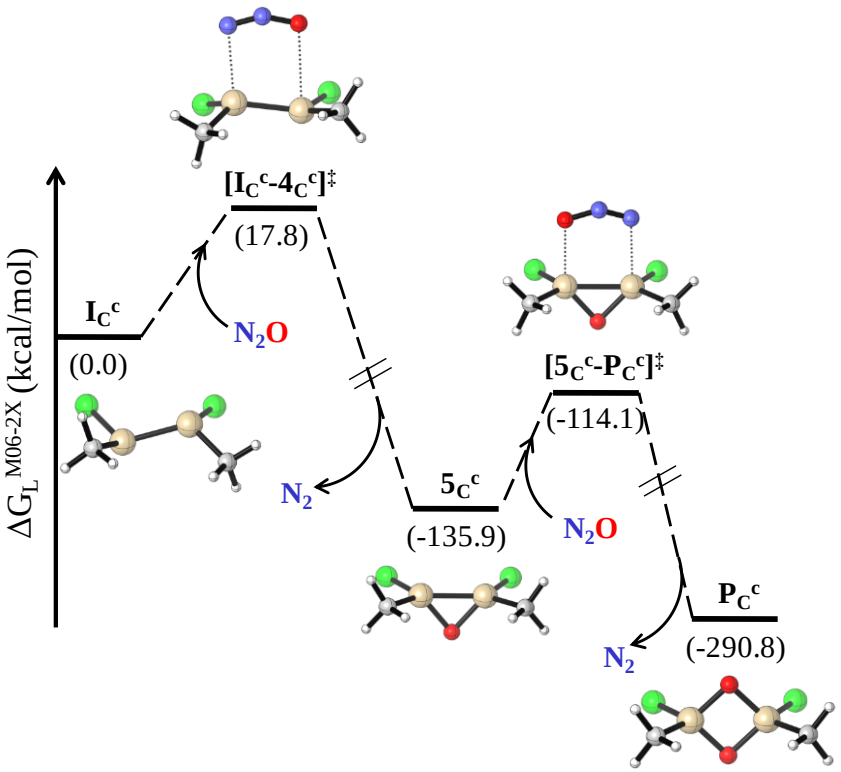

Figure S24. "Pathway IIb" energy profile diagram for $\mathbf{I_C^c}$.

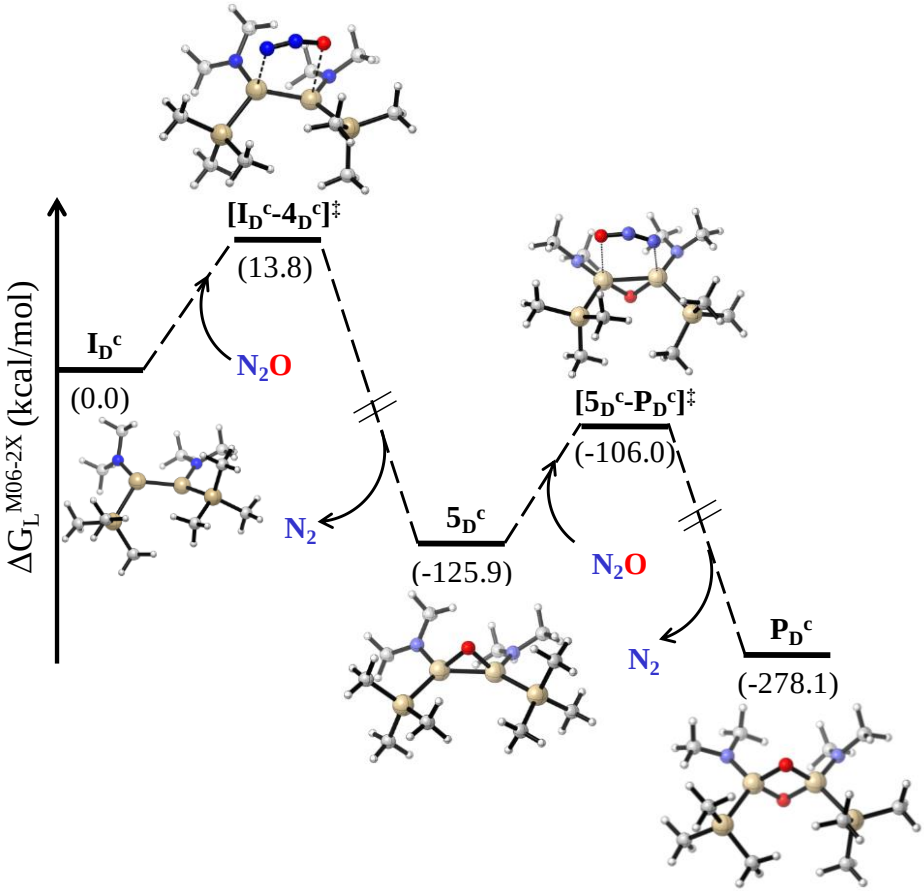

Figure S25. "Pathway IIb" energy profile diagram for $\mathbf{I_D^c}$.

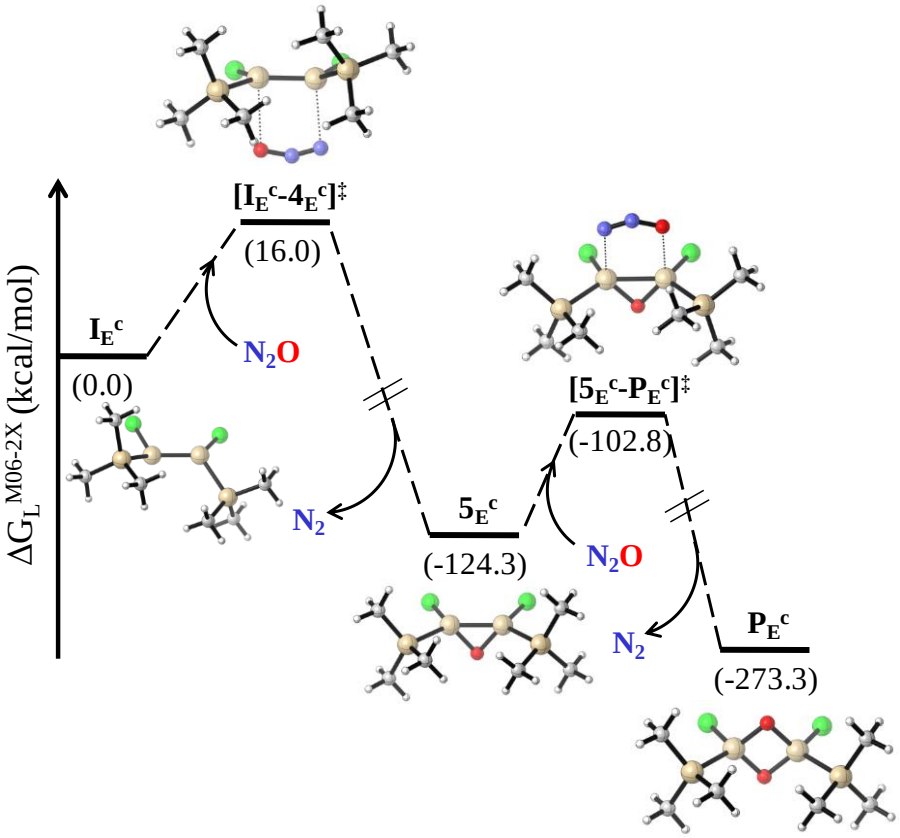

Figure S26. "Pathway IIb" energy profile diagram for $\mathbf{I_E^c}$.

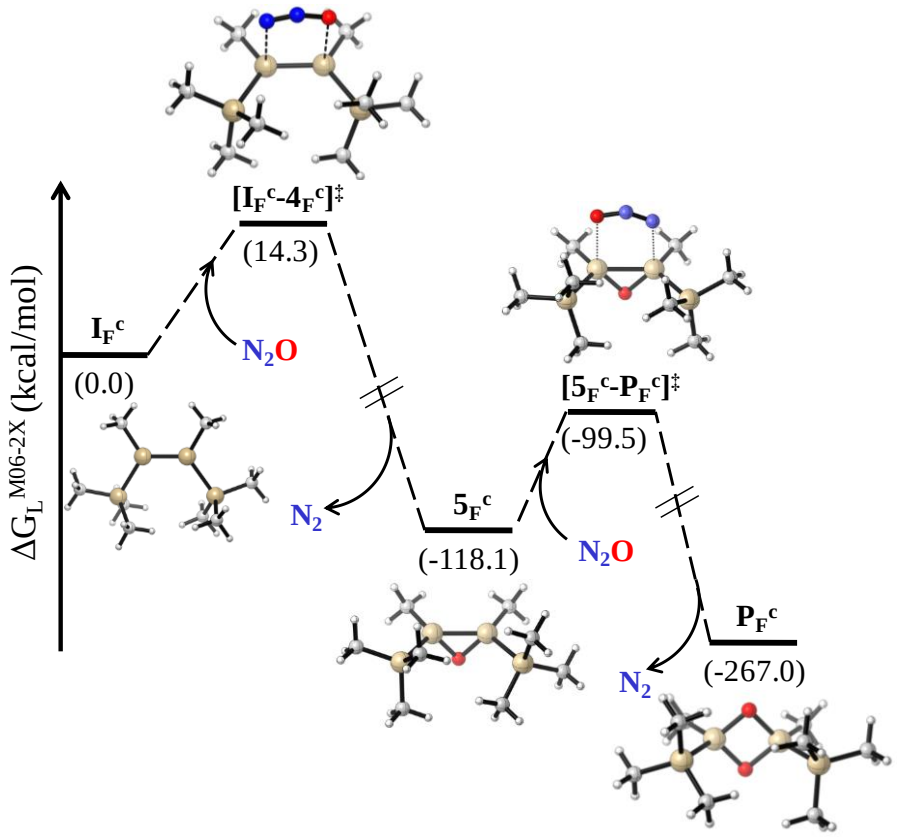

Figure S27. "Pathway IIb" energy profile diagram for $\mathbf{I_F^c}$.

Table S3. Energies (in kcal/mol) in the "Pathway IIb" for *cis*-disilenes.

Steps	$\mathbf{I_A^c}$	$\mathbf{I_B^c}$	$\mathbf{I_C^c}$	$\mathbf{I_D^c}$	$\mathbf{I_E^c}$	$\mathbf{I_F^c}$
$\mathbf{I_X^c + N_2O \rightarrow [I_X^c\text{-}4_X^c]^{\ddagger}}$	23.8	19.1	17.8	13.8	16.0	14.3
$\mathbf{[I_X^c\text{-}4_X^c]^{\ddagger} \rightarrow 5_X^c}$	-151.4	-154.6	-153.7	-139.7	-140.3	-132.4
$\mathbf{5_X^c + N_2O \rightarrow [5_X^c\text{-}P_X^c]^{\ddagger}}$	21.5	18.9	21.8	19.9	21.5	18.6
$\mathbf{[5_X^c\text{-}P_X^c]^{\ddagger} \rightarrow P_X^c + N_2}$	-176.3	-178.1	-176.7	-172.1	-169.5	-167.5

Table S4. Comparison of population between initial *trans*- and *cis*- disilenes, $\mathbf{I_X^t}$ and $\mathbf{I_X^c}$ respectively. $\Delta^{\ddagger}G(\mathbf{P_X^t})$ and $\Delta^{\ddagger}G(\mathbf{P_X^c})$ are the energy values for highest energy transition states $\mathbf{[I_X^t\text{-}4_X^t]^{\ddagger}}$ and $\mathbf{[I_X^c\text{-}4_X^c]^{\ddagger}}$ involved in $\mathbf{P_X^t}$ and $\mathbf{P_X^c}$ product formation respectively. All energy terms are Gibbs free energy at M06-2X/QZVP//ωB97xD/TZVP

	$\Delta\mathbf{G(I_X^t \rightarrow I_X^c)}$	$\mathbf{F(I_X^c)}/\mathbf{F(I_X^t)}$	$\Delta^{\ddagger}G(\mathbf{P_X^t})$	$\Delta^{\ddagger}G(\mathbf{P_X^c})$	$\lvert\Delta\Delta^{\ddagger}G\rvert$	product ratio
$\mathbf{I_A^t}$	1.4	0.155	26.0	23.8	2.2	10.09; $\mathbf{P_A^t < P_A^c}$
$\mathbf{I_B^t}$	0.6	0.363	19.7	19.1	0.6	2.75; $\mathbf{P_B^t < P_B^c}$
$\mathbf{I_C^t}$	0.6	0.363	17.3	17.8	0.5	2.29; $\mathbf{P_C^t > P_C^c}$
$\mathbf{I_D^t}$	-1.1	5.047	14.1	13.8	0.3	1.38; $\mathbf{P_D^t < P_D^c}$
$\mathbf{I_E^t}$	1.8	0.121	14.9	16.0	1.1	5.05; $\mathbf{P_E^t > P_E^c}$
$\mathbf{I_F^t}$	2.0	0.109	15.1	14.3	0.8	3.67; $\mathbf{P_F^t < P_F^c}$

[a] Φ is the population ration of $\mathbf{F(I_X^c)}$ and $\mathbf{F(I_X^t)}$, calculated using Boltzmann distribution.

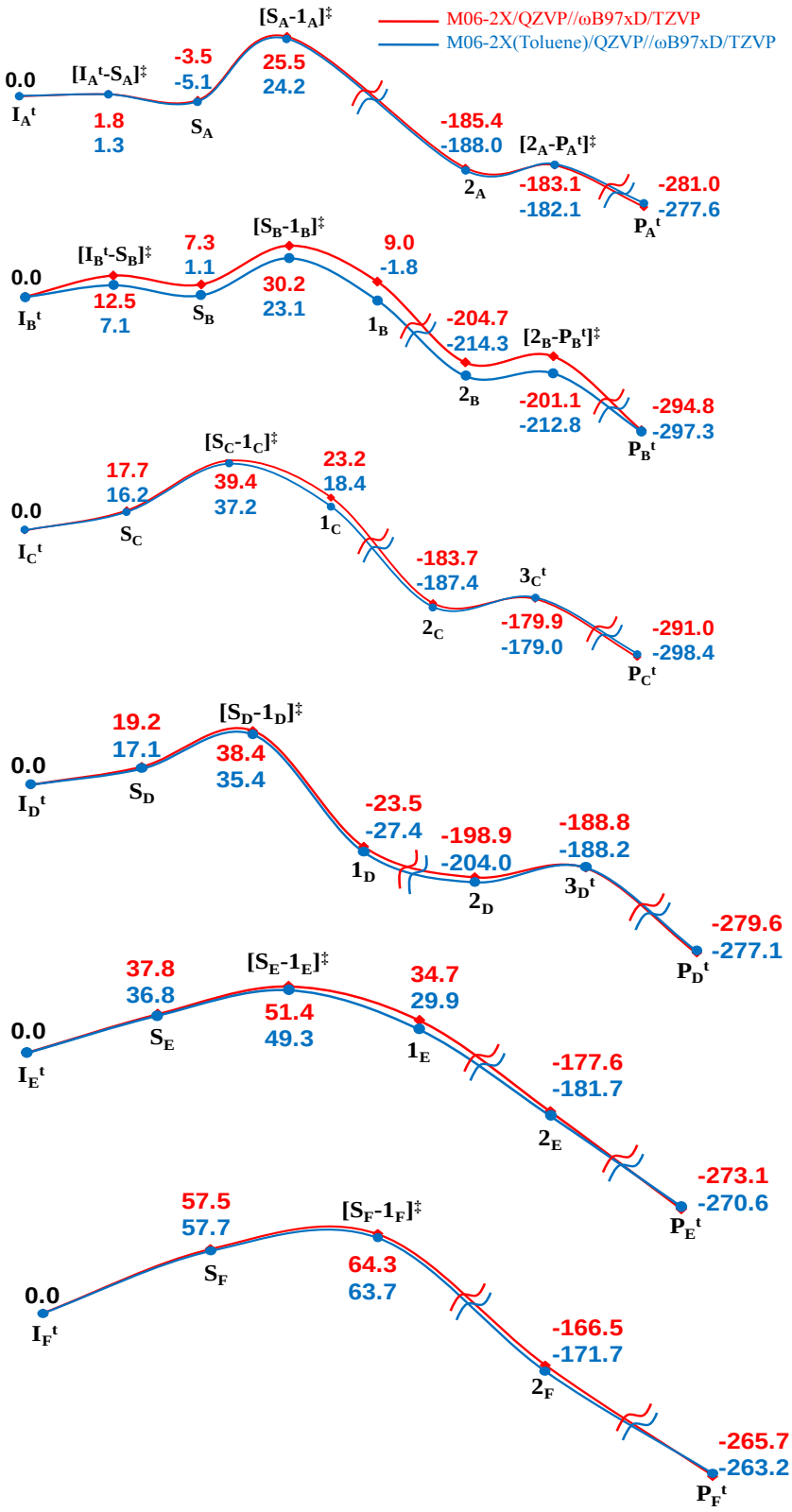

Figure 28. Computed energy profile (ΔG_L in kcal/mol) of "Pathway I" for $\mathbf{I_{A\text{-}F}}^t$ at gas phase and implicit solvation model (SMD).

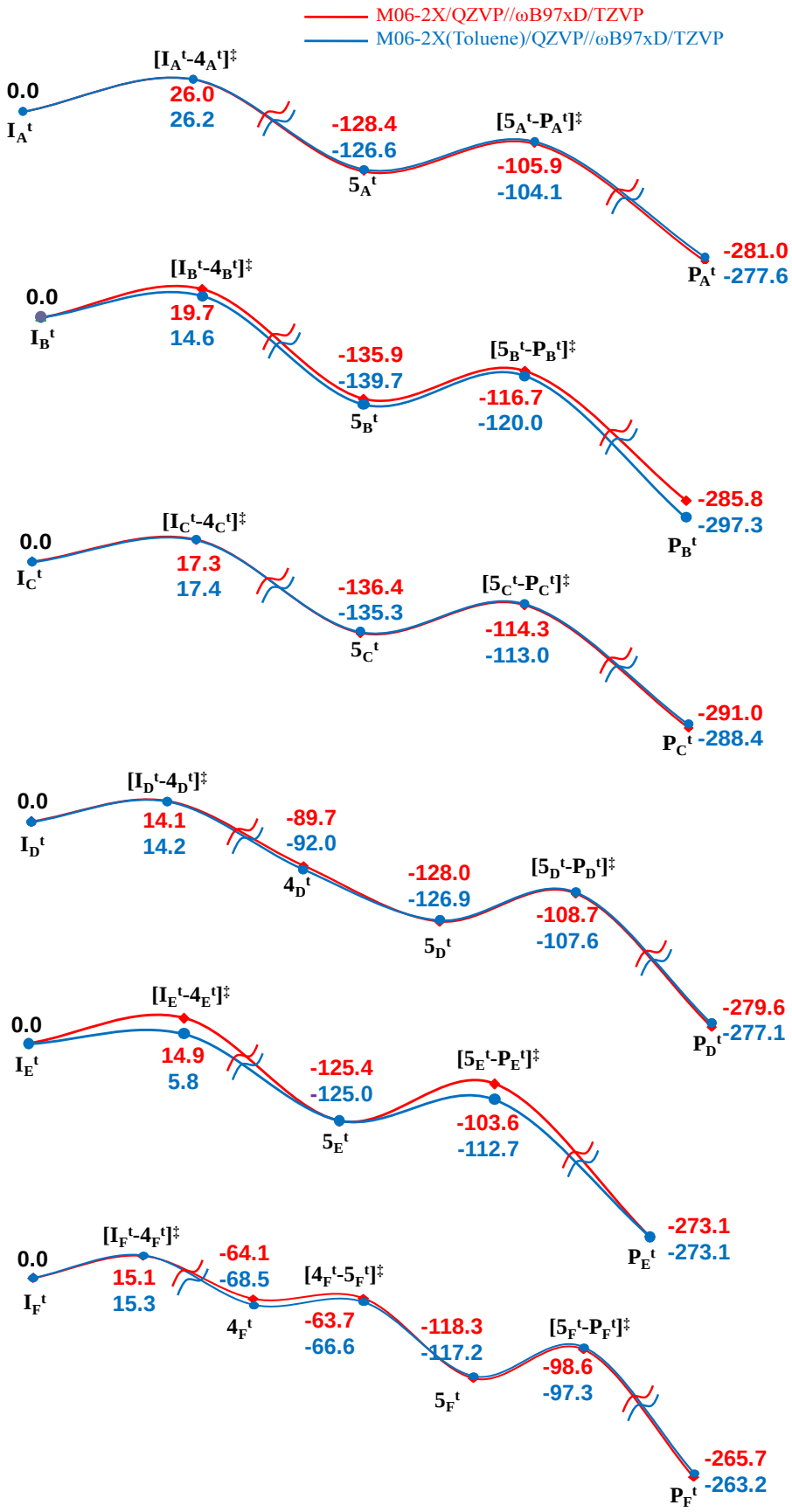

Figure 29. Computed energy profile (ΔG_L in kcal/mol) of "Pathway IIb" for $\mathbf{I_{A\text{-}F}}^t$ at gas phase and implicit solvation model (SMD).

Table S5. Cartesian coordinates (Å) of the optimized structures of all intermediates and transition states at ωB97xD/TZVP level of theory.

I_A^t

22

XYZ

Si	1.07476	0.29178	0.68922
Si	-1.07476	-0.29175	-0.68923
N	-2.41316	0.63630	-0.13948
N	2.41315	-0.63631	0.13950
C	-3.53658	0.25436	0.69276
H	-3.46337	0.73415	1.67596
H	-4.47722	0.56871	0.22941
H	-3.56408	-0.82317	0.83522
C	2.35875	-2.06825	0.39798
H	2.26401	-2.62851	-0.53863
H	3.26465	-2.40300	0.91293
H	1.49931	-2.31564	1.02466
C	-2.35880	2.06825	-0.39794
H	-3.26471	2.40299	-0.91286
H	-2.26405	2.62848	0.53869
H	-1.49937	2.31567	-1.02462
C	3.53658	-0.25441	-0.69273
H	4.47721	-0.56877	-0.22937
H	3.46337	-0.73421	-1.67592
H	3.56411	0.82312	-0.83521
Cl	1.56057	2.27864	0.10748
Cl	-1.56053	-2.27864	-0.10752

I_B^t

28

XYZ

Si	-0.89670	0.50102	-0.52435
Si	0.89669	-0.50101	0.52435
N	2.45979	0.18476	0.19395
N	-2.45979	-0.18477	-0.19396
C	3.49266	-0.43686	-0.60606
H	3.50555	-0.03751	-1.63058
H	4.48010	-0.25865	-0.16488
H	3.34489	-1.51378	-0.66749
C	-2.66971	-1.60584	-0.37145
H	-2.62692	-2.14784	0.58465
H	-3.64999	-1.79997	-0.82152
H	-1.90749	-2.02086	-1.03320
C	2.66973	1.60584	0.37141
H	3.65001	1.79997	0.82147
H	2.62695	2.14782	-0.58471
H	1.90751	2.02088	1.03314
C	-3.49266	0.43683	0.60606
H	-4.48010	0.25862	0.16489
H	-3.50554	0.03746	1.63058
H	-3.34489	1.51374	0.66752
C	1.02608	-2.37215	0.23717
H	0.06189	-2.83966	0.44397
H	1.31553	-2.63159	-0.78236
H	1.75945	-2.80285	0.92343
C	-1.02610	2.37216	-0.23712
H	-1.31556	2.63158	0.78241
H	-0.06192	2.83968	-0.44392
H	-1.75947	2.80287	-0.92338

I_C^t

12

XYZ

Si	-0.96264	0.43240	0.34663
Si	0.96264	-0.43231	-0.34662
Cl	-2.59358	-0.81609	-0.06078
Cl	2.59372	0.81599	0.06074
C	-1.43708	2.18633	-0.12684
H	-2.16975	2.57512	0.58271
H	-0.55265	2.82521	-0.09853
H	-1.87279	2.21955	-1.12577
C	1.43683	-2.18629	0.12690
H	1.87253	-2.21955	1.12582
H	0.55228	-2.82502	0.09862

H	2.16942	-2.57523	-0.58264

I_D^t

46

XYZ

Si	-0.90887	-0.70476	-0.19847
Si	0.90760	0.37067	0.48064
N	0.76126	2.10909	0.29763
N	-1.06800	-2.42521	-0.01993
C	1.30480	2.85637	-0.81262
H	0.51021	3.30700	-1.42549
H	1.95827	3.66914	-0.46720
H	1.88879	2.20782	-1.46619
C	0.10441	-3.26763	-0.12838
H	0.57507	-3.44783	0.84908
H	-0.16050	-4.23917	-0.55958
H	0.84466	-2.80320	-0.78236
C	0.05623	2.93389	1.25308
H	0.71378	3.71516	1.65813
H	-0.81337	3.43790	0.80693
H	-0.29890	2.32790	2.08712
C	-2.15303	-3.06162	0.69712
H	-2.44387	-3.99623	0.20459
H	-1.87370	-3.29789	1.73363
H	-3.02801	-2.41384	0.72857
Si	3.08931	-0.33331	-0.06438
Si	-2.94457	0.48979	-0.19513
C	-4.34119	-0.52624	-0.97187
H	-4.70849	-1.30579	-0.30242
H	-5.18193	0.13273	-1.20505
H	-4.01989	-1.00225	-1.90021
C	-2.63172	2.00223	-1.28359
H	-1.73230	2.53119	-0.96605
H	-2.49026	1.70485	-2.32456
H	-3.47527	2.69567	-1.23736
C	-3.46267	1.04357	1.53564
H	-2.70994	1.70355	1.97012
H	-4.41141	1.58561	1.49544
H	-3.58602	0.18993	2.20504
C	3.52494	-1.93012	0.85227
H	2.90882	-2.76869	0.52445
H	4.57082	-2.18998	0.66826
H	3.38740	-1.81294	1.92874
C	3.35097	-0.61756	-1.91837
H	4.38113	-0.92410	-2.12023
H	2.68144	-1.39637	-2.28897
H	3.14869	0.29008	-2.49053
C	4.25195	1.03959	0.52314
H	4.03496	1.98413	0.02069
H	4.14738	1.20321	1.59763
H	5.29303	0.77707	0.31804

I_E^t

30

XYZ

Si	0.91419	0.51156	-0.31692
Si	-0.91063	-0.50884	0.29413
Si	-3.11534	0.26423	-0.00661
C	-4.16158	-0.40662	1.41120
H	-5.20965	-0.13207	1.26678
H	-4.10323	-1.49561	1.46242
H	-3.83316	-0.00284	2.37052
C	-3.75186	-0.39700	-1.65220
H	-3.19436	0.03100	-2.48684
H	-3.65425	-1.48304	-1.70082
H	-4.80805	-0.14438	-1.77792
C	-3.06829	2.14608	0.01136
H	-2.66672	2.52650	0.95209
H	-2.44511	2.53221	-0.79696
H	-4.07813	2.54525	-0.11415
Si	3.11347	-0.26639	0.01123
C	3.10303	-2.13234	-0.23906
H	4.10847	-2.53416	-0.08925
H	2.43065	-2.62249	0.46697
H	2.77899	-2.39548	-1.24747
C	3.64975	0.19297	1.75852
H	4.70100	-0.06471	1.91267
H	3.53375	1.26438	1.93179
H	3.05190	-0.33767	2.50118
C	4.21915	0.59366	-1.25026

H	4.14977	1.67873	-1.15108
H	5.26208	0.30724	-1.09238
H	3.94425	0.32727	-2.27230
Cl	-0.81420	-2.58927	-0.02916
Cl	0.81813	2.58995	0.02221

I_F^t

36

XYZ

Si	0.86022	-0.64149	0.00028
Si	-0.86022	0.64149	-0.00030
C	-0.66579	2.52946	-0.00015
H	0.38481	2.81824	0.00017
H	-1.13924	2.96296	-0.88324
H	-1.13973	2.96283	0.88275
Si	-3.07517	-0.11877	0.00004
C	-3.96370	0.53740	-1.53608
H	-5.01649	0.24255	-1.52375
H	-3.92250	1.62786	-1.58190
H	-3.51017	0.14545	-2.44841
C	-3.96328	0.53871	1.53583
H	-3.50948	0.14765	2.44840
H	-3.92205	1.62922	1.58056
H	-5.01608	0.24387	1.52411
C	-3.12938	-2.00636	0.00065
H	-2.63875	-2.41590	-0.88443
H	-2.63841	-2.41548	0.88572
H	-4.16641	-2.35194	0.00090
C	0.66579	-2.52947	0.00015
Si	3.07517	0.11877	-0.00004
H	-0.38481	-2.81824	-0.00018
H	1.13973	-2.96284	-0.88275
H	1.13923	-2.96296	0.88325
C	3.12937	2.00636	-0.00066
H	4.16640	2.35195	-0.00089
H	2.63843	2.41547	-0.88575
H	2.63871	2.41591	0.88440
C	3.96331	-0.53871	-1.53581
H	5.01611	-0.24388	-1.52407
H	3.92209	-1.62922	-1.58054
H	3.50953	-0.14766	-2.44839
C	3.96368	-0.53739	1.53610
H	3.92248	-1.62785	1.58192
H	5.01647	-0.24253	1.52379
H	3.51013	-0.14544	2.44842

I_R

6

XYZ

Si	-1.06266	0.00015	-0.11632
Si	1.06266	-0.00015	0.11632
H	1.84744	1.24361	-0.05868
H	1.84710	-1.24412	-0.05874
H	-1.84744	-1.24361	0.05868
H	-1.84710	1.24412	0.05874

$[I_A^t\text{-}S_A]^‡$

22

XYZ

N	2.14638	0.90455	0.18473
Si	1.29034	-0.36658	0.96479
Si	-1.28198	0.28534	-0.98285
N	-2.18180	-0.89585	-0.11534
C	-1.89529	-2.28749	-0.44349
H	-1.46038	-2.80395	0.41836
H	-2.80940	-2.81026	-0.74005
H	-1.17957	-2.34968	-1.26592
C	-3.10012	-0.76383	0.99974
H	-4.03146	-1.29810	0.78810
H	-2.65692	-1.19302	1.90518
H	-3.33025	0.28167	1.18732
C	3.05668	0.88505	-0.94470
H	2.59803	1.38262	-1.80626
H	3.98097	1.41527	-0.69519
H	3.30226	-0.13636	-1.22316
C	1.83759	2.25765	0.63267
H	2.74514	2.76942	0.96647
H	1.38501	2.83801	-0.17741
H	1.12894	2.23527	1.46315
Cl	-1.95607	2.10636	-0.08959

Cl	2.01874	-2.09476	-0.05856

S_A

11

XYZ

Si	-0.30788	-1.05189	0.00001
N	0.99652	0.07289	0.00002
C	1.01247	1.52505	0.00001
H	1.53563	1.89905	0.88602
H	1.53565	1.89904	-0.88601
H	0.00040	1.92087	-0.00002
C	2.33921	-0.49591	-0.00002
H	2.89488	-0.17785	-0.88770
H	2.89503	-0.17761	0.88748
H	2.29248	-1.58708	0.00012
Cl	-1.99585	0.25088	-0.00001

$[S_A\text{-}1_A]^‡$

14

XYZ

N	-0.93424	1.07300	-0.04359
Si	0.00392	-0.32337	-0.33691
N	1.61329	-0.47962	1.02221
N	2.57561	-0.16911	0.44008
O	2.91379	0.16505	-0.66741
C	-0.24447	2.35626	-0.11097
H	-0.72279	3.01138	-0.84483
H	-0.26127	2.85322	0.86368
H	0.79718	2.21983	-0.40928
C	-2.34639	1.19876	0.27209
H	-2.47242	1.68316	1.24562
H	-2.85217	1.80871	-0.48251
H	-2.82276	0.22225	0.30746
Cl	-1.30991	-1.93481	-0.08951

2_A

12

XYZ

N	-1.10062	-0.26284	-0.00006
Si	0.34515	0.60001	0.00000
O	0.50645	2.11741	0.00004
C	-2.35362	0.48828	-0.00003
H	-2.94193	0.24186	-0.88880
H	-2.94218	0.24130	0.88843
H	-2.15114	1.55817	0.00035
C	-1.27845	-1.70459	0.00005
H	-1.83726	-2.01654	0.88747
H	-1.83736	-2.01666	-0.88728
H	-0.31940	-2.21670	0.00001
Cl	1.92014	-0.70547	-0.00001

$[2_A\text{-}P_A{}^c]^‡$

24

XYZ

Si	1.74855	0.08528	-0.81722
O	-0.78348	0.36241	1.95418
Si	-1.70400	-0.04847	0.80102
O	0.95773	0.79939	-1.91837
N	-2.15926	0.87577	-0.51883
N	2.21045	0.69634	0.67200
C	1.81162	2.06274	1.01551
H	1.01660	2.03219	1.76563
H	2.67435	2.60839	1.40696
H	1.44458	2.58113	0.13117
C	2.69810	-0.06661	1.81169
H	3.02156	-1.05963	1.50836
H	3.55040	0.45098	2.25982
H	1.90320	-0.16399	2.55550
C	-1.64778	2.24319	-0.62374
H	-1.19292	2.54725	0.31823
H	-0.89358	2.29154	-1.41219
H	-2.47295	2.92443	-0.84774
C	-2.82139	0.41605	-1.73008
H	-2.12035	0.45202	-2.56833
H	-3.18240	-0.60335	-1.61667
H	-3.67489	1.06200	-1.95321
Cl	2.38446	-1.84764	-1.02639
Cl	-2.54286	-1.90939	0.70169

$[2_A\text{-}P_A{}^t]^‡$

24
XYZ

Si	1.68549	0.04651	0.78005
O	-1.16154	-0.81155	-1.98321
Si	-1.69951	-0.06570	-0.75981
O	1.11468	0.74122	2.01835
N	-1.31872	1.49211	-0.26461
N	1.33141	-1.49327	0.21495
C	0.46497	-2.36226	1.00941
H	-0.39554	-2.67552	0.41227
H	1.01272	-3.25566	1.32177
H	0.11149	-1.84010	1.89802
C	1.73553	-2.08066	-1.05787
H	2.45492	-1.44453	-1.56726
H	2.19930	-3.05444	-0.87925
H	0.85848	-2.19592	-1.69926
C	-0.46218	2.31857	-1.11304
H	-0.12747	1.75391	-1.98269
H	-1.01014	3.20044	-1.45637
H	0.41136	2.65397	-0.54775
C	-1.69900	2.13770	0.98712
H	-2.15329	3.10880	0.77304
H	-2.41869	1.53276	1.53253
H	-0.81419	2.26842	1.61451
Cl	3.04028	0.95599	-0.45389
Cl	-3.03337	-0.91439	0.53683

P_A^c
24
XYZ

Si	-1.20487	-0.24413	-0.03279
O	0.02143	-0.22082	-1.17971
Si	1.20493	-0.24422	0.03289
O	-0.02139	-0.22098	1.17982
N	2.28433	1.05219	0.18391
N	-2.28426	1.05230	-0.18368
C	-1.81289	2.33627	-0.67810
H	-2.49654	2.71453	-1.44466
H	-1.75430	3.08060	0.12492
H	-0.82869	2.23583	-1.13485
C	-3.64081	1.08860	0.32888
H	-3.95625	0.10331	0.66658
H	-3.72580	1.78479	1.17096
H	-4.33272	1.41442	-0.45462
C	1.81283	2.33618	0.67821
H	0.82866	2.23573	1.13500
H	2.49647	2.71457	1.44473
H	1.75423	3.08043	-0.12489
C	3.64065	1.08890	-0.32919
H	4.33270	1.41534	0.45391
H	3.95645	0.10363	-0.66665
H	3.72502	1.78479	-1.17159
Cl	-2.25690	-2.00373	0.07228
Cl	2.25694	-2.00379	-0.07237

P_A^t
24
XYZ

Si	-1.17583	0.27723	0.00196
O	-0.00024	0.00611	-1.17701
Si	1.17583	-0.27723	-0.00196
O	0.00024	-0.00611	1.17701
N	2.53088	0.73211	-0.00328
N	-2.53088	-0.73211	0.00328
C	-2.32881	-2.17403	0.01244
H	-2.79423	-2.62224	0.89613
H	-2.76467	-2.63085	-0.88191
H	-1.26807	-2.42536	0.03215
C	-3.92722	-0.34366	-0.01521
H	-4.03374	0.73855	-0.01989
H	-4.42437	-0.74044	-0.90693
H	-4.44477	-0.73440	0.86747
C	2.32881	2.17403	-0.01245
H	1.26807	2.42536	-0.03218
H	2.76467	2.63086	0.88190
H	2.79424	2.62224	-0.89614
C	3.92722	0.34366	0.01522
H	4.42436	0.74044	0.90694
H	4.03374	-0.73855	0.01991
H	4.44478	0.73439	-0.86746

Cl	-1.78458	2.24534	0.00749
Cl	1.78458	-2.24534	-0.00748

$[I_B^t\text{-}S_B]^‡$

28

XYZ

Si	-1.07646	-0.54463	1.11088
Si	1.07640	0.97845	-0.86786
N	2.09346	-0.30524	-0.28904
N	-2.22859	0.21851	0.06611
C	2.89844	-0.35818	0.91594
H	2.49028	-1.09561	1.61820
H	3.92796	-0.65021	0.68089
H	2.92067	0.60611	1.41629
C	-2.45067	1.64857	0.19984
H	-2.07536	2.18271	-0.68242
H	-3.51799	1.87056	0.30445
H	-1.93082	2.02994	1.07987
C	2.13198	-1.56097	-1.02018
H	3.14970	-1.78500	-1.35848
H	1.79352	-2.39302	-0.39205
H	1.48387	-1.50506	-1.89597
C	-2.88602	-0.31722	-1.10970
H	-3.95007	-0.05761	-1.10635
H	-2.43732	0.09929	-2.02024
H	-2.79989	-1.40016	-1.14955
C	1.45681	2.38514	0.37707
H	0.87402	3.27002	0.11205
H	1.20113	2.11204	1.40414
H	2.51484	2.66666	0.35250
C	-1.06871	-2.34230	0.44434
H	-0.77270	-2.39220	-0.60754
H	-0.36240	-2.94385	1.02027
H	-2.05359	-2.81127	0.53821

S_B

14

XYZ

Si	0.77168	-0.92946	-0.00002
N	-0.66948	0.03390	-0.00002
C	-1.95981	-0.63912	0.00007
H	-2.54370	-0.36631	0.88653
H	-2.54382	-0.36632	-0.88632
H	-1.81842	-1.72042	0.00007
C	-0.82129	1.47715	0.00003
H	-1.37832	1.80773	-0.88419
H	-1.37760	1.80778	0.88468
H	0.14442	1.97568	-0.00039
C	2.13488	0.42199	-0.00005
H	2.08021	1.06607	0.88372
H	3.11700	-0.05506	0.00007
H	2.08033	1.06584	-0.88399

$[S_B\text{-}1_B]^‡$

17

XYZ

N	1.23571	-0.64516	-0.08117
Si	0.14104	0.60468	-0.53553
N	-1.48206	0.58004	0.76253
N	-2.44218	-0.00417	0.49165
O	-3.02036	-0.64830	-0.33759
C	1.02798	2.22944	-0.12737
H	0.36273	3.07032	-0.32951
H	1.32633	2.27997	0.92270
H	1.92179	2.35460	-0.74363
C	0.82647	-2.03460	-0.20868
H	1.53559	-2.59505	-0.82750
H	0.77542	-2.51895	0.77308
H	-0.15841	-2.09852	-0.67387
C	2.56112	-0.50548	0.49111
H	2.59266	-0.92243	1.50467
H	3.30136	-1.04009	-0.11405
H	2.85715	0.53980	0.54482

1_B

17

XYZ

N	1.06587	-0.70258	0.01789
Si	0.09842	0.68320	-0.01147
N	-1.47971	0.83805	0.46382

N	-2.48192	0.01856	0.29960
O	-2.40274	-0.79794	-0.61159
C	1.06848	2.25950	-0.16262
H	0.36717	3.09262	-0.13899
H	1.77608	2.37526	0.66021
H	1.62694	2.29366	-1.09938
C	0.50323	-2.04184	0.15617
H	0.92973	-2.70108	-0.60510
H	0.73175	-2.45627	1.14248
H	-0.57652	-2.01738	0.01784
C	2.51890	-0.68342	-0.03453
H	2.94175	-1.11325	0.87879
H	2.87551	-1.27032	-0.88615
H	2.89840	0.33178	-0.13964

2_B

15

XYZ

N	0.90313	0.07500	-0.00036
Si	-0.76401	-0.25125	0.00025
O	-1.33851	-1.67346	-0.00064
C	-1.76603	1.32089	0.00054
H	-2.82316	1.06015	0.02245
H	-1.53872	1.93823	0.87145
H	-1.57045	1.91477	-0.89420
C	1.51080	1.39068	-0.00044
H	2.13587	1.53044	0.88821
H	2.14371	1.52612	-0.88414
H	0.75368	2.17352	-0.00602
C	1.86227	-1.01936	0.00056
H	2.50278	-0.97225	-0.88659
H	2.50169	-0.97187	0.88848
H	1.33477	-1.97215	0.00044

$[2_B\text{-}P_B{}^c]^‡$

30

XYZ

Si	-1.30394	-0.11235	1.09493
O	0.90436	-1.42800	-1.55831
Si	1.79659	-0.58043	-0.63224
O	-0.92346	1.14499	1.89951
N	1.56595	1.07816	-0.39913
N	-2.28050	-0.07023	-0.28766
C	-2.86757	1.17596	-0.74879
H	-2.45850	1.46131	-1.72435
H	-3.95271	1.07267	-0.85154
H	-2.65905	1.97341	-0.03617
C	-2.47660	-1.18712	-1.19623
H	-2.05456	-2.10271	-0.78816
H	-3.54484	-1.34486	-1.37706
H	-1.97348	-1.00128	-2.14943
C	0.59781	1.82283	-1.19226
H	0.11542	1.15950	-1.90986
H	-0.16311	2.25605	-0.53729
H	1.09542	2.63182	-1.73639
C	2.15121	1.86156	0.67839
H	1.36833	2.14983	1.38659
H	2.90629	1.28660	1.21315
H	2.62958	2.75985	0.27605
C	-0.79341	-1.84875	1.53655
H	-0.14531	-1.82157	2.41181
H	-1.67040	-2.45497	1.77266
H	-0.27128	-2.32483	0.70407
C	3.17156	-1.25639	0.42478
H	3.36413	-2.28895	0.13707
H	4.08863	-0.67608	0.31593
H	2.88508	-1.23702	1.47845

$[2_B\text{-}P_B{}^t]^‡$

30

XYZ

Si	1.28532	0.66053	0.14785
O	0.03679	-0.30735	-1.91015
Si	-0.88576	-0.57695	-0.66841
O	1.32636	1.64115	1.33729
N	-1.26784	0.99044	0.00173
N	0.54839	-1.01890	0.55412
C	0.29280	-1.17985	2.00231
H	-0.47997	-1.93617	2.15848
H	1.20713	-1.50055	2.50435

H	-0.00545	-0.23035	2.43566
C	1.29667	-2.18852	0.03986
H	1.38146	-2.11335	-1.04155
H	2.29005	-2.23364	0.49161
H	0.75721	-3.10264	0.29729
C	-1.36536	2.15955	-0.86786
H	-0.87387	1.95293	-1.81743
H	-2.41252	2.42028	-1.06038
H	-0.87915	3.01507	-0.38889
C	-1.89981	1.21962	1.29031
H	-2.87882	1.69324	1.15947
H	-2.06091	0.28270	1.82502
H	-1.26771	1.86760	1.90570
C	2.61843	0.66119	-1.14558
H	2.69878	-0.29437	-1.65676
H	2.34979	1.40467	-1.89648
H	3.56227	0.94916	-0.68074
C	-2.18682	-1.89332	-0.47372
H	-2.99389	-1.71792	-1.18734
H	-1.77540	-2.88485	-0.66995
H	-2.61737	-1.88516	0.52978

P_B^t

30

XYZ

Si	1.09258	0.52623	-0.10487
O	0.01492	0.16743	1.17176
Si	-1.09258	-0.52623	0.10487
O	-0.01492	-0.16743	-1.17176
N	-2.59130	0.30174	0.11422
N	2.59130	-0.30174	-0.11423
C	1.35100	2.36292	-0.26840
H	1.73426	2.79083	0.65982
H	2.04489	2.60259	-1.07517
H	0.39449	2.84057	-0.48540
C	-1.35100	-2.36292	0.26840
H	-2.04489	-2.60259	1.07517
H	-1.73426	-2.79083	-0.65982
H	-0.39449	-2.84057	0.48539
C	2.64793	-1.74459	-0.23719
H	3.47056	-2.03724	-0.89894
H	2.80259	-2.23525	0.73293
H	1.72505	-2.12419	-0.67593
C	3.83444	0.28791	0.33463
H	3.75231	1.37313	0.39344
H	4.12813	-0.08153	1.32603
H	4.64558	0.05263	-0.36400
C	-2.64793	1.74459	0.23719
H	-1.72505	2.12419	0.67592
H	-2.80259	2.23525	-0.73293
H	-3.47056	2.03724	0.89894
C	-3.83444	-0.28791	-0.33462
H	-4.12814	0.08153	-1.32602
H	-3.75231	-1.37313	-0.39343
H	-4.64558	-0.05263	0.36400

P_B^c

30

XYZ

Si	-1.21615	-0.58174	0.03144
O	-0.01760	-0.55982	-1.18343
Si	1.21613	-0.58186	-0.03137
O	0.01753	-0.56032	1.18352
N	2.22904	0.78978	-0.18832
N	-2.22928	0.78970	0.18887
C	-2.22208	-2.14453	-0.07475
H	-2.98280	-2.18918	0.70550
H	-2.71078	-2.23592	-1.04634
H	-1.55672	-3.00148	0.04143
C	2.22201	-2.14466	0.07440
H	2.98176	-2.19000	-0.70674
H	2.71185	-2.23553	1.04547
H	1.55626	-3.00151	-0.04029
C	-1.71935	2.06691	0.64528
H	-1.63107	2.79216	-0.17452
H	-2.38859	2.49416	1.40080
H	-0.73917	1.94138	1.10447
C	-3.57708	0.85644	-0.33253
H	-3.93279	-0.13211	-0.62320
H	-4.26629	1.24737	0.42536

H	-3.64195	1.50928	-1.21263
C	1.71962	2.06696	-0.64535
H	0.73940	1.94165	-1.10449
H	1.63167	2.79261	0.17413
H	2.38910	2.49355	-1.40104
C	3.57711	0.85631	0.33241
H	3.64269	1.51046	1.21147
H	3.93221	-0.13202	0.62455
H	4.26638	1.24562	-0.42628

S_C

6

XYZ

Si	-0.48828	0.81346	-0.00000
Cl	1.33157	-0.26300	0.00000
C	-1.67834	-0.66453	-0.00001
H	-1.50522	-1.29541	0.87809
H	-2.72070	-0.33902	-0.00029
H	-1.50483	-1.29586	-0.87770

$[S_C\text{-}1_C]^{‡}$

9

XYZ

Si	0.47395	0.38042	-0.47985
N	-1.08006	0.47137	0.49222
N	-2.17508	0.07059	0.41313
O	-2.97548	-0.37998	-0.35442
C	1.56347	1.79292	0.11044
H	1.05784	2.74936	-0.03090
H	1.82170	1.67257	1.16399
H	2.49006	1.80029	-0.46680
Cl	1.48259	-1.35644	0.11100

1_C

9

XYZ

Si	0.48696	0.40374	0.00157
N	-1.04996	0.74246	0.25350
N	-2.20973	0.11275	0.47029
O	-2.77829	-0.29772	-0.50545
C	1.79317	1.70079	-0.14361
H	1.32541	2.68337	-0.10441
H	2.51318	1.60181	0.66975
H	2.32816	1.58617	-1.08709
Cl	1.25300	-1.49019	0.01990

2_C

7

XYZ

Si	-0.44168	0.21663	-0.00009
Cl	1.58067	-0.13301	0.00008
C	-1.32158	-1.41476	-0.00000
H	-1.03355	-1.99015	0.88145
H	-2.39840	-1.25450	-0.00023
H	-1.03321	-1.99046	-0.88113
O	-1.03665	1.61901	-0.00003

3_C^c

14

XYZ

Si	-1.94194	0.33448	-0.27862
O	1.04476	0.50173	1.53843
Si	1.94094	0.33434	0.27926
O	-1.04582	0.50717	-1.53714
C	2.05583	1.46040	-1.19573
H	2.92021	1.22805	-1.84556
H	1.09564	1.29440	-1.73945
H	2.08510	2.51722	-0.86202
C	-2.06315	1.45904	1.19729
H	-2.92758	1.22306	1.84584
H	-1.10368	1.29637	1.74311
H	-2.09613	2.51595	0.86420
Cl	3.16619	-1.32189	0.06331
Cl	-3.16074	-1.32673	-0.06537

3_C^t

14

XYZ

Si	1.89186	0.21374	0.52098
O	-0.99933	0.72134	-1.38516

Si	-1.89194	-0.21316	-0.52118
O	0.99884	-0.71945	1.38592
C	-1.62592	-2.01724	-0.15348
H	-0.79973	-2.02876	0.59549
H	-2.52808	-2.50737	0.25837
H	-1.27250	-2.54066	-1.06448
C	1.62660	2.01744	0.15090
H	2.52801	2.50576	-0.26472
H	0.79804	2.02845	-0.59549
H	1.27675	2.54300	1.06206
Cl	3.58364	-0.50592	-0.43566
Cl	-3.58372	0.50445	0.43690

P_C^c

14

XYZ

Si	1.20054	0.33218	-0.00010
O	0.00006	0.35070	-1.18585
Si	-1.20054	0.33218	-0.00024
O	-0.00007	0.35076	1.18553
C	-2.36237	1.76730	0.00003
H	-3.00019	1.73665	-0.88429
H	-2.99998	1.73510	0.88453
H	-1.80329	2.70366	0.00101
C	2.36237	1.76730	0.00022
H	2.99852	1.73664	0.88580
H	3.00164	1.73512	-0.88302
H	1.80328	2.70365	-0.00151
Cl	-2.26844	-1.42562	0.00015
Cl	2.26844	-1.42562	0.00004

P_C^t

14

XYZ

Si	-1.13148	0.39957	-0.00009
O	-0.00000	-0.00003	1.18628
Si	1.13148	-0.39958	-0.00010
O	-0.00000	-0.00000	-1.18645
C	1.74752	-2.13802	-0.00112
H	2.35607	-2.32409	-0.88689
H	2.35701	-2.32499	0.88384
H	0.90150	-2.82652	-0.00102
C	-1.74746	2.13803	-0.00108
H	-2.35596	2.32415	-0.88687
H	-2.35698	2.32499	0.88386
H	-0.90140	2.82649	-0.00092
Cl	-2.72021	-0.91364	0.00073
Cl	2.72017	0.91367	0.00075

S_D

23

XYZ

Si	-0.75053	-1.26208	-0.00084
N	-1.96584	-0.02641	-0.00031
C	-3.36904	-0.42710	0.00002
H	-3.88184	-0.03778	0.88647
H	-3.88243	-0.03711	-0.88578
H	-3.45054	-1.51337	-0.00036
C	-1.84566	1.42165	-0.00011
H	-2.33061	1.84930	-0.88482
H	-2.33058	1.84904	0.88473
H	-0.80485	1.72952	-0.00009
Si	1.32292	-0.00310	-0.00007
C	1.56660	1.07550	-1.54534
H	0.82891	1.87660	-1.61780
H	2.55871	1.53481	-1.52770
H	1.49459	0.47556	-2.45534
C	2.70098	-1.30557	-0.00079
H	2.63831	-1.95042	0.87894
H	2.64101	-1.94632	-0.88371
H	3.68450	-0.82870	0.00183
C	1.56486	1.07232	1.54771
H	1.49194	0.47051	2.45640
H	2.55690	1.53187	1.53217
H	0.82690	1.87310	1.62096

$[S_D\text{-}1_D]^‡$

26

XYZ

N	0.71713	1.88714	-0.15096

Si	0.55725	0.23933	-0.64389
N	1.65115	-0.87591	0.63175
N	2.45957	-1.67864	0.46308
O	3.24045	-2.23085	-0.25471
C	2.00439	2.55227	-0.27252
H	1.90519	3.49553	-0.82119
H	2.42663	2.77704	0.71430
H	2.70972	1.91705	-0.80915
C	-0.26917	2.71760	0.51227
H	0.00539	2.90182	1.55856
H	-0.35396	3.68798	0.01108
H	-1.24919	2.24607	0.49777
Si	-1.62694	-0.53420	-0.04217
C	-2.93973	0.31110	-1.11334
H	-3.92394	-0.11821	-0.90872
H	-2.99827	1.38450	-0.92199
H	-2.72916	0.17253	-2.17591
C	-1.61643	-2.38465	-0.43021
H	-0.87138	-2.91000	0.17150
H	-2.59238	-2.82607	-0.21316
H	-1.38809	-2.57020	-1.48175
C	-2.05388	-0.31090	1.78909
H	-2.11021	0.73946	2.07893
H	-3.02187	-0.77141	2.00517
H	-1.30251	-0.79194	2.41823

1_D

26

XYZ

N	1.72842	0.96837	-0.02266
Si	0.62662	-0.32903	-0.01547
N	0.90694	-1.75682	1.14770
N	1.07482	-2.48877	0.19872
O	1.08587	-1.60983	-1.04091
C	3.15920	0.73808	-0.14847
H	3.57299	1.34572	-0.95956
H	3.68320	0.99599	0.77851
H	3.35571	-0.30840	-0.38039
C	1.38051	2.35050	0.23763
H	1.82161	2.70356	1.17670
H	1.74028	2.99727	-0.56977
H	0.29979	2.47458	0.30907
Si	-1.66607	0.21216	-0.02815
C	-2.03193	1.30527	-1.52291
H	-3.10631	1.49062	-1.59794
H	-1.52934	2.27173	-1.45191
H	-1.70924	0.82434	-2.44821
C	-2.55286	-1.44227	-0.18060
H	-2.36499	-2.07113	0.69156
H	-3.63140	-1.28980	-0.26594
H	-2.21337	-1.98550	-1.06442
C	-2.15802	1.08495	1.57193
H	-1.66714	2.05414	1.67901
H	-3.23760	1.25445	1.58687
H	-1.90141	0.47857	2.44268

2_D

24

XYZ

Si	0.67956	0.78894	-0.00041
N	1.95387	-0.34864	-0.00014
C	3.34024	0.09058	0.00018
H	3.86301	-0.28132	0.88797
H	3.86338	-0.28121	-0.88744
H	3.38056	1.17928	0.00024
C	1.78833	-1.78630	-0.00014
H	2.24958	-2.23496	-0.88685
H	2.24930	-2.23497	0.88671
H	0.73213	-2.05683	-0.00032
Si	-1.50213	-0.12030	0.00003
C	-1.76451	-1.17582	-1.54499
H	-1.07953	-2.02490	-1.58244
H	-2.78429	-1.56912	-1.55543
H	-1.62204	-0.58877	-2.45411
C	-2.66082	1.35974	-0.00131
H	-2.49276	1.98526	0.87663
H	-2.49577	1.98118	-0.88272
H	-3.70264	1.02962	0.00120
C	-1.76444	-1.17310	1.54692
H	-1.62240	-0.58432	2.45499

H	-2.78406	-1.56681	1.55788
H	-1.07911	-2.02183	1.58606
O	0.94135	2.30731	0.00001

3_D^c

48

XYZ

Si	-2.07795	-0.94846	0.09405
O	0.94578	1.92403	-0.40182
Si	2.07606	0.94658	0.08896
O	-0.94476	-1.93472	-0.37232
N	2.96964	1.37929	1.51384
N	-3.00198	-1.36908	1.50351
C	-2.74296	-2.62388	2.20376
H	-2.41982	-2.44322	3.25607
H	-3.65624	-3.26333	2.23711
H	-1.94106	-3.17730	1.67577
C	-4.04389	-0.54400	2.09209
H	-4.17938	0.39229	1.51378
H	-5.02578	-1.07396	2.11568
H	-3.79650	-0.25794	3.14207
C	2.67811	2.62817	2.21191
H	1.87793	3.17015	1.66978
H	2.33776	2.43938	3.25735
H	3.58040	3.28173	2.26397
C	4.01900	0.57250	2.11436
H	3.76383	0.27825	3.16017
H	4.17992	-0.35873	1.53449
H	4.99000	1.12126	2.15188
Si	-2.67953	1.09442	-0.99149
Si	2.69953	-1.10085	-0.97353
C	-2.29545	2.56100	0.14500
H	-2.62903	3.50217	-0.34448
H	-2.78037	2.50338	1.14087
H	-1.19043	2.60475	0.26502
C	-4.52786	1.02196	-1.45529
H	-5.19592	0.97464	-0.57057
H	-4.79347	1.93937	-2.02516
H	-4.75336	0.14839	-2.10208
C	-1.59124	1.18972	-2.53103
H	-0.54797	1.36662	-2.19021
H	-1.63125	0.26558	-3.14221
H	-1.90742	2.04649	-3.16484
C	4.54635	-1.00574	-1.44040
H	5.21385	-0.88536	-0.56237
H	4.84007	-1.94512	-1.95818
H	4.74323	-0.16379	-2.13682
C	1.61948	-1.23501	-2.51588
H	0.57259	-1.40655	-2.18445
H	1.66469	-0.32504	-3.14776
H	1.94413	-2.10501	-3.12702
C	2.33442	-2.55202	0.18876
H	2.66664	-3.49946	-0.28941
H	2.83057	-2.47552	1.17781
H	1.23141	-2.59984	0.32400

3_D^t

48

XYZ

Si	1.71836	-0.71291	-0.61753
O	-0.48883	0.88491	1.57913
Si	-1.71961	0.71616	0.61473
O	0.48887	-0.87626	-1.58455
N	-2.48216	2.13732	-0.02625
N	2.47708	-2.13801	0.01952
C	2.00737	-3.46564	-0.36350
H	2.82514	-4.06252	-0.83185
H	1.63570	-4.03834	0.51848
H	1.18147	-3.36355	-1.09541
C	3.57637	-2.12909	0.97105
H	3.86670	-1.08981	1.22734
H	3.29846	-2.64119	1.92239
H	4.47795	-2.64610	0.56449
C	-2.01280	3.46716	0.34942
H	-1.18582	3.36922	1.08069
H	-1.64274	4.03567	-0.53594
H	-2.83028	4.06582	0.81599
C	-3.58362	2.12276	-0.97517
H	-3.30832	2.62984	-1.92995
H	-3.87418	1.08197	-1.22506

H	-4.48446	2.64149	-0.56917
Si	2.76843	1.35499	-0.08271
Si	-2.76527	-1.35602	0.08847
C	4.57862	1.31672	-0.67993
H	5.04513	2.31147	-0.50810
H	5.18811	0.56467	-0.13769
H	4.64711	1.09528	-1.76549
C	2.64474	1.69620	1.77393
H	2.96605	2.73782	1.99257
H	1.58060	1.56551	2.07097
H	3.27570	1.01113	2.37736
C	1.79656	2.63818	-1.08356
H	1.77706	2.38009	-2.16216
H	0.75001	2.68517	-0.72171
H	2.25191	3.64564	-0.97012
C	-2.64240	-1.70295	-1.76719
H	-1.57936	-1.56851	-2.06658
H	-2.95964	-2.74658	-1.98212
H	-3.27726	-1.02247	-2.37173
C	-1.78881	-2.63269	1.09323
H	-2.23941	-3.64245	0.98139
H	-0.74138	-2.67577	0.73342
H	-1.77220	-2.37207	2.17128
C	-4.57506	-1.32088	0.68707
H	-5.18685	-0.57201	0.14302
H	-5.03921	-2.31731	0.51864
H	-4.64323	-1.09627	1.77201

P_D[c]

48

XYZ

Si	-1.23758	0.55592	0.02186
O	-0.01280	0.62596	-1.16871
Si	1.21046	0.51375	0.00695
O	-0.00374	0.46829	1.20158
N	2.20707	1.91872	-0.08811
N	-2.19500	1.98496	0.04331
C	-1.60509	3.29718	-0.12894
H	-2.24121	3.92106	-0.76684
H	-1.47270	3.81445	0.83025
H	-0.63261	3.21501	-0.60980
C	-3.52455	2.03369	0.61137
H	-3.92853	1.03124	0.75603
H	-3.53039	2.53584	1.58762
H	-4.21057	2.57626	-0.04954
C	2.00619	3.01556	-1.00875
H	1.26476	2.74486	-1.75973
H	1.66857	3.92675	-0.49585
H	2.94238	3.25530	-1.52737
C	3.23235	2.16296	0.90244
H	2.98884	3.03299	1.52530
H	3.33890	1.30609	1.57110
H	4.20768	2.34236	0.43341
Si	-2.55121	-1.39525	-0.07495
Si	2.51288	-1.45540	0.01927
C	-4.03435	-1.17238	-1.22688
H	-4.55482	-2.12560	-1.35084
H	-4.75322	-0.44479	-0.84721
H	-3.70962	-0.83651	-2.21381
C	-3.13015	-1.87550	1.65856
H	-3.81861	-1.13618	2.07343
H	-3.64574	-2.83880	1.63606
H	-2.28061	-1.95817	2.33938
C	-1.46456	-2.76514	-0.78717
H	-1.15817	-2.51713	-1.80524
H	-0.56357	-2.92154	-0.19304
H	-2.01478	-3.70884	-0.81745
C	4.35289	-1.05216	0.20450
H	4.59569	-0.69659	1.20743
H	4.94724	-1.94978	0.01564
H	4.66125	-0.28577	-0.50937
C	2.27020	-2.31661	-1.64574
H	1.22117	-2.55028	-1.82845
H	2.61614	-1.67927	-2.46222
H	2.83951	-3.24913	-1.67764
C	1.98751	-2.58097	1.44343
H	2.52651	-3.53092	1.40641
H	2.20007	-2.10431	2.40261
H	0.91789	-2.79430	1.41960

P_D^t

48

XYZ

Si	-1.10542	0.52629	-0.01584
O	-0.04137	-0.08840	1.18389
Si	1.10546	-0.52629	0.01558
O	0.04138	0.08838	-1.18416
N	1.36606	-2.22691	0.06213
N	-1.36602	2.22692	-0.06256
C	-0.43452	3.16627	-0.64918
H	-0.96142	3.85851	-1.31654
H	0.07942	3.76350	0.11529
H	0.31191	2.63545	-1.23964
C	-2.42517	2.85992	0.69158
H	-3.10599	2.11585	1.10995
H	-2.03066	3.44904	1.52921
H	-3.01569	3.53030	0.05519
C	0.43396	-3.16634	0.64771
H	-0.31265	-2.63565	1.23805
H	-0.07968	-3.76303	-0.11739
H	0.96030	-3.85907	1.31499
C	2.42572	-2.85985	-0.69137
H	2.03174	-3.44890	-1.52930
H	3.10679	-2.11575	-1.10927
H	3.01583	-3.53028	-0.05466
Si	-3.15380	-0.63545	-0.07958
Si	3.15377	0.63547	0.07989
C	-4.39088	0.34743	-1.11830
H	-5.33967	-0.18987	-1.19326
H	-4.59146	1.32922	-0.68619
H	-4.00864	0.50092	-2.12957
C	-3.83236	-0.89991	1.66541
H	-4.75840	-1.47940	1.63094
H	-3.11272	-1.44328	2.28107
H	-4.04839	0.04695	2.16459
C	-2.86288	-2.31047	-0.90219
H	-2.35309	-2.19188	-1.86004
H	-2.25214	-2.96013	-0.27461
H	-3.81743	-2.81209	-1.07996
C	3.83362	0.89929	-1.66470
H	3.11471	1.44294	-2.28097
H	4.75995	1.47828	-1.62967
H	4.04953	-0.04777	-2.16357
C	2.86235	2.31078	0.90174
H	3.81679	2.81250	1.07989
H	2.25197	2.96021	0.27357
H	2.35202	2.19250	1.85934
C	4.39008	-0.34714	1.11979
H	4.59076	-1.32915	0.68822
H	5.33892	0.19004	1.19508
H	4.00720	-0.50013	2.13088

S_E

15

XYZ

Si	-1.04820	1.29374	0.00002
Si	0.97145	-0.04130	0.00000
C	0.99514	-1.13607	1.54343
H	0.12351	-1.79269	1.56662
H	1.89193	-1.76136	1.54301
H	1.00168	-0.54588	2.46226
C	2.49112	1.08732	0.00100
H	3.40887	0.49361	0.00103
H	2.51203	1.73119	-0.88123
H	2.51146	1.73039	0.88384
C	0.99607	-1.13458	-1.54446
H	1.89291	-1.75979	-1.54417
H	0.12451	-1.79124	-1.56877
H	1.00306	-0.54350	-2.46272
Cl	-2.36997	-0.36441	0.00000

$[S_E\text{-}1_E]^‡$

18

XYZ

Si	-0.42945	0.57465	-0.84184
N	-1.71545	-0.34828	-0.01186
N	-2.67434	-0.92504	0.28944
O	-3.77039	-1.29720	-0.01199
Si	1.48660	-0.54583	0.03743
C	2.99742	0.29807	-0.70798

H	3.02174	1.35809	-0.44759
H	3.91201	-0.16238	-0.32598
H	3.00660	0.21431	-1.79636
C	1.38147	-2.34828	-0.50684
H	2.25527	-2.89863	-0.14883
H	0.49257	-2.83588	-0.10146
H	1.35153	-2.43632	-1.59445
C	1.51145	-0.40664	1.91579
H	0.65089	-0.91141	2.35836
H	2.41963	-0.86395	2.31741
H	1.48862	0.63872	2.22809
Cl	-0.46173	2.44270	0.15998

$\mathbf{1}_{E}$

18

XYZ

Si	-0.53973	0.20700	0.04848
N	-1.70029	-0.88178	0.23331
N	-3.00035	-1.01328	0.46833
O	-3.70897	-1.14249	-0.49667
Si	1.74534	-0.36266	-0.02593
C	2.44106	0.39564	-1.59906
H	2.29502	1.47711	-1.61782
H	3.51470	0.20029	-1.65784
H	1.97216	-0.02921	-2.48800
C	1.80561	-2.23677	-0.03036
H	2.84467	-2.57518	-0.04918
H	1.32725	-2.64784	0.85962
H	1.29696	-2.64514	-0.90468
C	2.54114	0.38794	1.50380
H	2.12842	-0.04050	2.41846
H	3.61593	0.18979	1.49205
H	2.39919	1.46958	1.53673
Cl	-0.96608	2.22969	-0.00527

$\mathbf{2}_{E}$

16

XYZ

Si	-0.99859	0.66905	-0.00001
O	-1.49853	2.11560	-0.00000
Si	1.23265	-0.11586	0.00001
C	1.44505	-1.16209	1.54973
H	0.73337	-1.98926	1.56846
H	2.45324	-1.58362	1.57149
H	1.30833	-0.57086	2.45669
C	2.34013	1.39897	0.00017
H	3.39025	1.09643	0.00052
H	2.16158	2.01614	-0.88158
H	2.16106	2.01634	0.88168
C	1.44524	-1.16182	-1.54987
H	1.30854	-0.57043	-2.45673
H	2.45347	-1.58323	-1.57162
H	0.73364	-1.98906	-1.56882
Cl	-2.31616	-0.93896	-0.00002

$\mathbf{P}_{E}^{c}$

32

XYZ

Si	1.21053	0.65821	-0.00052
O	-0.00040	0.63284	-1.18782
Si	-1.21053	0.65821	0.00051
O	0.00040	0.63288	1.18781
Si	-2.78729	-1.07849	0.00236
C	-3.66496	-1.03485	-1.66420
H	-2.96179	-1.19373	-2.48379
H	-4.42588	-1.81755	-1.71163
H	-4.15777	-0.07372	-1.82190
C	-3.99170	-0.75433	1.41384
H	-3.48150	-0.75555	2.37882
H	-4.48492	0.21163	1.29273
H	-4.76167	-1.52930	1.43697
C	-1.88324	-2.71306	0.25319
H	-2.59794	-3.53959	0.25677
H	-1.15966	-2.89643	-0.54267
H	-1.35186	-2.72327	1.20684
Si	2.78728	-1.07850	-0.00237
C	3.66503	-1.03473	1.66415
H	4.42601	-1.81739	1.71157
H	4.15779	-0.07357	1.82179
H	2.96191	-1.19362	2.48378

C	1.88320	-2.71308	-0.25301
H	1.15957	-2.89629	0.54283
H	1.35188	-2.72343	-1.20669
H	2.59788	-3.53964	-0.25640
C	3.99165	-0.75446	-1.41392
H	4.48491	0.21149	-1.29287
H	4.76158	-1.52946	-1.43705
H	3.48140	-0.75569	-2.37887
Cl	-2.21263	2.47955	-0.00820
Cl	2.21264	2.47955	0.00820

P_E^t

32

XYZ

Si	-1.07158	-0.56215	-0.00679
O	-0.00001	0.00006	-1.19583
Si	1.07158	0.56215	-0.00675
O	0.00001	-0.00006	1.18226
Si	3.23014	-0.35238	0.00142
C	4.03776	0.09106	1.64479
H	3.44957	-0.28211	2.48511
H	5.03397	-0.35389	1.70591
H	4.14259	1.17182	1.75597
C	4.18949	0.37751	-1.44619
H	3.69054	0.17587	-2.39577
H	4.29561	1.45866	-1.34036
H	5.19025	-0.05899	-1.49186
C	3.01336	-2.21412	-0.17930
H	3.98584	-2.71242	-0.17175
H	2.41576	-2.62191	0.63810
H	2.51079	-2.46092	-1.11621
Si	-3.23014	0.35238	0.00151
C	-4.03775	-0.09124	1.64484
H	-5.03396	0.35370	1.70601
H	-4.14257	-1.17201	1.75591
H	-3.44956	0.28185	2.48519
C	-3.01337	2.21414	-0.17902
H	-2.41576	2.62185	0.63842
H	-2.51080	2.46104	-1.11590
H	-3.98585	2.71244	-0.17142
C	-4.18950	-0.37736	-1.44617
H	-4.29563	-1.45852	-1.34045
H	-5.19026	0.05915	-1.49180
H	-3.69055	-0.17563	-2.39574
Cl	1.12246	2.64405	-0.00329
Cl	-1.12246	-2.64405	-0.00354

S_F

18

XYZ

Si	1.48743	-1.07642	-0.08532
Si	-0.66141	0.00422	-0.01247
C	-2.07029	-1.17402	-0.47025
H	-2.08226	-2.04434	0.18978
H	-3.03926	-0.67507	-0.38734
H	-1.96639	-1.53785	-1.49494
C	-0.72715	1.51326	-1.16097
H	-1.69892	2.00788	-1.08308
H	0.04229	2.24217	-0.89804
H	-0.58094	1.23229	-2.20636
C	-0.93384	0.60415	1.77001
H	-1.90790	1.09371	1.85256
H	-0.91764	-0.22121	2.48519
H	-0.17226	1.32688	2.07094
C	2.50551	0.54337	0.00963
H	2.12726	1.27682	0.72796
H	3.56493	0.36970	0.20022
H	2.42139	1.01916	-0.97832

$[S_F\text{-}1_F]^‡$

21

XYZ

Si	-0.38354	1.01674	-0.77290
N	-1.77706	0.13885	0.01995
N	-2.68532	-0.52202	0.23988
O	-3.71663	-1.06240	-0.02411
C	-0.30912	2.61163	0.28070
H	-1.19329	3.23323	0.13272
H	-0.18584	2.41787	1.34744
H	0.55589	3.19183	-0.05352

Si	1.35171	-0.40548	0.01416
C	2.94681	0.05695	-0.89015
H	3.22964	1.09375	-0.69435
H	3.77041	-0.58034	-0.55820
H	2.83903	-0.06496	-1.96974
C	0.89692	-2.19821	-0.37388
H	1.70461	-2.86929	-0.07087
H	-0.00594	-2.50599	0.15839
H	0.72331	-2.33997	-1.44238
C	1.62190	-0.21028	1.87700
H	0.71831	-0.46662	2.43423
H	2.42827	-0.86350	2.22107
H	1.89177	0.81731	2.12957

2_F

19

XYZ

Si	-1.37180	0.23684	0.00730
C	-2.39271	-1.33754	0.00455
H	-3.45023	-1.12025	-0.14422
H	-2.04760	-2.01815	-0.77845
H	-2.26799	-1.85739	0.95906
Si	0.97968	-0.03886	0.00860
C	1.42198	-1.71000	0.77227
H	0.95003	-2.53479	0.23401
H	2.50328	-1.86501	0.73619
H	1.11238	-1.76836	1.81778
C	1.72597	1.38237	0.99150
H	2.81494	1.37978	0.90033
H	1.34965	2.33794	0.62264
H	1.47272	1.30915	2.05064
C	1.56816	0.01816	-1.78556
H	1.31506	0.97169	-2.25216
H	2.65432	-0.09896	-1.82261
H	1.12654	-0.78155	-2.38363
O	-1.99798	1.64453	-0.00735

P_F^c

38

XYZ

Si	-1.21822	1.12531	0.00684
O	0.00706	1.13492	1.19396
Si	1.21614	1.12759	-0.01008
O	-0.00975	1.14219	-1.19719
Si	2.49960	-0.85450	0.00097
C	1.80921	-2.00181	1.33518
H	0.74867	-2.20501	1.17571
H	2.34086	-2.95645	1.34171
H	1.90862	-1.54624	2.32226
C	4.30459	-0.44429	0.39304
H	4.72295	0.24185	-0.34668
H	4.40236	0.02261	1.37552
H	4.91370	-1.35167	0.39132
C	2.39059	-1.67715	-1.69625
H	2.93740	-2.62338	-1.70213
H	1.35264	-1.87957	-1.96583
H	2.81418	-1.03570	-2.47181
C	2.22755	2.70099	-0.02457
H	2.90085	2.73481	0.83512
H	2.83714	2.75048	-0.93030
H	1.57869	3.57818	0.00432
C	-2.23670	2.69410	0.02653
H	-2.89909	2.73267	-0.84145
H	-2.85733	2.73265	0.92530
H	-1.59162	3.57447	0.01335
Si	-2.49774	-0.85636	-0.00200
C	-1.60383	-2.15361	-1.04549
H	-2.19436	-3.07072	-1.11127
H	-1.42836	-1.78336	-2.05733
H	-0.63528	-2.41040	-0.61274
C	-2.69048	-1.47760	1.77206
H	-1.71435	-1.61445	2.24177
H	-3.25660	-0.77089	2.38248
H	-3.21672	-2.43523	1.79004
C	-4.19857	-0.50482	-0.75239
H	-4.11004	-0.14607	-1.78018
H	-4.80846	-1.41156	-0.76492
H	-4.73545	0.25287	-0.17744

P_F^t

38

XYZ

Si	-0.98920	-0.71092	0.01379
O	0.00002	-0.00010	-1.18312
Si	0.98920	0.71091	0.01371
O	-0.00002	0.00009	1.21029
Si	3.17684	-0.15324	-0.00426
C	4.07935	0.34151	1.58209
H	3.53940	-0.00692	2.46481
H	5.08011	-0.09712	1.60452
H	4.18756	1.42558	1.65901
C	4.10731	0.52637	-1.50416
H	3.58071	0.29715	-2.43281
H	4.22270	1.61058	-1.43986
H	5.10603	0.08697	-1.56666
C	3.05880	-2.03484	-0.11682
H	4.05331	-2.48395	-0.17382
H	2.55289	-2.44482	0.75981
H	2.49959	-2.33529	-1.00535
C	0.88100	2.57796	0.01353
H	1.37029	2.99068	0.89896
H	1.37547	2.98973	-0.86946
H	-0.16083	2.90320	0.00994
C	-0.88101	-2.57797	0.01392
H	-1.37039	-2.99054	0.89936
H	-1.37539	-2.98988	-0.86905
H	0.16082	-2.90321	0.01050
Si	-3.17684	0.15324	-0.00428
C	-4.07911	-0.34085	1.58241
H	-5.07987	0.09779	1.60481
H	-4.18730	-1.42489	1.65981
H	-3.53902	0.00796	2.46490
C	-3.05879	2.03480	-0.11760
H	-2.55287	2.44511	0.75888
H	-2.49960	2.33490	-1.00625
H	-4.05330	2.48389	-0.17474
C	-4.10754	-0.52696	-1.50376
H	-4.22293	-1.61115	-1.43900
H	-5.10628	-0.08758	-1.56628
H	-3.58110	-0.29812	-2.43260

S_R

3

XYZ

Si	0.00000	0.00000	0.13288
H	0.00000	-1.09599	-0.93017
H	0.00000	1.09599	-0.93017

$[S_R\text{-}1_R]^‡$

6

XYZ

Si	-1.15213	-0.18862	-0.00690
N	0.05740	0.96306	-0.04740
N	1.21497	0.41785	0.20207
O	1.36090	-0.73988	-0.18036
H	-1.17779	-1.28342	0.98479
H	-2.48616	0.17679	-0.52803

1_R

6

XYZ

Si	-0.88773	0.10723	-0.00000
N	0.67472	1.02976	0.00007
N	1.28364	-0.02542	-0.00004
O	0.26479	-1.13285	0.00002
H	-1.69953	0.26553	1.22574
H	-1.69903	0.26573	-1.22607

2_R

7

XYZ

Si	-1.10105	-0.25340	0.00001
O	0.00000	1.06165	0.00000
Si	1.10105	-0.25340	-0.00001
H	-1.93898	-0.34937	1.22016
H	-1.93761	-0.34959	-1.22110
H	1.93898	-0.34937	-1.22016
H	1.93761	-0.34959	1.22110

P_R

8

XYZ

Si	-1.20333	-0.00001	0.00017
O	-0.00002	-1.19067	-0.00061
Si	1.20338	0.00004	0.00017
O	-0.00014	1.19060	-0.00061
H	-2.03764	-0.00001	1.22282
H	-2.04059	0.00000	-1.22041
H	2.03786	0.00009	1.22269
H	2.04089	0.00011	-1.22022

$[I_A^t\text{-}5_A^t]_{IIa}^{\ddagger}$

25

XYZ

Si	-1.69483	-0.40739	-0.73745
Si	0.66897	0.28107	0.35844
O	2.02319	0.33236	1.85079
N	3.20192	0.10679	1.44272
N	3.73685	-0.27280	0.51352
N	1.83631	-0.65675	-0.62867
N	-2.86323	0.64569	-0.02968
C	2.16501	-0.31340	-2.00735
H	3.03505	-0.88866	-2.32985
H	1.32152	-0.54738	-2.66818
H	2.39291	0.74602	-2.09115
C	1.69788	-2.10372	-0.44713
H	2.64826	-2.59827	-0.65866
H	1.40431	-2.33627	0.57812
H	0.93241	-2.51003	-1.11711
C	-3.69314	0.45975	1.14275
H	-3.33394	1.08234	1.97183
H	-4.72771	0.74623	0.92684
H	-3.68219	-0.57972	1.46142
C	-2.89526	2.00976	-0.53490
H	-3.91171	2.28875	-0.83122
H	-2.54864	2.71955	0.22483
H	-2.24623	2.11165	-1.40747
Cl	-2.07340	-2.27313	0.24419
Cl	1.00649	2.26140	-0.33625

5_A^t

23

XYZ

Si	1.06883	-0.28276	-0.02701
O	0.00002	0.00010	1.27150
Si	-1.06879	0.28261	-0.02703
N	-2.49197	-0.65387	0.01172
N	2.49195	0.65383	0.01204
C	2.39770	2.06321	0.36358
H	2.58122	2.70399	-0.50631
H	1.41257	2.30027	0.76420
H	3.13625	2.30690	1.13358
C	3.79833	0.26950	-0.48576
H	4.56306	0.47864	0.26948
H	3.83276	-0.79404	-0.71203
H	4.05553	0.82645	-1.39422
C	-3.79857	-0.26907	-0.48514
H	-4.56277	-0.47653	0.27112
H	-3.83235	0.79418	-0.71286
H	-4.05708	-0.82704	-1.39260
C	-2.39797	-2.06330	0.36306
H	-2.58210	-2.70391	-0.50683
H	-1.41270	-2.30074	0.76313
H	-3.13621	-2.30691	1.13338
Cl	1.62589	-2.27777	-0.21242
Cl	-1.62564	2.27767	-0.21266

$[5_A^t\text{-}P_A^t]_{IIa}^{\ddagger}$

26

XYZ

Si	-0.76556	0.22068	-0.29550
O	0.50257	0.03272	-1.48950
Si	1.44053	-0.29729	-0.15231
N	-3.24383	0.40811	2.10326
N	-2.14112	0.38530	2.23592
O	-0.88583	0.22036	1.64927
N	2.81109	0.69310	0.03209
N	-2.10293	-0.82621	-0.57470
C	3.98356	0.38286	0.82786
H	4.89022	0.61246	0.25925

H	4.00185	0.97147	1.75212
H	4.00962	-0.67284	1.09018
C	2.73327	2.09091	-0.36963
H	2.69466	2.75329	0.50237
H	3.61263	2.35400	-0.96520
H	1.84912	2.26968	-0.98033
C	-2.89098	-0.71867	-1.79163
H	-2.47913	-1.33206	-2.60290
H	-3.91510	-1.05152	-1.59770
H	-2.93554	0.31567	-2.13113
C	-2.06452	-2.18163	-0.04598
H	-3.07624	-2.50952	0.21356
H	-1.65135	-2.89386	-0.77134
H	-1.45097	-2.22906	0.85430
Cl	2.01535	-2.27662	0.08096
Cl	-1.41322	2.18235	-0.60635

$[I_C^t\text{-}5_C^t]_{IIa}^‡$

15

XYZ

Si	1.79331	-0.63613	-0.24923
Si	-0.43096	-0.08320	-0.44183
O	-1.04685	0.79357	1.13339
N	-2.32704	1.16065	1.26532
N	-3.37712	1.15709	0.88136
Cl	2.78421	1.23999	-0.12885
Cl	-1.68824	-1.75128	-0.50540
C	2.15036	-1.50422	1.39554
H	2.00122	-0.83829	2.24617
H	3.18457	-1.85324	1.40772
H	1.49706	-2.37305	1.50239
C	-0.96348	1.06465	-1.81313
H	-0.38381	1.98848	-1.76682
H	-0.79469	0.59764	-2.78407
H	-2.02607	1.30566	-1.73663

5_C^t

13

XYZ

Si	-1.02396	-0.39804	-0.06087
O	0.00001	-0.00004	1.24636
Si	1.02396	0.39805	-0.06085
C	-1.62464	-2.15517	-0.09891
H	-2.28898	-2.33054	0.74986
H	-2.17573	-2.35618	-1.01806
H	-0.77629	-2.83713	-0.03270
C	1.62464	2.15518	-0.09878
H	2.17571	2.35625	-1.01793
H	0.77630	2.83714	-0.03249
H	2.28901	2.33047	0.74999
Cl	2.66378	-0.86956	-0.19062
Cl	-2.66379	0.86957	-0.19051

$[5_C^t\text{-}P_C^t]_{IIa}^‡$

16

XYZ

Si	-0.55007	-0.21664	0.59545
O	0.88495	-1.05244	1.06633
Si	1.53766	-0.25651	-0.26934
N	-3.38145	1.39958	-1.04973
N	-2.28276	1.49134	-1.15179
O	-0.96446	1.05488	-0.88934
Cl	-1.95111	-1.67075	0.06098
Cl	2.94335	1.17795	0.25640
C	-1.19823	0.76221	2.03450
H	-1.20957	0.12555	2.92057
H	-0.53979	1.61099	2.22683
H	-2.20876	1.13211	1.85712
C	2.25539	-1.33704	-1.59949
H	3.13497	-1.85442	-1.20931
H	1.51687	-2.07719	-1.90894
H	2.55461	-0.74219	-2.46262

$[I_E^t\text{-}5_E^t]_{IIa}^‡$

33

XYZ

Si	1.20154	0.89182	-0.68434
Si	-0.66606	-0.31818	-0.36869
O	-0.32878	-1.20671	1.34398
N	-1.25328	-2.00038	1.89570

N	-2.28877	-2.42545	1.84966
Si	3.19448	-0.20587	-0.04269
Si	-2.77133	0.75848	-0.21450
C	4.66519	0.78150	-0.69051
H	4.65419	0.84148	-1.78029
H	4.65795	1.79901	-0.29455
H	5.60178	0.30788	-0.38477
C	3.27134	-0.31226	1.83805
H	3.19412	0.67952	2.28709
H	2.45191	-0.92212	2.22053
H	4.21889	-0.75813	2.15322
C	3.15478	-1.92597	-0.81522
H	2.31240	-2.50732	-0.43604
H	3.06784	-1.87649	-1.90211
H	4.07571	-2.46331	-0.57386
C	-2.96900	1.34528	1.56644
H	-2.12264	1.96589	1.86679
H	-3.87912	1.94276	1.66253
H	-3.04521	0.50943	2.26451
C	-4.13452	-0.44874	-0.69446
H	-3.98556	-0.82497	-1.70806
H	-4.17082	-1.30578	-0.01969
H	-5.10462	0.05327	-0.65603
C	-2.72126	2.23040	-1.38746
H	-2.56767	1.91091	-2.41960
H	-3.66324	2.78276	-1.33729
H	-1.91063	2.91005	-1.11803
Cl	0.93412	2.57406	0.60443
Cl	-0.78003	-1.99755	-1.62513

5_E^t

31

XYZ

Si	0.97740	0.52406	-0.08836
O	-0.00001	0.00006	1.22472
Si	3.17062	-0.31827	-0.01194
C	4.02996	0.50452	1.44939
H	3.49122	0.31648	2.37969
H	5.04383	0.11091	1.55888
H	4.09810	1.58450	1.30708
C	4.04734	0.09619	-1.62716
H	3.54753	-0.36408	-2.48140
H	4.07968	1.17495	-1.79116
H	5.07595	-0.27210	-1.60019
C	3.01214	-2.17684	0.23967
H	2.45115	-2.39901	1.14922
H	2.49259	-2.64824	-0.59650
H	4.00091	-2.63382	0.32865
Si	-0.97739	-0.52405	-0.08833
Si	-3.17063	0.31826	-0.01199
C	-3.01218	2.17685	0.23947
H	-2.45117	2.39911	1.14899
H	-2.49265	2.64819	-0.59675
H	-4.00095	2.63382	0.32843
C	-4.02995	-0.50443	1.44941
H	-3.49121	-0.31632	2.37969
H	-5.04382	-0.11081	1.55888
H	-4.09809	-1.58442	1.30718
C	-4.04734	-0.09635	-1.62718
H	-5.07597	0.27190	-1.60022
H	-3.54756	0.36389	-2.48145
H	-4.07964	-1.17512	-1.79111
Cl	-1.00036	-2.61687	-0.24222
Cl	1.00037	2.61687	-0.24241

$[5_E^t\text{-}P_E^t]_{IIa}^{\ddagger}$

34

XYZ

Si	0.85067	-0.19436	-0.38415
O	-0.23454	0.78819	-1.31458
Si	2.94241	0.84941	-0.21771
C	2.66585	2.51851	0.60871
H	2.24164	2.39931	1.60742
H	3.61070	3.05984	0.70111
H	1.97670	3.13145	0.02494
C	3.60691	1.05644	-1.96799
H	3.74768	0.08832	-2.45214
H	2.91641	1.64244	-2.57726
H	4.56983	1.57301	-1.95148
C	4.08949	-0.23601	0.81386

H	3.72965	-0.32748	1.84064
H	4.17976	-1.23746	0.38808
H	5.08945	0.20305	0.85042
Si	-1.19762	0.68049	0.08026
Si	-3.32232	-0.29213	-0.18667
C	-4.37114	0.87103	-1.23416
H	-4.49016	1.84001	-0.74612
H	-3.91715	1.03547	-2.21289
H	-5.36533	0.44368	-1.38831
C	-4.07119	-0.52782	1.52473
H	-4.18035	0.42812	2.04026
H	-5.06082	-0.98428	1.44401
H	-3.44789	-1.17753	2.14181
C	-3.03654	-1.93653	-1.05573
H	-3.98819	-2.44436	-1.23113
H	-2.54456	-1.79010	-2.01896
H	-2.40460	-2.59441	-0.45625
N	1.92352	-3.08397	1.79719
N	1.34585	-2.15287	1.96590
O	0.60561	-1.05150	1.47207
Cl	1.00370	-2.02710	-1.41152
Cl	-1.33553	2.52086	1.06879

$[I_A^t\text{-}4_A^t]^‡$

25

XYZ

Si	-1.12623	-0.47941	-0.91063
Si	1.03641	0.31894	0.07621
O	1.54935	0.76769	2.20960
N	0.40590	0.78339	2.67219
N	-0.67734	0.61057	2.36002
N	2.29316	-0.75425	-0.36762
N	-2.54302	0.43066	-0.59898
C	3.12599	-0.69713	-1.55199
H	4.17081	-0.89024	-1.28826
H	2.81321	-1.44898	-2.28712
H	3.06964	0.28477	-2.01709
C	2.37829	-2.02108	0.34224
H	3.40148	-2.19448	0.69003
H	1.72288	-2.01991	1.21521
H	2.08049	-2.85780	-0.29969
C	-3.66308	0.11040	0.26462
H	-3.62600	0.71457	1.17793
H	-4.60689	0.31642	-0.24965
H	-3.64523	-0.93935	0.54730
C	-2.54826	1.81213	-1.05689
H	-3.45845	2.02618	-1.62534
H	-2.49764	2.50309	-0.20789
H	-1.69004	2.00907	-1.70278
Cl	-1.48068	-2.38503	-0.07042
Cl	1.42302	2.14287	-0.89398

$[5_A^t\text{-}P_A^t]^‡$

26

XYZ

Si	-1.14322	0.31290	-0.24871
Si	1.10597	-0.29141	-0.30081
O	1.21734	-0.20057	2.17095
N	0.07170	-0.08873	2.52340
N	-1.01785	0.03933	2.21829
N	2.51276	0.63290	-0.54072
N	-2.56476	-0.59125	-0.50064
C	3.73446	0.41100	0.20977
H	4.59880	0.47112	-0.45869
H	3.85891	1.15712	1.00312
H	3.73584	-0.57749	0.66803
C	2.45841	1.91965	-1.21571
H	3.29021	2.00245	-1.92198
H	1.53043	2.02054	-1.77625
H	2.52864	2.74979	-0.50279
C	-3.78949	-0.36793	0.24423
H	-4.65072	-0.41829	-0.42933
H	-3.92386	-1.11973	1.03100
H	-3.78715	0.61673	0.71013
C	-2.51292	-1.87866	-1.17452
H	-2.58403	-2.70949	-0.46206
H	-3.34517	-1.96083	-1.88043
H	-1.58624	-1.98210	-1.73713
Cl	-1.62256	2.33084	-0.10116
Cl	1.56691	-2.31541	-0.26289

O	-0.03658	0.04266	-1.50175

[I_B^t-4_B^t]‡

31

XYZ

Si	0.87709	0.07683	1.01061
Si	-0.94541	0.52586	-0.22776
O	-0.74481	-0.81217	-2.37680
N	0.18033	-1.52911	-2.07575
N	0.96441	-1.85099	-1.31832
C	1.00271	-1.54838	1.95805
H	-0.00167	-1.89824	2.20250
H	1.50832	-2.33334	1.39594
H	1.53947	-1.38589	2.89517
C	-1.09154	2.24342	-0.98100
H	-1.36786	3.00451	-0.25030
H	-0.13717	2.52937	-1.42567
H	-1.84138	2.22977	-1.77466
N	-2.47606	-0.00365	0.38501
N	2.43969	0.63065	0.50631
C	-3.47530	0.90145	0.91214
H	-4.48083	0.54834	0.65731
H	-3.41491	0.98854	2.00661
H	-3.35853	1.89862	0.48849
C	-2.65851	-1.37148	0.81990
H	-3.65069	-1.73675	0.53195
H	-1.91465	-2.02084	0.35484
H	-2.56803	-1.47585	1.91116
C	3.53491	-0.25740	0.17494
H	3.60185	-0.43453	-0.90716
H	4.48616	0.17109	0.50962
H	3.41255	-1.22387	0.66175
C	2.59283	1.95370	-0.06038
H	3.54603	2.39555	0.25043
H	2.57597	1.93773	-1.16026
H	1.79129	2.60938	0.28410

5_B^t

29

XYZ

Si	0.97991	-0.49778	-0.12944
O	0.01014	-0.17574	1.27736
Si	-0.99036	0.51248	0.08950
N	-2.53453	-0.25354	-0.00815
N	2.50916	0.29362	-0.25082
C	-1.23680	2.36708	0.20848
H	-0.30685	2.82743	0.54447
H	-1.50565	2.80958	-0.75223
H	-2.01756	2.60676	0.93389
C	1.24183	-2.34877	-0.29747
H	0.28252	-2.84435	-0.44926
H	1.89221	-2.59430	-1.13829
H	1.68235	-2.75355	0.61730
C	2.60200	1.73323	-0.37135
H	3.39336	2.00842	-1.07807
H	1.66491	2.14384	-0.75028
H	2.82459	2.21789	0.58879
C	3.77340	-0.32979	0.08249
H	4.16317	0.02730	1.04516
H	3.67010	-1.41244	0.14591
H	4.52632	-0.10986	-0.68367
C	-3.70350	0.37138	-0.58783
H	-4.59219	0.15932	0.01792
H	-3.58573	1.45378	-0.63422
H	-3.90140	0.00962	-1.60621
C	-2.65511	-1.69199	0.11305
H	-2.73831	-2.18561	-0.86561
H	-1.79285	-2.10187	0.63849
H	-3.54707	-1.94922	0.69483

[5_B^t-P_B^t]‡

32

XYZ

Si	-1.06116	0.63667	0.12400
Si	1.02170	-0.33130	0.57639
O	1.11203	-1.37146	-1.82179
N	0.06624	-1.01180	-2.29776
N	-0.90767	-0.43547	-2.16945
C	-1.26338	2.35089	-0.59400
H	-0.27908	2.79853	-0.74074

H	-1.77216	2.33583	-1.55813
H	-1.83045	2.97876	0.09709
C	1.22559	-2.04716	1.28454
H	1.65864	-1.98040	2.28527
H	0.25002	-2.52991	1.35889
H	1.86239	-2.67424	0.66075
N	2.53538	0.48229	0.42774
N	-2.59633	-0.03241	0.54907
C	3.68551	-0.17544	-0.15810
H	3.78641	0.04323	-1.22953
H	4.60301	0.15138	0.34281
H	3.61492	-1.25728	-0.04465
C	2.59336	1.92752	0.33490
H	2.59307	2.27815	-0.70769
H	1.74676	2.37434	0.85523
H	3.50811	2.29623	0.81041
C	-3.75055	0.11683	-0.31332
H	-3.87504	-0.73569	-0.99500
H	-4.66216	0.20325	0.28796
H	-3.66845	1.01970	-0.91865
C	-2.67441	-1.19341	1.41246
H	-3.59189	-1.15558	2.00888
H	-2.68175	-2.13704	0.84667
H	-1.83343	-1.20722	2.10551
O	-0.04410	0.62510	1.49223

[I_C^t-4_C^t]‡

15

XYZ

Si	-1.05025	-0.36269	0.36054
Si	0.93215	-0.68346	-0.54226
O	1.09039	2.15388	-0.11712
N	0.10984	2.40931	0.51729
N	-0.87547	2.14561	1.01710
Cl	2.50415	-0.87876	0.80463
Cl	-2.58100	-0.38284	-1.05869
C	1.51832	-0.16827	-2.24029
H	1.99725	-1.01350	-2.73703
H	0.65532	0.13966	-2.83326
H	2.22419	0.65858	-2.18008
C	-1.56597	-1.25379	1.92203
H	-1.96976	-2.24085	1.69772
H	-0.69957	-1.36315	2.57678
H	-2.32530	-0.67032	2.44454

[5_C^t-P_C^t]‡

16

XYZ

Si	-1.12557	-0.44486	-0.29488
Si	1.06185	-0.33957	0.45253
O	1.10758	2.07177	0.11758
N	0.11017	2.33241	-0.50367
N	-0.86433	1.95846	-0.95563
Cl	2.58457	-0.66406	-0.91910
Cl	-2.67332	-0.07835	1.04324
C	1.74809	-0.14140	2.16215
H	2.52356	0.62327	2.18801
H	0.94696	0.13697	2.84850
H	2.16977	-1.09467	2.48745
C	-1.81931	-0.96344	-1.93492
H	-2.33474	-1.91907	-1.81889
H	-2.52245	-0.22263	-2.31444
H	-1.00788	-1.08961	-2.65342
O	-0.06606	-1.60155	0.35704

[I_D^t-4_D^t]‡

49

XYZ

Si	-0.95549	0.43710	0.11544
Si	0.91763	-0.58645	-0.48576
O	1.21522	-1.08610	2.37884
N	0.16477	-0.70930	2.82033
N	-0.85942	-0.22224	2.75260
N	1.03155	-2.30351	-0.68394
N	-0.81581	2.18102	0.12090
C	2.10337	-3.08328	-0.09784
H	1.81038	-3.50812	0.87126
H	2.38560	-3.90584	-0.76408
H	2.98461	-2.46526	0.06667
C	-0.15141	-3.09102	-0.95873

H	-0.60922	-3.48238	-0.03871
H	-0.89550	-2.48900	-1.48283
H	0.09959	-3.94537	-1.59667
C	-1.31276	3.00518	-0.95755
H	-1.95310	3.81176	-0.57631
H	-0.49604	3.47069	-1.52883
H	-1.90070	2.41152	-1.65897
C	-0.10441	2.92734	1.13297
H	0.80013	3.41105	0.73539
H	-0.73927	3.71788	1.55442
H	0.19799	2.27225	1.94962
Si	2.93217	0.63561	-0.50344
Si	-3.13276	-0.27351	-0.39413
C	4.32774	-0.37140	-1.28878
H	3.99875	-0.87060	-2.20207
H	5.15498	0.29496	-1.54717
H	4.71557	-1.13096	-0.60783
C	3.44597	1.20287	1.21993
H	4.36103	1.79875	1.16447
H	2.66629	1.81752	1.67315
H	3.62309	0.35166	1.87850
C	2.58237	2.14616	-1.58346
H	1.71123	2.69047	-1.21508
H	3.43823	2.82614	-1.58315
H	2.37836	1.85172	-2.61470
C	-3.49674	-1.91620	0.46560
H	-3.32574	-1.83703	1.54065
H	-4.54022	-2.19963	0.30443
H	-2.86857	-2.72152	0.08183
C	-3.43966	-0.47132	-2.25081
H	-2.77375	-1.22128	-2.68261
H	-4.47070	-0.78440	-2.43719
H	-3.26954	0.46710	-2.78247
C	-4.28142	1.06072	0.29265
H	-4.13747	1.17744	1.36850
H	-4.08868	2.02749	-0.17653
H	-5.32695	0.79736	0.11305

4_D^t

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XYZ

Si	0.82671	0.06605	0.37938
Si	-1.45836	0.91485	-0.25831
O	-1.41126	2.34255	0.38973
N	1.76606	3.89594	-0.33316
N	1.88671	2.87693	-0.69843
N	-1.53125	0.79126	-1.99308
N	1.45623	0.63491	1.85577
C	-0.99380	1.85620	-2.81021
H	-0.06304	1.55843	-3.31808
H	-1.71179	2.15451	-3.58388
H	-0.79167	2.72844	-2.18800
C	-1.94833	-0.36760	-2.73972
H	-1.11531	-0.83639	-3.28328
H	-2.37597	-1.12311	-2.07879
H	-2.71583	-0.10464	-3.47896
C	2.70026	0.22899	2.48725
H	3.40434	1.06655	2.52192
H	2.51077	-0.09594	3.51466
H	3.16586	-0.59429	1.94988
C	0.76361	1.68236	2.61316
H	0.44984	1.29290	3.58673
H	1.45019	2.51751	2.78427
H	-0.10485	2.04809	2.05706
Si	-2.63152	-0.84228	0.79944
Si	2.33051	-1.48788	-0.63555
C	-4.43818	-1.00727	0.26531
H	-4.52370	-1.24277	-0.79735
H	-4.93972	-1.79736	0.83010
H	-4.97217	-0.07147	0.44145
C	-2.53854	-0.45210	2.64735
H	-3.03396	-1.22207	3.24395
H	-1.49804	-0.38436	2.97591
H	-3.00942	0.51025	2.85527
C	-1.74188	-2.50408	0.52273
H	-0.74006	-2.49169	0.96421
H	-2.29148	-3.31730	1.00374
H	-1.63697	-2.75151	-0.53587
C	1.51382	-1.88773	-2.28923
H	1.34287	-0.97966	-2.87191

H	2.14182	-2.55770	-2.88117
H	0.54634	-2.37262	-2.14130
C	2.50737	-3.07518	0.37707
H	1.53528	-3.54504	0.53979
H	3.13547	-3.78735	-0.16459
H	2.96556	-2.89989	1.35208
C	4.02038	-0.69634	-0.93937
H	3.91760	0.24781	-1.47768
H	4.55145	-0.49454	-0.00770
H	4.64166	-1.36249	-1.54354

$5_D{}^t$

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XYZ

Si	-0.98376	-0.45343	-0.08743
O	-0.04571	0.15040	1.26656
Si	1.01951	0.55160	-0.00093
N	1.30075	2.26089	-0.10235
N	-1.14044	-2.17360	-0.26078
C	-0.19342	-3.00124	-0.97383
H	-0.69126	-3.57169	-1.76860
H	0.57748	-2.38403	-1.43634
H	0.29735	-3.72360	-0.30789
C	-2.17521	-2.94473	0.39508
H	-1.75216	-3.63394	1.13746
H	-2.87470	-2.29394	0.92049
H	-2.74675	-3.54174	-0.32749
C	2.28978	2.80897	-1.00245
H	2.85838	3.60962	-0.51446
H	3.00083	2.04192	-1.31625
H	1.83503	3.22681	-1.91119
C	0.32318	3.23000	0.34011
H	-0.27385	3.62798	-0.49234
H	-0.35154	2.77652	1.06601
H	0.82236	4.07418	0.82934
Si	3.08128	-0.59282	0.12048
Si	-3.12914	0.52571	-0.04436
C	2.77776	-2.14549	1.14859
H	2.12306	-2.84525	0.62852
H	3.72226	-2.65396	1.35805
H	2.30337	-1.88978	2.09758
C	3.74032	-1.06595	-1.58786
H	4.67350	-1.62667	-1.49085
H	3.02697	-1.69100	-2.12906
H	3.94376	-0.18473	-2.20022
C	4.34004	0.50060	1.01223
H	5.28758	-0.03092	1.13325
H	4.53745	1.42501	0.46710
H	3.97453	0.77205	2.00454
C	-3.06026	2.33112	-0.59889
H	-2.54750	2.95395	0.13459
H	-2.54506	2.44128	-1.55504
H	-4.07614	2.71774	-0.71556
C	-3.83964	0.47042	1.70854
H	-3.14358	0.92625	2.41558
H	-4.78465	1.01796	1.75520
H	-4.02899	-0.55204	2.04142
C	-4.25236	-0.41885	-1.23810
H	-4.34109	-1.47155	-0.96463
H	-5.25480	0.01681	-1.24280
H	-3.85986	-0.37136	-2.25621

$[5_D{}^t\text{-}P_D{}^t]^‡$

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XYZ

Si	-1.09605	-0.62142	-0.26930
Si	0.99652	0.45736	-0.12051
O	1.11084	0.27663	2.42647
N	0.08335	-0.30136	2.68912
N	-0.88335	-0.75476	2.28737
N	1.03266	2.18831	-0.05291
N	-1.37471	-2.32418	-0.38159
C	1.80860	2.95306	-1.00615
H	1.16629	3.57959	-1.63843
H	2.52791	3.60983	-0.49958
H	2.36987	2.29170	-1.66978
C	0.29300	3.00509	0.88027
H	-0.36646	3.71378	0.36092
H	-0.32713	2.38337	1.52536
H	0.96515	3.58751	1.52307

C	-2.39993	-2.95428	0.42209
H	-2.91536	-3.73132	-0.15321
H	-1.98735	-3.41583	1.32896
H	-3.14643	-2.22385	0.73913
C	-0.33914	-3.23711	-0.81578
H	0.19660	-3.68699	0.03302
H	-0.77575	-4.05098	-1.40471
H	0.38059	-2.71643	-1.44725
Si	3.13632	-0.49531	-0.29514
Si	-3.04749	0.69676	-0.36731
C	4.35952	0.64763	0.57817
H	4.08074	0.78025	1.62528
H	5.37070	0.23449	0.54321
H	4.37921	1.63365	0.10952
C	3.59715	-0.69499	-2.11755
H	4.54775	-1.22453	-2.22039
H	2.82914	-1.26092	-2.64837
H	3.69673	0.27328	-2.61275
C	3.14205	-2.18778	0.54303
H	2.45741	-2.87896	0.04879
H	4.14347	-2.62425	0.50900
H	2.84381	-2.10364	1.58976
C	-2.58130	2.14316	-1.48593
H	-2.34168	1.78575	-2.48901
H	-3.40196	2.86098	-1.55880
H	-1.69916	2.66131	-1.10642
C	-3.52883	1.31867	1.34871
H	-2.72009	1.90006	1.79586
H	-4.41129	1.96047	1.28779
H	-3.75509	0.49074	2.02324
C	-4.48665	-0.25997	-1.13297
H	-4.19440	-0.71138	-2.08287
H	-4.83942	-1.05770	-0.47705
H	-5.32584	0.41461	-1.32164
O	0.04030	-0.15850	-1.43377

$[I_E^t\text{-}4_E^t]^‡$

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XYZ

Si	-1.00130	0.51236	-0.05975
Si	0.89970	-0.52168	-0.34918
O	1.27341	-0.32146	2.38468
N	0.20613	0.07352	2.75889
N	-0.85808	0.44075	2.61734
Si	3.11235	0.26030	-0.50009
C	3.11805	2.02205	0.15996
H	2.42580	2.65898	-0.39311
H	2.83234	2.04306	1.21264
H	4.12066	2.44791	0.06857
C	4.20262	-0.88000	0.52375
H	3.92125	-0.84998	1.57685
H	4.12372	-1.91276	0.17957
H	5.24768	-0.57160	0.43554
C	3.62849	0.21577	-2.31192
H	2.99125	0.86019	-2.91990
H	4.66032	0.56194	-2.41503
H	3.57125	-0.79723	-2.71468
Si	-3.18007	-0.27625	-0.41514
C	-3.67605	0.07296	-2.19820
H	-3.59773	1.13801	-2.42411
H	-3.03710	-0.47049	-2.89606
H	-4.71125	-0.23470	-2.36847
C	-4.30461	0.65248	0.77566
H	-5.34133	0.33331	0.64076
H	-4.01930	0.46524	1.81203
H	-4.25655	1.72891	0.60046
C	-3.16732	-2.12314	-0.05237
H	-2.48797	-2.65546	-0.71993
H	-2.85569	-2.32250	0.97442
H	-4.17145	-2.53328	-0.18776
Cl	0.72564	-2.60994	-0.25355
Cl	-0.81248	2.59084	-0.33562

$[5_E^t\text{-}P_E^t]^‡$

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XYZ

Si	1.05400	-0.53713	-0.10386
Si	-1.03158	0.53318	-0.17399
O	-1.14320	0.51454	2.30569
N	-0.05996	0.13029	2.67230

N	0.96563	-0.25803	2.35661
Si	-3.18709	-0.37246	-0.38483
C	-3.04593	-2.19210	0.07725
H	-2.32023	-2.70516	-0.55649
H	-2.72952	-2.31035	1.11530
H	-4.01246	-2.68819	-0.04091
C	-4.34700	0.55243	0.77179
H	-4.03236	0.44708	1.81116
H	-4.37351	1.61681	0.53150
H	-5.36210	0.15801	0.68048
C	-3.68950	-0.16121	-2.18771
H	-2.96853	-0.64208	-2.85108
H	-4.66910	-0.61313	-2.36282
H	-3.75002	0.89428	-2.45936
Si	3.22584	0.31472	-0.36314
C	3.75112	-0.06159	-2.13252
H	3.79796	-1.13783	-2.30872
H	3.04740	0.36921	-2.84687
H	4.74034	0.35830	-2.33152
C	4.36250	-0.51500	0.88591
H	5.38272	-0.13886	0.77657
H	4.03401	-0.31863	1.90776
H	4.38144	-1.59635	0.73842
C	3.10665	2.17126	-0.06764
H	2.39445	2.63413	-0.75331
H	2.78168	2.38831	0.95180
H	4.08090	2.64253	-0.21924
Cl	-1.01242	2.62545	-0.22573
Cl	1.04106	-2.63344	-0.01704
O	0.02656	-0.04294	-1.37807

$[I_F^t\text{-}4_F^t]^‡$

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XYZ

Si	0.89960	-0.30449	0.63202
Si	-0.85909	-0.31800	-0.64788
O	-1.02631	2.45114	-0.49339
N	-0.04539	2.69734	0.14690
N	0.89665	2.44643	0.72544
Si	-3.06276	-0.48751	0.12971
C	-3.12655	-0.13359	1.98367
H	-2.59857	-0.90295	2.55027
H	-2.68031	0.83442	2.21944
H	-4.16461	-0.11958	2.32560
C	-4.13132	0.76087	-0.80213
H	-3.78614	1.78056	-0.62519
H	-4.10385	0.57740	-1.87847
H	-5.17237	0.68707	-0.47666
C	-3.72694	-2.22749	-0.19835
H	-3.13757	-2.97963	0.32942
H	-4.76405	-2.30834	0.13822
H	-3.70122	-2.46659	-1.26368
Si	3.09550	-0.43539	-0.16791
C	3.77429	-2.18165	0.08830
H	3.75138	-2.46286	1.14336
H	3.18865	-2.91589	-0.46802
H	4.81155	-2.24181	-0.25224
C	4.16524	0.78254	0.80319
H	5.20284	0.73336	0.46242
H	3.80891	1.80608	0.67681
H	4.15246	0.55278	1.87090
C	3.14744	-0.00647	-2.00667
H	2.61207	-0.75004	-2.60015
H	2.70412	0.97222	-2.20079
H	4.18322	0.01757	-2.35492
C	-0.66581	-0.25001	-2.53176
H	-0.95549	-1.20061	-2.98385
H	-1.30430	0.53286	-2.94431
H	0.36403	-0.03561	-2.81593
C	0.70046	-0.49483	2.50905
H	-0.33157	-0.32417	2.81477
H	0.99491	-1.49410	2.83426
H	1.33127	0.23175	3.02453

4_F^t

39

XYZ

Si	-0.74889	0.27098	-0.52633
Si	1.27512	1.00895	0.66549
O	1.35270	2.50940	0.19698

N	-1.65558	3.24471	-0.33441
N	-1.48039	2.17810	-0.47637
Si	2.78392	-0.61738	-0.15686
C	3.27600	-0.23990	-1.94325
H	2.41230	-0.27345	-2.61099
H	3.70804	0.75995	-2.01446
H	4.01188	-0.96151	-2.30742
C	4.34062	-0.70454	0.91671
H	4.86494	0.25319	0.91388
H	4.09237	-0.94630	1.95257
H	5.02881	-1.46879	0.54613
C	1.93510	-2.32200	-0.11080
H	1.06954	-2.36217	-0.77949
H	2.62443	-3.10902	-0.42725
H	1.58939	-2.56714	0.89656
Si	-2.70674	-0.84629	0.20306
C	-2.18054	-2.64239	0.46033
H	-1.82377	-3.09654	-0.46651
H	-1.38069	-2.71633	1.19990
H	-3.02585	-3.23512	0.81847
C	-4.10095	-0.74659	-1.06724
H	-4.98510	-1.27817	-0.70636
H	-4.39083	0.28837	-1.26111
H	-3.80320	-1.19703	-2.01622
C	-3.24682	-0.08565	1.84363
H	-2.43335	-0.10866	2.57159
H	-3.56155	0.95325	1.72311
H	-4.09035	-0.64045	2.26138
C	0.87963	0.59054	2.47722
H	0.67845	-0.47711	2.60885
H	1.73490	0.85311	3.10552
H	0.02004	1.15824	2.84067
C	-0.58351	0.19293	-2.40826
H	0.14569	0.92675	-2.75460
H	-0.19597	-0.79951	-2.65828
H	-1.52502	0.32748	-2.94122

[4_F^t-5_F^t]‡

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XYZ

Si	-0.73278	0.05669	-0.49107
Si	1.22681	0.79362	0.64471
O	0.90854	2.22523	0.03151
N	-2.12798	3.23777	-0.14242
N	-1.74090	2.22469	-0.23469
Si	3.05324	-0.46798	-0.15910
C	3.08457	-0.39575	-2.05038
H	2.19949	-0.86948	-2.48170
H	3.10821	0.64095	-2.39236
H	3.96484	-0.90786	-2.44710
C	4.68727	0.21229	0.51201
H	4.81778	1.25823	0.22749
H	4.72155	0.15426	1.60218
H	5.53392	-0.35570	0.11761
C	2.87344	-2.27772	0.38415
H	1.93446	-2.70981	0.02824
H	3.69034	-2.88595	-0.01271
H	2.88958	-2.36524	1.47292
Si	-2.80311	-0.89789	0.16534
C	-2.56484	-2.76893	0.01583
H	-2.36906	-3.06937	-1.01575
H	-1.73461	-3.11666	0.63425
H	-3.46732	-3.28845	0.34753
C	-4.22825	-0.33962	-0.94206
H	-5.15909	-0.82467	-0.63733
H	-4.38289	0.73977	-0.88479
H	-4.04200	-0.59902	-1.98622
C	-3.14175	-0.43458	1.96308
H	-2.31259	-0.73585	2.60656
H	-3.28177	0.64201	2.08072
H	-4.04692	-0.92990	2.32278
C	1.00262	0.48294	2.50135
H	0.99031	-0.58809	2.72255
H	1.83359	0.93124	3.05284
H	0.07874	0.93088	2.87308
C	-0.66015	0.24568	-2.36136
H	0.14785	0.92590	-2.63072
H	-0.43921	-0.73837	-2.78907
H	-1.59700	0.59422	-2.79749

5_F^t

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XYZ

Si	0.89330	-0.66666	0.03668
O	0.00000	0.00000	-1.28755
Si	3.10162	0.13530	0.08290
C	3.06919	2.01095	-0.13278
H	2.58274	2.49415	0.71719
H	4.08360	2.40945	-0.21279
H	2.52413	2.28467	-1.03847
C	4.07197	-0.65041	-1.33854
H	4.15714	-1.73154	-1.20945
H	3.58442	-0.46197	-2.29705
H	5.08300	-0.23744	-1.38626
C	3.92563	-0.31258	1.72551
H	3.38598	0.11890	2.57098
H	3.96697	-1.39468	1.86809
H	4.95038	0.06671	1.75250
Si	-0.89331	0.66667	0.03668
Si	-3.10162	-0.13530	0.08290
C	-3.06918	-2.01095	-0.13278
H	-2.52412	-2.28466	-1.03848
H	-2.58273	-2.49415	0.71718
H	-4.08359	-2.40945	-0.21280
C	-4.07198	0.65041	-1.33854
H	-3.58444	0.46196	-2.29705
H	-5.08302	0.23744	-1.38624
H	-4.15715	1.73153	-1.20945
C	-3.92563	0.31257	1.72551
H	-4.95036	-0.06677	1.75253
H	-3.38594	-0.11887	2.57098
H	-3.96701	1.39467	1.86807
C	0.77182	-2.54543	0.12679
H	1.31279	-2.99395	-0.71047
H	1.21678	-2.91589	1.05338
H	-0.26481	-2.87954	0.08256
C	-0.77182	2.54543	0.12679
H	-1.21678	2.91590	1.05338
H	0.26482	2.87954	0.08257
H	-1.31278	2.99396	-0.71047

$[5_F^t\text{-}P_F^t]^‡$

40

XYZ

Si	-0.95713	-0.49152	-0.55789
Si	0.92693	-0.02464	0.74653
O	0.92857	2.42661	-0.08556
N	0.06863	2.43054	-0.92870
N	-0.74378	1.85178	-1.47976
Si	3.10572	-0.37958	-0.05672
C	3.04052	-0.66696	-1.92246
H	2.48943	-1.58070	-2.15382
H	2.55454	0.16437	-2.43754
H	4.04974	-0.77250	-2.32815
C	4.17232	1.12894	0.33357
H	3.76642	2.02892	-0.13130
H	4.22984	1.30322	1.41022
H	5.19012	0.98173	-0.03649
C	3.81508	-1.91313	0.79031
H	3.16984	-2.77856	0.62754
H	4.80638	-2.14711	0.39362
H	3.91146	-1.76278	1.86767
Si	-3.14332	-0.20671	0.25290
C	-3.92117	-1.91325	0.49030
H	-4.02140	-2.43926	-0.46152
H	-3.30962	-2.52879	1.15287
H	-4.91732	-1.82385	0.93132
C	-4.16514	0.80130	-0.97529
H	-5.18456	0.93486	-0.60453
H	-3.72849	1.78856	-1.13576
H	-4.22403	0.30025	-1.94393
C	-3.06430	0.68451	1.91684
H	-2.50997	0.09076	2.64659
H	-2.57376	1.65600	1.82442
H	-4.06964	0.85032	2.31181
C	0.80797	0.62208	2.50606
H	1.11261	-0.16380	3.20205
H	1.46273	1.48466	2.64156
H	-0.21093	0.92121	2.75325
C	-0.84745	-1.22249	-2.28735

H	0.17637	-1.21042	-2.66231
H	-1.19293	-2.25904	-2.26534
H	-1.47476	-0.66130	-2.98231
O	-0.03530	-1.43220	0.55307

$[I_R\text{-}4_R]^‡$

9

XYZ

Si	-1.16112	-1.05483	0.00000
Si	-1.07725	1.10383	0.00001
O	1.55810	1.05660	0.00000
N	1.81796	-0.11310	-0.00002
N	1.57739	-1.21997	0.00000
H	-1.42426	-1.79306	-1.25326
H	-1.02341	1.88939	-1.25013
H	-1.02340	1.88959	1.25002
H	-1.42402	-1.79319	1.25326

5_R

7

XYZ

Si	-1.10105	-0.25340	0.00001
O	0.00000	1.06165	0.00000
Si	1.10105	-0.25340	-0.00001
H	-1.93898	-0.34937	1.22016
H	-1.93761	-0.34959	-1.22110
H	1.93898	-0.34937	-1.22016
H	1.93761	-0.34959	1.22110

$[5_R\text{-}P_R]^‡$

10

XYZ

Si	0.85703	1.12566	-0.00016
Si	0.64691	-1.17004	0.00010
O	-1.80221	-1.00656	-0.00033
N	-2.03878	0.17288	0.00008
N	-1.63174	1.23514	0.00030
H	0.93561	1.95586	-1.22503
H	0.57061	-1.98949	-1.23032
H	0.56970	-1.98874	1.23092
H	0.93583	1.95642	1.22429
O	2.00555	-0.13955	0.00012

$[4_F{}^t\text{-}5_F{}^c]^‡$

39

XYZ

Si	-0.92439	0.75071	-0.47150
Si	1.50051	1.21250	-0.37989
O	1.59248	1.74980	-1.85430
N	-1.91692	2.64629	1.83057
N	-1.74569	1.96349	0.99359
Si	2.49258	-0.87006	0.12989
C	2.31384	-2.02417	-1.35684
H	1.26525	-2.21241	-1.59718
H	2.77295	-1.56756	-2.23568
H	2.79660	-2.98742	-1.17307
C	4.33182	-0.62603	0.50794
H	4.84227	-0.15917	-0.33673
H	4.47342	0.01436	1.38149
H	4.81713	-1.58444	0.71044
C	1.67760	-1.66636	1.65046
H	0.61561	-1.85702	1.48083
H	2.15109	-2.62198	1.89000
H	1.76526	-1.02130	2.52809
Si	-2.32852	-1.10719	0.03687
C	-1.55669	-2.64942	-0.72803
H	-1.40975	-2.53762	-1.80425
H	-0.59011	-2.88177	-0.27854
H	-2.21629	-3.50626	-0.56893
C	-4.04669	-0.82504	-0.69441
H	-4.69472	-1.68009	-0.48562
H	-4.52037	0.06456	-0.27346
H	-3.99702	-0.69756	-1.77762
C	-2.45714	-1.30974	1.91151
H	-1.47443	-1.37113	2.38291
H	-3.00358	-0.48236	2.36958
H	-2.99718	-2.23005	2.14736
C	1.69591	2.37494	1.11089
H	1.38943	1.89342	2.04456
H	2.74959	2.64993	1.20914

H	1.12988	3.30062	0.98344
C	-1.64148	1.69670	-1.93091
H	-1.13150	2.65283	-2.04810
H	-1.37618	1.10823	-2.81458
H	-2.72451	1.81871	-1.90746

5_F^c

37

XYZ

Si	1.11396	1.16531	-0.06134
Si	-1.11062	1.16145	-0.09089
O	-0.01480	1.24142	1.24787
Si	-2.43750	-0.78282	-0.04040
C	-1.58251	-2.04479	1.07486
H	-0.63647	-2.37997	0.64599
H	-1.37016	-1.61012	2.05345
H	-2.21593	-2.92385	1.21717
C	-4.14099	-0.36376	0.66897
H	-4.05652	0.04790	1.67688
H	-4.65702	0.37178	0.04797
H	-4.76724	-1.25811	0.72071
C	-2.64050	-1.49061	-1.78186
H	-1.66936	-1.69474	-2.23745
H	-3.20470	-2.42618	-1.75169
H	-3.17673	-0.79705	-2.43327
Si	2.43945	-0.78507	-0.04353
C	2.35148	-1.55916	1.67663
H	2.77307	-0.88794	2.42741
H	1.31804	-1.76277	1.96130
H	2.90824	-2.49926	1.70612
C	4.23219	-0.34306	-0.45751
H	4.85917	-1.23832	-0.45066
H	4.31246	0.11439	-1.44602
H	4.64230	0.35986	0.27076
C	1.78682	-1.99892	-1.33899
H	0.72828	-2.21478	-1.18172
H	1.89337	-1.58563	-2.34429
H	2.33463	-2.94372	-1.29989
C	-2.09804	2.75266	-0.31208
H	-2.62863	2.74227	-1.26738
H	-2.83981	2.85231	0.48416
H	-1.44675	3.62725	-0.28947
C	2.09729	2.76310	-0.25021
H	1.43986	3.63314	-0.23014
H	2.82419	2.86113	0.55986
H	2.64570	2.76434	-1.19520

$[5_F^c\text{-}P_F^c]^‡$

40

XYZ

Si	-1.15898	-0.84803	-0.58505
Si	1.17655	-0.81580	-0.63859
O	1.27284	-1.90916	1.69478
N	0.12145	-1.91342	2.04728
N	-0.96421	-1.68074	1.78835
Si	2.42997	1.06109	0.04349
C	2.22459	1.36879	1.89431
H	1.17620	1.51857	2.15866
H	2.59852	0.52155	2.47177
H	2.77947	2.26079	2.19596
C	4.25698	0.75676	-0.33904
H	4.63426	-0.11021	0.20745
H	4.41649	0.57862	-1.40447
H	4.85712	1.62293	-0.04892
C	1.80035	2.54343	-0.94276
H	0.73422	2.70646	-0.77379
H	2.33380	3.45356	-0.65760
H	1.93856	2.38444	-2.01377
Si	-2.52974	0.94860	0.06175
C	-4.14867	0.26219	0.75358
H	-4.67996	-0.32856	0.00430
H	-3.96156	-0.37840	1.61787
H	-4.80741	1.07448	1.07073
C	-2.85714	2.02461	-1.45551
H	-3.43717	2.91032	-1.18432
H	-1.91711	2.35360	-1.90308
H	-3.41358	1.47629	-2.21839
C	-1.66646	1.97767	1.39060
H	-1.43000	1.36811	2.26512
H	-0.73686	2.41161	1.01753

H	-2.31077	2.79890	1.71441
C	2.15949	-2.27719	-1.29297
H	2.62027	-2.00595	-2.24611
H	2.94568	-2.56139	-0.59178
H	1.51619	-3.14225	-1.46033
C	-2.09402	-2.37957	-1.15450
H	-1.41257	-3.20468	-1.36711
H	-2.80522	-2.70351	-0.39258
H	-2.64658	-2.15175	-2.06942
O	-0.02192	-0.36542	-1.78304

$[I_A^t-I_A^c]^T$

22

XYZ

Si	-1.15542	-0.24337	-0.78938
Si	1.15552	0.24350	-0.78950
N	1.70988	0.90634	0.71720
N	-1.70981	-0.90636	0.71722
C	3.12246	1.04373	1.02367
H	3.47263	2.07083	0.86462
H	3.30182	0.78231	2.07149
H	3.71943	0.37491	0.40466
C	-0.85939	-1.74616	1.54196
H	-1.03222	-1.51648	2.59872
H	-1.06335	-2.81247	1.38944
H	0.19431	-1.56527	1.33004
C	0.85947	1.74629	1.54181
H	1.03294	1.51728	2.59861
H	1.06284	2.81262	1.38860
H	-0.19425	1.56479	1.33050
C	-3.12241	-1.04407	1.02349
H	-3.47242	-2.07115	0.86394
H	-3.30185	-0.78318	2.07143
H	-3.71944	-0.37502	0.40479
Cl	-2.17566	1.58906	-1.05988
Cl	2.17548	-1.58904	-1.06006

$[I_B^t-I_B^c]^T$

28

XYZ

Si	-1.16791	0.06802	-0.93747
Si	1.16774	-0.06700	-0.93769
N	1.87968	0.48735	0.56921
N	-1.87951	-0.48776	0.56908
C	3.27161	0.24754	0.88719
H	3.91202	1.10035	0.62130
H	3.38942	0.06651	1.96177
H	3.64349	-0.63133	0.36065
C	-1.31521	-1.59717	1.30748
H	-1.43444	-1.43003	2.38409
H	-1.79777	-2.55374	1.06372
H	-0.24741	-1.68787	1.10454
C	1.31594	1.59643	1.30850
H	1.43509	1.42842	2.38499
H	1.79895	2.55298	1.06550
H	0.24819	1.68785	1.10564
C	-3.27166	-0.24915	0.88704
H	-3.91140	-1.10232	0.62069
H	-3.38972	-0.06869	1.96169
H	-3.64415	0.62970	0.36090
C	1.81306	-1.82401	-1.25710
H	1.20747	-2.28671	-2.03838
H	2.84993	-1.82936	-1.59781
H	1.74500	-2.44070	-0.35667
C	-1.81358	1.82520	-1.25518
H	-1.74405	2.44147	-0.35457
H	-1.20936	2.28828	-2.03728
H	-2.85105	1.83069	-1.59408

$[I_C^t-I_C^c]^T$

12

XYZ

Si	1.08322	0.72219	-0.28245
Si	-1.13640	0.06517	-0.67653
Cl	2.31971	-0.95540	-0.41482
Cl	-1.75631	-1.39669	0.69503
C	1.40824	1.54794	1.38280
H	2.46184	1.81171	1.48411
H	0.80869	2.45466	1.48117
H	1.14206	0.86056	2.18934

C	-2.33014	1.51871	-0.54140
H	-2.31345	1.93466	0.46902
H	-2.05125	2.30181	-1.24884
H	-3.34971	1.19931	-0.76100

$[I_D^t - I_D^c]^T$

46

XYZ

Si	-0.93567	-0.68874	0.34829
Si	0.93580	0.68910	0.34919
N	1.06918	1.69318	-1.09058
N	-1.06834	-1.69092	-1.09292
C	2.21812	2.54475	-1.31080
H	2.57199	2.45883	-2.34539
H	1.98794	3.60190	-1.12144
H	3.04033	2.26334	-0.65152
C	0.05851	-2.03089	-1.93253
H	0.47074	-3.02258	-1.69817
H	-0.24258	-2.03798	-2.98692
H	0.85293	-1.29278	-1.81939
C	-0.05745	2.03506	-1.92973
H	-0.46836	3.02711	-1.69459
H	0.24339	2.04249	-2.98420
H	-0.85276	1.29786	-1.81690
C	-2.21659	-2.54322	-1.31401
H	-2.57052	-2.45652	-2.34851
H	-1.98559	-3.60038	-1.12571
H	-3.03904	-2.26314	-0.65447
Si	2.97461	-0.43693	0.72280
Si	-2.97525	0.43547	0.72291
C	-3.84041	0.83859	-0.91421
H	-4.03103	-0.06514	-1.49648
H	-4.80027	1.32764	-0.72695
H	-3.23384	1.50856	-1.52635
C	-2.58169	2.04370	1.63478
H	-2.05863	1.84953	2.57324
H	-1.94405	2.68922	1.02706
H	-3.50210	2.58733	1.86412
C	-4.15371	-0.60071	1.78119
H	-3.70243	-0.83067	2.74829
H	-5.08638	-0.05882	1.95916
H	-4.40425	-1.54750	1.29772
C	2.57991	-2.04600	1.63269
H	1.94225	-2.69064	1.02405
H	3.50004	-2.59024	1.86177
H	2.05661	-1.85266	2.57117
C	3.83986	-0.83861	-0.91464
H	4.79963	-1.32802	-0.72784
H	3.23319	-1.50786	-1.52746
H	4.03066	0.06567	-1.49599
C	4.15353	0.59725	1.78252
H	4.40479	1.54438	1.30006
H	3.70217	0.82655	2.74974
H	5.08581	0.05460	1.96017

$[I_E^t - I_E^c]^T$

30

XYZ

Si	-0.89141	-0.75731	0.59272
Si	0.89141	0.75732	0.59273
Si	-3.03254	0.16595	0.21273
Si	3.03254	-0.16595	0.21274
C	-3.13699	1.74105	1.24417
H	-2.37945	2.46204	0.93030
H	-4.11775	2.20679	1.11767
H	-2.99608	1.53789	2.30748
C	-4.34690	-1.07896	0.73873
H	-5.34457	-0.68413	0.53040
H	-4.23531	-2.01990	0.19662
H	-4.28269	-1.29321	1.80705
C	-3.18928	0.55477	-1.62511
H	-3.07396	-0.34866	-2.22641
H	-4.17345	0.98252	-1.83444
H	-2.42902	1.27252	-1.93766
C	4.34688	1.07897	0.73872
H	4.28265	1.29327	1.80703
H	5.34456	0.68413	0.53043
H	4.23530	2.01988	0.19656
C	3.18927	-0.55478	-1.62510
H	2.42900	-1.27252	-1.93765

H	3.07396	0.34865	-2.22641
H	4.17344	-0.98254	-1.83444
C	3.13699	-1.74106	1.24418
H	4.11775	-2.20680	1.11766
H	2.99610	-1.53790	2.30748
H	2.37945	-2.46204	0.93031
Cl	0.53600	2.27865	-0.84201
Cl	-0.53598	-2.27865	-0.84201

$[I_F^t\text{-}I_F^c]^T$

36

XYZ

Si	0.97236	1.10726	0.47111
Si	-0.99582	0.98661	-0.76402
C	-1.88472	2.65996	-0.96148
H	-1.21322	3.41622	-1.36980
H	-2.74582	2.56895	-1.62648
H	-2.24371	3.01732	0.00813
Si	-2.47722	-0.67067	0.00523
C	-3.83198	-1.00978	-1.27010
H	-4.54670	-1.74184	-0.88477
H	-4.38296	-0.09823	-1.51149
H	-3.40947	-1.40317	-2.19665
C	-3.28328	-0.05813	1.60788
H	-2.53198	0.11097	2.38235
H	-3.81916	0.87992	1.44858
H	-3.99820	-0.79554	1.98332
C	-1.53172	-2.26490	0.37278
H	-1.05560	-2.66571	-0.52363
H	-0.75086	-2.09279	1.11685
H	-2.21039	-3.02615	0.76598
C	0.69269	0.99837	2.35803
Si	2.70993	-0.29279	-0.25972
H	-0.02412	1.74759	2.69751
H	0.30328	0.01312	2.63105
H	1.63051	1.15040	2.89611
C	3.40360	0.36527	-1.88967
H	4.18041	-0.30244	-2.27143
H	2.61933	0.43657	-2.64647
H	3.83942	1.35799	-1.76252
C	2.10346	-2.06438	-0.54455
H	2.92920	-2.69597	-0.88388
H	1.69369	-2.50305	0.36705
H	1.32307	-2.08870	-1.30787
C	4.06976	-0.31587	1.05616
H	3.69106	-0.69821	2.00665
H	4.89401	-0.96071	0.74052
H	4.47170	0.68431	1.23031

$[I_A^t\text{-}6_A^t]^‡$

22

XYZ

Si	1.31584	-1.24361	-0.06722
Si	-0.78176	0.14554	-0.49583
N	-2.33705	-0.55002	-0.44869
N	2.60695	-0.09724	-0.25002
C	-2.43782	-1.98875	-0.66259
H	-2.72474	-2.49951	0.26233
H	-3.18677	-2.20744	-1.42937
H	-1.48220	-2.39968	-0.99220
C	2.67357	1.30121	0.12165
H	3.64460	1.52808	0.57475
H	2.54771	1.95142	-0.75396
H	1.90188	1.54837	0.84767
C	-3.58593	0.04764	-0.01107
H	-4.37231	-0.14633	-0.74665
H	-3.89894	-0.37788	0.94842
H	-3.48072	1.12342	0.10556
C	3.72739	-0.51430	-1.07682
H	3.77460	0.05908	-2.01085
H	4.67472	-0.37439	-0.54429
H	3.64176	-1.57236	-1.33585
Cl	-1.05963	2.20423	-0.22497
Cl	0.31439	-0.42799	1.84974

6_A^t

22

XYZ

Si	1.30988	-1.38103	-0.29951
Si	-0.62070	0.06130	-0.02245

N	-2.05483	-0.84624	-0.32055
N	2.61301	-0.28425	-0.05661
C	-3.34743	-0.21766	-0.53562
H	-3.96358	-0.85248	-1.17962
H	-3.88592	-0.06260	0.40829
H	-3.23033	0.74650	-1.02775
C	2.65537	1.13245	0.27886
H	3.22566	1.28051	1.20098
H	3.14683	1.69432	-0.52128
H	1.66303	1.54477	0.42697
C	-2.17688	-2.16978	0.26998
H	-2.65544	-2.13802	1.25754
H	-2.77877	-2.81283	-0.37927
H	-1.19945	-2.64345	0.38306
C	3.96506	-0.82002	-0.20872
H	4.49693	-0.29403	-1.00764
H	4.53035	-0.69584	0.72001
H	3.92897	-1.88104	-0.45520
Cl	-0.64019	1.65804	-1.38464
Cl	-0.73692	0.98631	1.88431

6_A^c

22

XYZ

Si	1.45484	-1.10764	-0.81894
Si	-0.69326	-0.28353	-0.03558
N	-1.02191	1.40365	-0.17960
N	2.51935	-0.01878	-0.00631
C	-2.26038	1.98934	0.30290
H	-2.08017	3.01328	0.64521
H	-3.03013	2.01824	-0.47841
H	-2.64993	1.41945	1.14615
C	2.26904	1.08503	0.91058
H	2.72143	0.87700	1.88511
H	2.71722	2.00512	0.52076
H	1.20510	1.25601	1.05105
C	-0.40573	2.16547	-1.25008
H	-1.04268	2.22398	-2.14211
H	-0.20012	3.18701	-0.91354
H	0.54709	1.71914	-1.54412
C	3.95422	-0.21386	-0.20574
H	4.40818	0.68849	-0.62731
H	4.44720	-0.43089	0.74695
H	4.13477	-1.04421	-0.88821
Cl	-1.00871	-0.79461	1.97610
Cl	-2.14806	-1.39988	-1.07509

$[6_A^c\text{-}I_A^c]^‡$

22

XYZ

Si	1.43790	-1.21196	-0.37753
Si	-0.89548	-0.16942	-0.57590
N	-1.56989	1.35179	-0.18829
N	2.52836	0.13000	-0.16176
C	-2.83746	1.63018	0.46314
H	-2.67139	2.01709	1.47457
H	-3.39806	2.37915	-0.10473
H	-3.44182	0.72902	0.53293
C	2.43926	1.31816	0.65830
H	3.30148	1.38796	1.33140
H	2.42720	2.22563	0.04029
H	1.54034	1.30101	1.27130
C	-0.73535	2.53296	-0.34382
H	-1.25942	3.29324	-0.93100
H	-0.47382	2.96585	0.62803
H	0.19047	2.28223	-0.86385
C	3.73394	0.10357	-0.97423
H	3.75994	0.94145	-1.68161
H	4.62949	0.16211	-0.34502
H	3.78907	-0.82314	-1.55042
Cl	0.24033	-1.03573	1.60549
Cl	-2.49322	-1.51745	-0.59512

I_A^c

22

XYZ

Si	-1.13701	-0.52968	-0.63159
Si	1.13682	-0.52926	0.63049
N	1.90641	0.99661	0.39068
N	-1.90688	0.99594	-0.39054

C	3.04267	1.35349	-0.43576
H	2.74811	2.09208	-1.19059
H	3.84049	1.79194	0.17313
H	3.43887	0.47777	-0.94358
C	-3.04136	1.35238	0.43852
H	-2.74549	2.09154	1.19228
H	-3.84108	1.78994	-0.16852
H	-3.43560	0.47657	0.94774
C	1.36138	2.12852	1.12414
H	2.08614	2.51300	1.84974
H	1.09901	2.94198	0.44038
H	0.45912	1.83584	1.66674
C	-1.36451	2.12788	-1.12590
H	-2.09126	2.51137	-1.85004
H	-1.10118	2.94199	-0.44327
H	-0.46332	1.83562	-1.67050
Cl	2.39872	-1.88766	-0.38574
Cl	-2.39737	-1.88858	0.38603

$[I_B^t\text{-}6_B^t]^‡$

28

XYZ

Si	1.02349	-1.10905	0.10416
Si	-0.71025	0.33694	-0.37297
N	-2.30880	-0.31589	-0.32349
N	2.49334	-0.12347	0.02447
C	-3.47709	0.38850	0.16428
H	-4.34478	0.16785	-0.46712
H	-3.73091	0.09556	1.19224
H	-3.32265	1.46623	0.14792
C	2.58954	1.31489	0.02716
H	1.84950	1.75264	0.69992
H	3.57607	1.63391	0.38280
H	2.44118	1.75341	-0.97310
C	-2.52347	-1.74827	-0.42521
H	-2.72629	-2.20025	0.55485
H	-3.37904	-1.95968	-1.07617
H	-1.64446	-2.23818	-0.84387
C	3.67524	-0.76506	-0.51694
H	3.86712	-0.48338	-1.56269
H	4.56510	-0.49839	0.06689
H	3.56503	-1.85098	-0.48126
C	-0.87659	2.22174	-0.42955
H	0.10494	2.68812	-0.50401
H	-1.44384	2.49316	-1.32307
H	-1.39074	2.64216	0.43656
C	0.01778	-0.04023	1.72511
H	0.97165	0.04065	2.25107
H	-0.46046	0.93765	1.87060
H	-0.60695	-0.78489	2.21578

6_B^t

28

XYZ

Si	0.96015	-1.19507	0.00007
Si	-0.74731	0.53649	0.00008
N	-2.31360	-0.28282	-0.00004
N	2.44855	-0.30680	-0.00007
C	-2.72649	-0.98152	-1.20075
H	-2.26799	-1.97862	-1.30224
H	-3.81351	-1.12034	-1.20128
H	-2.47385	-0.40217	-2.09040
C	2.69377	1.12546	-0.00000
H	3.26971	1.41887	0.88503
H	3.26993	1.41891	-0.88488
H	1.76200	1.68279	-0.00011
C	-2.72641	-0.98201	1.20042
H	-3.81341	-1.12095	1.20088
H	-2.26780	-1.97909	1.30154
H	-2.47383	-0.40295	2.09027
C	3.70659	-1.04616	-0.00015
H	4.30143	-0.79860	-0.88655
H	4.30165	-0.79843	0.88604
H	3.51167	-2.11775	-0.00002
C	-0.71793	1.63578	-1.54348
H	0.07650	2.38175	-1.47694
H	-0.55500	1.06736	-2.46097
H	-1.67100	2.16302	-1.63410
C	-0.71804	1.63552	1.54383
H	-0.55530	1.06689	2.46122

H	0.07648	2.38142	1.47756
H	-1.67108	2.16283	1.63441

6_B^c

28

XYZ

Si	1.30007	-1.30029	-0.41604
Si	-0.99426	-0.67149	0.10777
N	-1.46145	0.96981	-0.31955
N	2.20930	0.09438	0.06313
C	-1.96269	1.97295	0.58628
H	-1.22227	2.76709	0.77736
H	-2.85916	2.45939	0.17993
H	-2.23259	1.53429	1.54619
C	1.76890	1.35070	0.64840
H	2.20290	1.48294	1.64593
H	2.09564	2.19550	0.03116
H	0.68598	1.38330	0.72632
C	-1.09533	1.50227	-1.61039
H	-1.94983	1.98689	-2.09962
H	-0.28852	2.24864	-1.53808
H	-0.74866	0.70819	-2.27634
C	3.65902	0.07394	-0.09571
H	3.98703	0.88259	-0.75832
H	4.15636	0.20739	0.87145
H	3.97707	-0.87643	-0.52296
C	-1.33608	-0.91704	1.95257
H	-1.08084	-1.94026	2.23816
H	-0.74635	-0.24072	2.57452
H	-2.39367	-0.76550	2.18308
C	-2.07049	-1.89142	-0.86103
H	-1.95231	-1.75448	-1.93877
H	-1.80121	-2.92576	-0.63114
H	-3.12589	-1.74578	-0.61888

$[6_B^c\text{-}I_B^c]^‡$

28

XYZ

Si	1.20623	-1.22526	-0.43040
Si	-0.95937	-0.48317	-0.43766
N	-1.66280	1.00023	0.05115
N	1.99055	0.37703	-0.00829
C	-0.83698	2.16919	0.31984
H	-1.09426	2.99396	-0.35393
H	-0.99219	2.51226	1.34942
H	0.21788	1.91687	0.21073
C	2.33233	1.16399	-1.17950
H	2.66225	2.16622	-0.88036
H	3.13983	0.72274	-1.78842
H	1.45924	1.28334	-1.82709
C	-3.06196	1.21067	0.36917
H	-3.19814	1.40496	1.44026
H	-3.45186	2.07456	-0.17987
H	-3.66393	0.34424	0.10161
C	3.12747	0.27657	0.88690
H	3.99275	-0.24448	0.44099
H	3.46433	1.27668	1.18283
H	2.85828	-0.25369	1.80309
C	0.16001	-1.53282	1.36759
H	-0.12257	-2.58300	1.43503
H	1.00960	-1.36412	2.03304
H	-0.64728	-0.93768	1.82218
C	-2.32193	-1.77165	-0.59861
H	-3.01741	-1.50460	-1.39755
H	-1.86936	-2.73055	-0.85582
H	-2.89109	-1.89635	0.32429

I_B^c

28

XYZ

Si	-1.07984	0.79802	-0.41116
Si	1.07985	0.79798	0.41100
N	1.96952	-0.69055	0.31661
N	-1.96967	-0.69041	-0.31673
C	3.13415	-0.94683	-0.50086
H	3.92713	-1.42244	0.08887
H	2.89563	-1.61699	-1.33878
H	3.53446	-0.02269	-0.91425
C	-1.47101	-1.88052	-0.97448
H	-1.22444	-2.66579	-0.24871

H	-2.21535	-2.28824	-1.66973
H	-0.56704	-1.64904	-1.54067
C	1.47061	-1.88064	0.97419
H	1.22424	-2.66588	0.24832
H	2.21472	-2.28842	1.66966
H	0.56649	-1.64914	1.54012
C	-3.13387	-0.94670	0.50137
H	-3.92681	-1.42311	-0.08775
H	-2.89473	-1.61615	1.33970
H	-3.53450	-0.02247	0.91423
C	2.15644	2.15777	-0.35733
H	1.61585	3.10620	-0.33001
H	3.07771	2.27977	0.21747
H	2.42219	1.95774	-1.39632
C	-2.15625	2.15785	0.35739
H	-2.42167	1.95780	1.39646
H	-1.61566	3.10628	0.32994
H	-3.07770	2.27986	-0.21712

$[I_C^t\text{-}6_C^t]^‡$

28

XYZ

Si	-1.07984	0.79802	-0.41116
Si	1.07985	0.79798	0.41100
N	1.96952	-0.69055	0.31661
N	-1.96967	-0.69041	-0.31673
C	3.13415	-0.94683	-0.50086
H	3.92713	-1.42244	0.08887
H	2.89563	-1.61699	-1.33878
H	3.53446	-0.02269	-0.91425
C	-1.47101	-1.88052	-0.97448
H	-1.22444	-2.66579	-0.24871
H	-2.21535	-2.28824	-1.66973
H	-0.56704	-1.64904	-1.54067
C	1.47061	-1.88064	0.97419
H	1.22424	-2.66588	0.24832
H	2.21472	-2.28842	1.66966
H	0.56649	-1.64914	1.54012
C	-3.13387	-0.94670	0.50137
H	-3.92681	-1.42311	-0.08775
H	-2.89473	-1.61615	1.33970
H	-3.53450	-0.02247	0.91423
C	2.15644	2.15777	-0.35733
H	1.61585	3.10620	-0.33001
H	3.07771	2.27977	0.21747
H	2.42219	1.95774	-1.39632
C	-2.15625	2.15785	0.35739
H	-2.42167	1.95780	1.39646
H	-1.61566	3.10628	0.32994
H	-3.07770	2.27986	-0.21712

6_C^t

12

XYZ

Si	-1.83007	-0.59323	0.86796
Si	0.45443	-0.05937	0.36080
Cl	0.77469	1.85000	-0.44145
C	-2.59098	0.53958	-0.45651
H	-3.66536	0.38581	-0.55691
H	-2.41152	1.58582	-0.17945
H	-2.11935	0.41047	-1.43588
C	1.79273	-0.34240	1.63297
H	1.70563	0.38754	2.44027
H	1.70159	-1.34430	2.05641
H	2.77928	-0.23983	1.17877
Cl	0.75815	-1.45190	-1.19176

6_C^c

12

XYZ

Si	-1.63482	-0.90891	-0.87561
Si	0.31463	-0.07233	0.24168
Cl	0.35475	1.86582	-0.58186
C	-2.84237	-0.20344	0.42978
H	-3.88354	-0.33673	0.13531
H	-2.69271	-0.70320	1.39469
H	-2.66714	0.86320	0.60820
C	0.39748	0.11083	2.10255
H	-0.48412	0.63756	2.47219
H	0.44436	-0.87129	2.57724

H	1.28740	0.67383	2.38831
Cl	2.06570	-1.04055	-0.35313

[6_C^c-I_C^c]‡

12

XYZ

Si	1.23312	-0.94430	0.49124
Si	-0.78919	-0.00031	-0.37537
Cl	1.64786	1.23705	0.67461
Cl	-2.56914	-0.68817	0.43988
C	2.22824	-1.34008	-1.10396
H	3.26510	-1.50756	-0.80133
H	1.86393	-2.27222	-1.54432
H	2.22083	-0.56040	-1.86451
C	-1.22039	1.69541	-1.03972
H	-0.36754	2.13689	-1.55451
H	-2.06986	1.60838	-1.72112
H	-1.51276	2.35650	-0.22057

I_C^c

12

XYZ

Si	-1.06137	0.41548	0.33437
Si	1.06137	0.41549	-0.33442
Cl	-2.09889	-1.36233	0.00801
C	-2.16322	1.83146	-0.23603
H	-3.01574	1.92353	0.43953
H	-1.61042	2.77264	-0.22082
H	-2.54140	1.65649	-1.24359
C	2.16302	1.83160	0.23605
H	1.60997	2.77264	0.22115
H	2.54137	1.65649	1.24352
H	3.01544	1.92405	-0.43959
Cl	2.09900	-1.36224	-0.00799

[I_D^t-6_D^t]‡

46

XYZ

Si	1.70938	-0.44832	1.32122
Si	-0.47516	-0.26384	0.71812
N	-1.37987	-1.67947	1.19762
N	2.43356	1.13547	1.10184
C	-2.50096	-2.20808	0.44992
H	-2.22730	-3.10350	-0.12392
H	-3.31880	-2.48242	1.12717
H	-2.88408	-1.47471	-0.25748
C	1.79036	2.42487	1.01728
H	0.77563	2.36533	1.40654
H	2.33947	3.16801	1.60829
H	1.73800	2.79908	-0.01474
C	-0.86535	-2.64345	2.15144
H	-1.68534	-3.03505	2.76458
H	-0.37869	-3.49668	1.65892
H	-0.13301	-2.18029	2.81186
C	3.86064	1.20558	0.85235
H	4.08033	1.51976	-0.17804
H	4.34182	1.92267	1.52843
H	4.32174	0.22900	1.00967
Si	-2.04451	1.27759	-0.21206
Si	1.11426	-0.87149	-1.20665
C	-3.53326	1.28096	0.95405
H	-4.29754	1.97040	0.58566
H	-3.98168	0.29026	1.04160
H	-3.24111	1.60325	1.95552
C	-2.62192	0.81293	-1.95583
H	-3.14458	-0.14426	-1.98790
H	-3.31501	1.58007	-2.31225
H	-1.78931	0.76236	-2.65909
C	-1.36458	3.03728	-0.30598
H	-1.14413	3.44174	0.68296
H	-0.45772	3.10185	-0.90837
H	-2.12101	3.67725	-0.76820
C	-0.11133	-2.02268	-2.10198
H	-1.10736	-1.59090	-2.20565
H	0.26669	-2.25416	-3.10186
H	-0.21066	-2.96450	-1.55712
C	1.31581	0.73521	-2.20052
H	2.11003	1.34552	-1.76558
H	1.60361	0.49567	-3.22783
H	0.40980	1.34089	-2.23806

C	2.77811	-1.77509	-1.40729
H	2.92782	-1.99553	-2.46973
H	3.61682	-1.17020	-1.05995
H	2.78911	-2.71314	-0.85101

6_D^t

46

XYZ

Si	-1.72192	-0.81930	1.56859
Si	0.29524	0.02162	0.52072
N	1.42373	0.29278	1.87578
N	-2.84335	-0.91547	0.25327
C	2.77267	0.72259	1.57224
H	3.17993	1.32414	2.39376
H	3.46176	-0.12408	1.41503
H	2.79390	1.33624	0.67171
C	-2.67634	-0.60761	-1.15420
H	-1.64329	-0.36079	-1.37643
H	-2.95793	-1.46510	-1.77503
H	-3.30854	0.23923	-1.44663
C	1.39983	-0.54789	3.05620
H	1.93806	-1.49988	2.91643
H	1.87369	-0.02655	3.89596
H	0.37812	-0.78221	3.35628
C	-4.20946	-1.34093	0.53797
H	-4.92445	-0.56179	0.25174
H	-4.45718	-2.24973	-0.02141
H	-4.32714	-1.54466	1.60167
Si	1.33718	-1.47676	-0.99981
Si	-0.14977	2.13264	-0.47978
C	1.97210	-2.94964	0.00857
H	2.50645	-3.65937	-0.62850
H	2.65984	-2.61328	0.78805
H	1.15190	-3.48121	0.49626
C	2.82863	-0.65259	-1.83427
H	3.57510	-0.34490	-1.10002
H	3.30667	-1.34942	-2.52837
H	2.53343	0.23327	-2.40110
C	0.20613	-2.12443	-2.37539
H	-0.65734	-2.65480	-1.96957
H	-0.16007	-1.31563	-3.01181
H	0.76352	-2.81956	-3.00899
C	1.20803	3.39575	-0.10065
H	2.13919	3.15982	-0.61989
H	0.88555	4.38799	-0.42791
H	1.41655	3.44150	0.96977
C	-0.30434	2.00571	-2.36662
H	-1.16863	1.41551	-2.67535
H	-0.41895	3.00491	-2.79547
H	0.58574	1.55399	-2.80937
C	-1.77983	2.80827	0.21128
H	-2.03207	3.76592	-0.25147
H	-2.60474	2.11536	0.03034
H	-1.70644	2.96365	1.29011

6_D^c

46

XYZ

Si	1.57900	-0.99470	-1.32780
Si	-0.10177	-0.17963	0.20481
N	0.19869	-0.47649	1.93520
N	3.07125	-0.75723	-0.48437
C	-0.61060	0.20087	2.92682
H	-1.60007	-0.26148	3.06991
H	-0.10156	0.19500	3.89756
H	-0.76973	1.24381	2.64863
C	3.33310	-0.19323	0.83208
H	2.40598	0.04363	1.34994
H	3.90186	-0.90299	1.44382
H	3.93548	0.71794	0.74021
C	0.52662	-1.83142	2.32971
H	1.02421	-1.83378	3.30640
H	-0.35616	-2.48676	2.40775
H	1.21386	-2.28114	1.60901
C	4.31275	-1.12544	-1.15586
H	4.96517	-0.25227	-1.26604
H	4.85585	-1.88079	-0.57746
H	4.10303	-1.53092	-2.14538
Si	-0.21191	2.14481	-0.19543
Si	-2.12814	-1.14124	-0.54705

C	1.13664	3.01827	0.80433
H	1.10137	4.09872	0.64262
H	1.02326	2.83061	1.87403
H	2.12540	2.66155	0.50810
C	-1.89970	2.87850	0.25432
H	-2.14069	2.72856	1.30875
H	-1.91491	3.95344	0.05543
H	-2.69353	2.41691	-0.33711
C	0.09084	2.44818	-2.04035
H	1.10345	2.15503	-2.32803
H	-0.60717	1.88134	-2.65983
H	-0.03304	3.50812	-2.27711
C	-3.54058	-0.74880	0.65416
H	-3.64879	0.32698	0.80713
H	-4.48902	-1.13412	0.26991
H	-3.36320	-1.20904	1.62883
C	-2.55589	-0.43298	-2.25167
H	-1.74883	-0.60796	-2.96706
H	-3.46151	-0.90172	-2.64556
H	-2.73170	0.64401	-2.19926
C	-1.97361	-3.02366	-0.69253
H	-2.90541	-3.46459	-1.05684
H	-1.17731	-3.29730	-1.38860
H	-1.74380	-3.47586	0.27505

$[6_D^c\text{-}I_D^c]^‡$

46

XYZ

Si	-1.18174	-0.73524	-1.26130
Si	0.43858	0.56834	-0.40453
N	0.67844	2.19114	0.19336
N	-2.77221	-0.01092	-1.23539
C	1.45321	2.46675	1.38635
H	2.10080	3.33858	1.23560
H	0.80966	2.67404	2.25317
H	2.08763	1.61895	1.64009
C	-3.16897	1.36329	-1.02283
H	-2.32860	1.95631	-0.67623
H	-3.55814	1.81407	-1.94506
H	-3.96112	1.43105	-0.26580
C	-0.13630	3.31332	-0.21926
H	-0.94429	3.53331	0.49446
H	0.48184	4.21430	-0.30526
H	-0.58110	3.12600	-1.19657
C	-3.91295	-0.87110	-1.49857
H	-4.59380	-0.90066	-0.63750
H	-4.48495	-0.51710	-2.36516
H	-3.58326	-1.89030	-1.70520
Si	-0.80622	-0.77631	1.33822
Si	2.47531	-0.59661	-0.70443
C	-1.89808	0.56527	2.12286
H	-2.11102	0.29995	3.16189
H	-1.41064	1.54256	2.11530
H	-2.84895	0.65663	1.59715
C	0.60490	-1.10604	2.57730
H	1.16389	-0.19731	2.80811
H	0.18117	-1.48600	3.51145
H	1.31126	-1.85071	2.20581
C	-1.81407	-2.38912	1.37657
H	-2.75359	-2.30123	0.82974
H	-1.24878	-3.21706	0.94619
H	-2.04304	-2.62808	2.42035
C	3.75450	-0.24446	0.64673
H	3.39080	-0.51479	1.63947
H	4.65452	-0.83285	0.44774
H	4.04431	0.80806	0.65977
C	2.17380	-2.45902	-0.79152
H	1.49325	-2.70678	-1.60712
H	3.12181	-2.97777	-0.95934
H	1.73762	-2.84416	0.13180
C	3.19765	-0.00515	-2.34942
H	4.16126	-0.48556	-2.53904
H	2.52782	-0.24556	-3.17729
H	3.35465	1.07568	-2.34499

I_D^c

46

XYZ

Si	1.02025	0.42933	-0.42642
Si	-1.02896	0.41699	0.44839

N	-1.84195	1.96091	0.59832
N	1.85801	1.93853	-0.61395
C	-2.76947	2.50549	-0.36697
H	-3.65824	2.92061	0.12512
H	-2.30987	3.31598	-0.95361
H	-3.09763	1.73918	-1.06611
C	1.15192	3.13786	-1.01574
H	1.13037	3.87967	-0.20727
H	1.63577	3.60261	-1.88355
H	0.12158	2.90177	-1.28322
C	-1.37744	2.95058	1.54777
H	-0.88960	3.80066	1.04994
H	-2.21532	3.34906	2.13417
H	-0.66007	2.50901	2.24020
C	3.23058	2.19459	-0.23831
H	3.76211	2.71348	-1.04498
H	3.29413	2.82029	0.66250
H	3.76097	1.26551	-0.03535
Si	-2.48114	-1.33691	-0.19090
Si	2.45849	-1.33595	0.18777
C	3.83646	-1.56122	-1.09104
H	4.49236	-0.69070	-1.15180
H	4.45275	-2.42492	-0.82709
H	3.41958	-1.73517	-2.08507
C	1.44218	-2.92760	0.25415
H	0.52710	-2.79510	0.83357
H	1.16935	-3.26463	-0.74726
H	2.02685	-3.72105	0.72647
C	3.22483	-1.03438	1.89141
H	2.44276	-0.97729	2.65064
H	3.90061	-1.85343	2.15303
H	3.79387	-0.10361	1.92813
C	-1.85799	-2.27596	-1.70796
H	-0.86753	-2.69672	-1.53019
H	-2.53703	-3.09760	-1.95231
H	-1.78971	-1.61276	-2.57185
C	-2.62764	-2.54947	1.25673
H	-3.31399	-3.36106	0.99989
H	-1.66366	-2.99263	1.51317
H	-3.01216	-2.04954	2.14815
C	-4.22427	-0.68570	-0.54885
H	-4.56088	0.01008	0.22204
H	-4.27755	-0.17674	-1.51302
H	-4.92507	-1.52452	-0.57585

$[I_E{}^t\text{-}6_E{}^t]^‡$

30

XYZ

Si	0.56679	-0.37368	-0.67728
Si	-1.29994	0.58903	-1.47005
Si	-2.38539	-0.35414	0.49347
C	-3.87901	0.77920	0.70910
H	-4.46624	0.45763	1.57394
H	-3.56419	1.81111	0.87406
H	-4.52013	0.75626	-0.17365
C	-1.43569	-0.35853	2.13448
H	-0.65904	-1.12763	2.14754
H	-0.96641	0.61189	2.31272
H	-2.11643	-0.55735	2.96705
C	-2.93784	-2.10656	0.07474
H	-3.55619	-2.11686	-0.82436
H	-2.09067	-2.77466	-0.08800
H	-3.53052	-2.50824	0.90120
Si	2.58268	0.28209	0.40131
C	2.59900	2.14328	0.65349
H	3.51626	2.43658	1.17091
H	2.55509	2.67536	-0.29773
H	1.74602	2.46840	1.25069
C	4.01566	-0.29028	-0.68008
H	4.96290	-0.07436	-0.17900
H	3.96688	-1.36485	-0.86412
H	4.02049	0.22290	-1.64326
C	2.58590	-0.63438	2.04918
H	2.51118	-1.71357	1.90341
H	3.51798	-0.42896	2.58196
H	1.75763	-0.31494	2.68416
Cl	-0.82276	2.57724	-0.69678
Cl	0.74802	-2.43967	-0.97424

$6_E{}^t$

30

XYZ

Si	0.03919	-0.05929	0.64141
Si	-0.30771	2.15268	1.45657
Si	2.05626	-0.33889	-0.56142
C	2.05116	0.73723	-2.11053
H	2.99315	0.60926	-2.65033
H	1.23653	0.46595	-2.78425
H	1.94114	1.79497	-1.86601
C	2.17137	-2.16274	-1.03509
H	2.09164	-2.80234	-0.15406
H	1.37487	-2.43904	-1.72937
H	3.12818	-2.37008	-1.52118
C	3.49886	0.13494	0.55861
H	3.48477	1.20273	0.78835
H	3.46167	-0.41537	1.50058
H	4.45043	-0.08972	0.07013
Si	-1.85150	-0.87725	-0.52505
C	-1.68556	-0.39618	-2.34256
H	-2.58385	-0.68531	-2.89402
H	-1.54793	0.68070	-2.45673
H	-0.83265	-0.89894	-2.80356
C	-3.42064	-0.12268	0.20583
H	-4.30724	-0.54553	-0.27337
H	-3.49203	-0.32170	1.27720
H	-3.44388	0.95894	0.05437
C	-1.88104	-2.75326	-0.33857
H	-1.92959	-3.03919	0.71350
H	-2.75295	-3.17114	-0.84845
H	-0.98538	-3.20678	-0.76766
Cl	-0.59756	2.99876	-0.47614
Cl	0.25644	-1.27128	2.39129

6_E^c

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XYZ

Si	0.19318	-0.14846	0.19339
Si	1.83171	-0.79275	-1.41759
Si	-1.81159	-1.34470	-0.17061
C	-2.12661	-1.42212	-2.03341
H	-3.07943	-1.91970	-2.23155
H	-2.17259	-0.42546	-2.47681
H	-1.34313	-1.98237	-2.54847
C	-3.23443	-0.44331	0.68281
H	-3.02622	-0.29890	1.74477
H	-3.40363	0.53804	0.23428
H	-4.16031	-1.01727	0.59349
C	-1.63081	-3.08370	0.53548
H	-0.83045	-3.63343	0.03590
H	-1.39834	-3.04774	1.60139
H	-2.55990	-3.64495	0.40769
Si	-0.17476	2.16848	-0.13430
C	-1.17941	2.39221	-1.72078
H	-1.32751	3.45564	-1.92504
H	-0.67763	1.95239	-2.58549
H	-2.16493	1.93019	-1.63084
C	1.47897	3.06675	-0.28975
H	1.32475	4.14712	-0.34929
H	2.11791	2.86312	0.57188
H	2.01616	2.75687	-1.18943
C	-1.13636	2.83416	1.34431
H	-0.58595	2.66901	2.27210
H	-1.30532	3.90827	1.23203
H	-2.10702	2.34395	1.43867
Cl	3.43209	-1.29442	-0.15629
Cl	0.75120	-0.41232	2.22101

$[6_E^c\text{-}I_E^c]^‡$

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XYZ

Si	-0.49943	-0.79664	-0.18645
Si	1.36484	-0.45950	-1.38041
Si	1.69703	1.29125	0.31468
C	3.54903	1.60064	0.11052
H	3.86830	2.37466	0.81444
H	4.12243	0.69499	0.31388
H	3.78299	1.93217	-0.90242
C	1.38945	0.88823	2.13847
H	0.32546	0.89713	2.38863
H	1.78474	-0.09875	2.38824

H	1.89120	1.62125	2.77642
C	0.75420	2.86141	-0.15208
H	0.83980	3.07811	-1.21827
H	-0.30469	2.80148	0.10202
H	1.17701	3.70603	0.39871
Si	-2.54303	0.40958	-0.25904
C	-3.92385	-0.85655	-0.46045
H	-4.89172	-0.34844	-0.45910
H	-3.83208	-1.40341	-1.40056
H	-3.91810	-1.58006	0.35631
C	-2.51719	1.59653	-1.72104
H	-3.44738	2.16998	-1.74732
H	-1.68791	2.30233	-1.66611
H	-2.43204	1.04952	-2.66177
C	-2.73093	1.31351	1.38577
H	-1.94406	2.05287	1.54308
H	-3.69180	1.83357	1.41511
H	-2.70529	0.60831	2.21899
Cl	2.67055	-1.98689	-0.61324
Cl	-0.80777	-2.38605	1.12440

I_E^c

30

XYZ

Si	-1.01375	0.65331	-0.41059
Si	1.01369	0.65326	0.41058
Si	2.62351	-0.98150	-0.13508
C	3.83163	-1.10292	1.30736
H	4.62653	-1.81422	1.06865
H	4.29483	-0.13578	1.51168
H	3.33495	-1.44199	2.21816
C	3.52491	-0.40540	-1.68634
H	2.84298	-0.35049	-2.53640
H	3.96490	0.58241	-1.53948
H	4.32901	-1.10399	-1.93304
C	1.78589	-2.64318	-0.43621
H	1.25606	-2.99897	0.44838
H	1.07477	-2.58512	-1.26199
H	2.54264	-3.38779	-0.69625
Si	-2.62350	-0.98152	0.13506
C	-3.52491	-0.40560	1.68638
H	-4.32898	-1.10426	1.93298
H	-2.84298	-0.35076	2.53644
H	-3.96495	0.58220	1.53961
C	-1.78573	-2.64315	0.43612
H	-2.54235	-3.38770	0.69670
H	-1.25631	-2.99913	-0.44863
H	-1.07422	-2.58491	1.26156
C	-3.83167	-1.10295	-1.30734
H	-3.33498	-1.44175	-2.21824
H	-4.62644	-1.81443	-1.06873
H	-4.29504	-0.13585	-1.51145
Cl	1.98207	2.51415	0.44012
Cl	-1.98210	2.51420	-0.44008

$[I_F^t\text{-}6_F^t]^‡$

36

XYZ

Si	0.45763	-0.26692	0.92367
Si	-1.23347	1.09267	1.39341
C	-0.74673	2.71108	0.43138
H	-0.38110	2.55382	-0.58444
H	-1.62139	3.36248	0.37396
H	0.02354	3.25318	0.98506
C	0.37076	-2.06906	1.49860
Si	2.47150	0.03689	-0.28503
H	-0.51711	-2.25531	2.10291
H	0.37039	-2.75223	0.64517
H	1.25100	-2.30737	2.10221
C	2.37042	1.60551	-1.32783
H	3.29622	1.74849	-1.89080
H	1.54714	1.54847	-2.04312
H	2.21032	2.48692	-0.70464
C	2.71764	-1.46449	-1.40814
H	3.64998	-1.36827	-1.97053
H	2.76896	-2.38901	-0.82915
H	1.90061	-1.55905	-2.12638
C	3.91831	0.15916	0.92737
H	4.00212	-0.74041	1.54069
H	4.85667	0.27947	0.37956

H	3.80694	1.01514	1.59567
Si	-2.22614	-0.29228	-0.35183
C	-3.14015	-1.76675	0.39500
H	-3.76717	-1.45276	1.23057
H	-3.77779	-2.22833	-0.36417
H	-2.45004	-2.53069	0.75737
C	-3.47142	0.93875	-1.07658
H	-4.04088	0.45999	-1.87854
H	-4.16837	1.28624	-0.31231
H	-2.96590	1.81110	-1.49549
C	-1.25061	-0.94336	-1.85774
H	-1.94467	-1.31412	-2.61807
H	-0.65157	-0.15134	-2.31447
H	-0.58056	-1.76646	-1.59645

H	3.57380	1.14549	0.86852
Si	-1.82406	-0.73577	-0.23835
C	-2.04894	-2.45103	0.52777
H	-2.24065	-2.37870	1.60034
H	-2.89279	-2.97125	0.06701
H	-1.15487	-3.06252	0.38823
C	-3.41416	0.26401	0.01028
H	-4.27280	-0.25588	-0.42251
H	-3.61888	0.42706	1.07064
H	-3.34304	1.24277	-0.47166
C	-1.52903	-0.93128	-2.09815
H	-2.38982	-1.41814	-2.56415
H	-1.38722	0.03322	-2.59036
H	-0.64788	-1.54377	-2.30010

6_F^t

36

XYZ

Si	0.00868	0.31885	0.82851
Si	-0.46263	2.63829	0.69280
C	-0.20041	2.86717	-1.19191
H	-0.37116	1.99690	-1.82730
H	-0.75779	3.72070	-1.58123
H	0.86548	3.12081	-1.29288
C	0.04238	-0.27729	2.64571
Si	1.97643	-0.45558	-0.21387
H	-0.88586	-0.02124	3.16073
H	0.17018	-1.36045	2.70324
H	0.86470	0.18844	3.19252
C	2.17699	0.20106	-1.97601
H	3.05792	-0.24791	-2.44227
H	1.30975	-0.04056	-2.59336
H	2.30602	1.28470	-1.99025
C	1.91534	-2.34816	-0.27994
H	2.84525	-2.74999	-0.69110
H	1.77614	-2.77507	0.71572
H	1.09318	-2.69427	-0.91038
C	3.47865	0.05868	0.81631
H	3.39871	-0.32013	1.83760
H	4.39876	-0.34036	0.38141

6_F^c

36

XYZ

Si	0.07785	-0.56049	0.41047
Si	0.98013	-2.13085	-1.11374
C	2.06033	-3.10918	0.13126
H	2.83933	-2.42558	0.49521
H	1.51134	-3.43969	1.01755
H	2.55592	-3.96712	-0.32442
C	0.27358	-0.95629	2.27145
Si	-2.14737	0.02391	-0.09275
H	1.32030	-1.13675	2.52454
H	-0.08371	-0.12816	2.88733
H	-0.29469	-1.84801	2.54413
C	-2.38867	0.11312	-1.96541
H	-3.41840	0.39146	-2.20461
H	-1.72507	0.85299	-2.41690
H	-2.17918	-0.84983	-2.43562
C	-2.56885	1.70830	0.66432
H	-3.62127	1.95211	0.49720
H	-2.38871	1.71860	1.74162
H	-1.96561	2.50093	0.21600
C	-3.32187	-1.27426	0.62808
H	-3.18341	-1.37859	1.70643
H	-4.36358	-0.99618	0.44819

H	-3.15210	-2.25204	0.17165
Si	1.42200	1.33039	-0.07195
C	1.23860	2.56768	1.34824
H	1.59899	2.13965	2.28622
H	1.81544	3.47435	1.14736
H	0.19427	2.85333	1.48942
C	3.24531	0.82690	-0.19642
H	3.88363	1.70770	-0.30394
H	3.56766	0.28944	0.69868
H	3.42403	0.18021	-1.05960
C	0.89929	2.14533	-1.69566
H	1.58353	2.95859	-1.95092
H	0.90490	1.42732	-2.51845
H	-0.10653	2.56416	-1.62085

[6_F^c-I_F^c]‡

36

a_Sic_sF.log Energy: -927040.9925441

Si	-0.41331	1.11849	0.02368
Si	1.36285	1.00840	-1.30377
C	2.51957	2.36526	-0.52602
H	2.54392	2.38001	0.56566
H	3.54154	2.21415	-0.88024
H	2.20142	3.35359	-0.86644
C	-0.71540	2.35160	1.42976
Si	-2.31129	-0.27796	-0.17671
H	0.14983	2.99495	1.59143
H	-1.57932	2.98210	1.20118
H	-0.93784	1.82005	2.35891
C	-2.31993	-1.15451	-1.84554
H	-3.18510	-1.81806	-1.92275
H	-2.37496	-0.42643	-2.65709
H	-1.41850	-1.74894	-1.99873
C	-3.82241	0.85625	-0.05241
H	-4.74036	0.27103	-0.15156
H	-3.85541	1.36974	0.91091
H	-3.82223	1.61266	-0.84006
C	-2.39339	-1.52492	1.24394
H	-2.37763	-1.01981	2.21240
H	-3.32397	-2.09498	1.18072
H	-1.56387	-2.23301	1.22069
Si	1.76385	-0.90481	0.16426
C	1.07403	-2.51272	-0.55037
H	1.29573	-2.58937	-1.61591
H	1.53351	-3.36363	-0.03970
H	-0.00581	-2.59630	-0.42316
C	3.65730	-0.95705	0.07209
H	4.02999	-1.79500	0.66860
H	3.99677	-1.08176	-0.95734
H	4.09872	-0.03980	0.46640
C	1.37460	-0.88357	2.03060
H	1.88966	-1.71116	2.52776
H	1.72135	0.04482	2.49157
H	0.30704	-0.98462	2.24003

I_F^c

36

XYZ

Si	1.06567	1.24535	0.02713
Si	-1.07842	1.24761	-0.03077
C	-2.05968	2.87340	-0.06146
H	-1.39259	3.73075	0.03468
H	-2.61137	2.97425	-0.99804
H	-2.78019	2.90505	0.75787
Si	-2.35542	-0.71840	0.00742
C	-2.37930	-1.56496	-1.68243
H	-2.97416	-2.48155	-1.64350
H	-2.81332	-0.90877	-2.43956
H	-1.37053	-1.82507	-2.00747
C	-4.12343	-0.23287	0.47531
H	-4.15844	0.23264	1.46243
H	-4.54285	0.47340	-0.24450
H	-4.76827	-1.11526	0.49481
C	-1.67446	-1.91114	1.30695
H	-0.61870	-2.12908	1.13772
H	-1.76579	-1.47901	2.30523
H	-2.22241	-2.85685	1.28899
C	2.05098	2.86868	0.06440
Si	2.35644	-0.71141	-0.00766
H	1.38566	3.72861	-0.02037

H	2.60864	2.96047	0.99848
H	2.76636	2.90508	-0.75927
C	1.57041	-2.02123	-1.12073
H	2.21694	-2.90102	-1.17782
H	0.60068	-2.34563	-0.74005
H	1.42312	-1.63650	-2.13142
C	2.57933	-1.42519	1.72876
H	3.16736	-2.34628	1.69234
H	3.09639	-0.71794	2.38049
H	1.61435	-1.65308	2.18548
C	4.05189	-0.24425	-0.70629
H	4.53799	0.51553	-0.09043
H	4.70616	-1.11930	-0.73827
H	3.96464	0.15071	-1.72062

$[I_A^c\text{-}4_A^c]^‡$

25

XYZ

Si	1.08159	-0.33039	-0.00361
Si	-1.08510	-0.28336	-1.16392
O	-0.98809	0.02443	2.61244
N	0.05624	-0.57197	2.63854
N	0.96941	-0.95644	2.04142
N	-2.03640	1.08107	-0.72562
N	1.95436	1.14123	-0.04679
C	-3.09885	1.14555	0.25622
H	-2.72459	1.58412	1.19090
H	-3.92597	1.75802	-0.11532
H	-3.47703	0.15169	0.48179
C	-1.61145	2.38445	-1.20599
H	-1.31650	3.03211	-0.37269
H	-0.75709	2.28633	-1.88020
H	-2.41904	2.88060	-1.75383
C	3.19029	1.44100	-0.74288
H	3.03724	2.24964	-1.46644
H	3.96338	1.75783	-0.03470
H	3.55455	0.56625	-1.27673
C	1.42747	2.26345	0.71352
H	2.11716	2.55196	1.51393
H	1.26976	3.13224	0.06578
H	0.46821	2.00678	1.17035
Cl	2.27035	-1.78314	-0.89647
Cl	-2.14601	-1.97124	-0.48913

5_A^c

23

XYZ

Si	1.11215	-0.24300	-0.05164
O	0.02668	-0.21485	1.28587
Si	-1.09326	-0.27930	0.02030
N	-2.24200	0.98020	0.09331
N	2.15570	1.08681	-0.28527
C	1.58078	2.38042	-0.60818
H	2.10822	2.83133	-1.45523
H	0.53124	2.27645	-0.89030
H	1.63686	3.07344	0.23957
C	3.58413	1.13236	-0.03693
H	3.81398	1.76242	0.83011
H	3.97720	0.13561	0.15108
H	4.10564	1.54510	-0.90686
C	-3.50965	1.00276	-0.61124
H	-3.50946	1.76572	-1.39828
H	-3.71899	0.03782	-1.06896
H	-4.32472	1.23034	0.08360
C	-1.91301	2.24149	0.73600
H	-0.97361	2.16216	1.28164
H	-1.82929	3.05351	0.00305
H	-2.69324	2.51155	1.45466
Cl	-2.11868	-2.06275	-0.22676
Cl	2.26862	-1.95876	0.00872

$[5_A^c\text{-}P_A^c]$

26

XYZ

Si	1.18766	-0.11629	-0.31881
Si	-1.14287	-0.12871	-0.33438
O	-1.20540	-0.66694	2.08276
N	-0.05026	-0.76044	2.40686
N	1.04365	-0.70713	2.09785
N	-2.29031	1.12103	-0.18725

N	2.31892	1.14746	-0.12263
C	-3.47457	0.99730	0.64143
H	-3.39596	1.61212	1.54544
H	-4.35998	1.31657	0.08255
H	-3.63035	-0.03655	0.94748
C	-2.05357	2.46179	-0.68799
H	-1.85274	3.16929	0.12631
H	-1.21062	2.46863	-1.37648
H	-2.93304	2.81518	-1.23560
C	3.55010	0.98743	0.62891
H	4.37960	1.45953	0.09310
H	3.47701	1.44578	1.62251
H	3.79268	-0.06647	0.75756
C	1.95402	2.53240	-0.35577
H	1.76560	3.06897	0.58322
H	2.76407	3.04621	-0.88264
H	1.06381	2.59497	-0.97891
Cl	2.19596	-1.85591	-0.81999
Cl	-2.08256	-1.91333	-0.80978
O	0.02731	0.30854	-1.47740

$[I_B^c\text{-}4_B^c]^‡$

31

XYZ

Si	-1.09067	-0.06969	-0.98957
Si	1.07924	-0.35522	-0.47866
O	1.19004	-2.07696	1.38858
N	0.02767	-2.07918	1.72174
N	-1.03296	-1.69792	1.57095
C	-2.13102	-1.57653	-1.44293
H	-1.47835	-2.35542	-1.84299
H	-2.67496	-1.99706	-0.59711
H	-2.84797	-1.30564	-2.22091
C	2.12250	-1.22725	-1.77779
H	3.01861	-1.64396	-1.31358
H	1.54988	-2.05138	-2.20761
H	2.42232	-0.56813	-2.59332
N	1.94765	0.94901	0.24791
N	-2.04255	1.14866	-0.21613
C	3.05511	1.64633	-0.36700
H	2.77202	2.66198	-0.67665
H	3.89580	1.73168	0.33187
H	3.40998	1.11452	-1.24911
C	1.50458	1.54953	1.48776
H	1.20210	2.59486	1.34494
H	0.64783	1.00649	1.89044
H	2.30317	1.53003	2.23947
C	-3.19142	0.87243	0.61975
H	-2.93896	0.93838	1.68689
H	-3.99539	1.58893	0.41596
H	-3.57765	-0.12833	0.43249
C	-1.54702	2.50183	-0.07660
H	-2.31074	3.22779	-0.38009
H	-1.26562	2.72668	0.96071
H	-0.66744	2.65097	-0.70517

5_B^c

29

XYZ

Si	-1.12306	0.63609	-0.12430
O	-0.03030	0.75541	1.22821
Si	1.09928	0.64902	-0.03216
N	2.13610	-0.71913	0.14902
N	-2.08056	-0.79090	-0.29303
C	2.14019	2.17034	-0.36662
H	1.50421	3.05442	-0.30345
H	2.93913	2.26439	0.37249
H	2.58676	2.15002	-1.36220
C	-2.25991	2.12891	-0.09108
H	-1.67707	3.03961	-0.23427
H	-3.02753	2.08159	-0.86453
H	-2.74631	2.20546	0.88498
C	-1.53010	-2.04693	-0.75416
H	-2.17694	-2.49130	-1.52040
H	-0.54505	-1.88988	-1.19517
H	-1.42597	-2.77802	0.05892
C	-3.42913	-0.91729	0.21981
H	-3.46994	-1.57801	1.09583
H	-3.82817	0.05254	0.51597
H	-4.09788	-1.33378	-0.54332

C	3.43490	-0.84110	-0.47473
H	3.42659	-1.56916	-1.29697
H	3.76949	0.11478	-0.87706
H	4.18288	-1.17384	0.25489
C	1.66681	-1.95380	0.74279
H	0.70884	-1.79757	1.23763
H	1.54881	-2.75003	-0.00498
H	2.37813	-2.30662	1.49832

[5_B^c-P_B^c]

32

XYZ

Si	-1.21971	-0.36148	-0.47949
Si	1.10743	-0.29575	-0.65513
O	1.26760	-1.24591	1.78061
N	0.15729	-1.67997	1.96298
N	-0.91403	-1.77584	1.58658
C	-2.41869	-1.56525	-1.25959
H	-2.87458	-1.12155	-2.14797
H	-1.88154	-2.45947	-1.57905
H	-3.20266	-1.86311	-0.56292
C	2.10902	-1.76587	-1.21975
H	2.84651	-2.07264	-0.47846
H	1.44435	-2.61066	-1.40723
H	2.62218	-1.51680	-2.15153
N	2.09636	1.06556	-0.29983
N	-2.07231	0.90265	0.32520
C	3.30528	0.94596	0.48757
H	4.10075	1.56680	0.06103
H	3.14848	1.26142	1.52734
H	3.66106	-0.08413	0.50381
C	1.59741	2.42275	-0.39100
H	2.33344	3.06398	-0.88829
H	0.67815	2.44937	-0.97506
H	1.39460	2.85030	0.60034
C	-3.40825	1.32974	-0.03236
H	-4.05643	1.36048	0.85211
H	-3.40719	2.33156	-0.48152
H	-3.85883	0.64402	-0.74952
C	-1.44843	1.74569	1.32094
H	-1.31920	2.77564	0.96322
H	-2.05308	1.78138	2.23557
H	-0.46171	1.36082	1.58511
O	-0.12156	0.14828	-1.71582

[I_C^c-4_C^c]‡

15

XYZ

Si	-1.12552	0.00726	0.41349
Si	1.01744	-0.40589	0.72960
O	1.23075	1.84463	-1.09173
N	0.09459	2.13815	-1.31948
N	-1.02921	2.01718	-1.20131
Cl	2.01718	-1.55345	-0.67229
Cl	-2.13968	-1.43244	-0.68683
C	2.19697	0.67308	1.70595
H	2.87699	1.21040	1.04671
H	1.62972	1.39586	2.29539
H	2.77915	0.05272	2.38943
C	-2.17142	0.60145	1.85105
H	-2.53757	-0.23495	2.44611
H	-1.58390	1.26241	2.49120
H	-3.02584	1.16309	1.47025

5_C^c

13

XYZ

Si	1.10001	0.37171	-0.08929
Si	-1.10008	0.37171	-0.08935
O	-0.00005	0.50862	1.20943
C	-2.31922	1.76923	-0.23424
H	-2.89777	1.68338	-1.15458
H	-3.00938	1.73789	0.61155
H	-1.79688	2.72644	-0.22789
C	2.31909	1.76929	-0.23418
H	1.79676	2.72650	-0.22791
H	3.00918	1.73800	0.61167
H	2.89773	1.68337	-1.15446
Cl	2.15223	-1.41179	-0.08304
Cl	-2.15208	-1.41193	-0.08298

[5_C^c-P_C^c]

16

XYZ

Si	1.19118	-0.02484	0.45885
Si	-1.12628	-0.10968	0.49852
O	-1.27411	1.70570	-1.12656
N	-0.13938	1.99300	-1.40544
N	0.96970	1.80342	-1.23910
Cl	-2.06564	-1.46610	-0.74860
Cl	2.21734	-1.31749	-0.79367
C	-2.37078	0.73976	1.58182
H	-2.78178	0.01015	2.28292
H	-1.89178	1.53696	2.15211
H	-3.18102	1.16318	0.98932
C	2.40416	0.92503	1.49686
H	2.92161	0.23011	2.16184
H	3.13940	1.43193	0.87250
H	1.88180	1.66464	2.10565
O	0.07560	-0.88021	1.41289

[I_D^c-4_D^c]‡

XYZ

Si	-1.12724	0.39552	0.11604
Si	0.97734	0.36537	-0.61854
O	1.60106	0.87268	2.26378
N	0.53787	0.62211	2.76344
N	-0.56240	0.33803	2.73420
N	1.70035	1.86962	-1.09133
N	-1.95169	1.92673	0.04739
C	2.90561	2.42283	-0.51191
H	3.59262	2.76883	-1.29380
H	2.67610	3.27857	0.13781
H	3.42224	1.68168	0.09274
C	0.98268	2.81941	-1.91806
H	1.58649	3.11108	-2.78623
H	0.05076	2.38441	-2.28015
H	0.73750	3.73237	-1.36025
C	-3.23108	2.15320	-0.58295
H	-3.95228	2.58292	0.12448
H	-3.14445	2.84527	-1.43216
H	-3.65116	1.22205	-0.96200
C	-1.37779	3.12426	0.62210
H	-1.28640	3.92077	-0.12734
H	-1.99709	3.50800	1.44360
H	-0.37929	2.92303	1.01272
Si	2.44767	-1.43196	-0.21160
Si	-2.51668	-1.45173	-0.28286
C	4.24496	-0.86511	-0.06816
H	4.40432	-0.27548	0.83636
H	4.89407	-1.74343	-0.01539
H	4.55504	-0.26984	-0.92889
C	2.31896	-2.60191	-1.69412
H	2.97941	-3.46266	-1.55841
H	1.30067	-2.97401	-1.82410
H	2.60683	-2.09589	-2.61804
C	1.97631	-2.36428	1.36058
H	0.90873	-2.57967	1.40418
H	2.51382	-3.31533	1.40381
H	2.24280	-1.77925	2.24165
C	-1.56606	-3.02965	0.13389
H	-1.32675	-3.07589	1.19766
H	-2.17667	-3.90217	-0.11223
H	-0.63543	-3.10473	-0.43146
C	-3.08291	-1.55198	-2.08501
H	-2.22198	-1.64125	-2.75018
H	-3.72290	-2.42666	-2.23115
H	-3.64845	-0.66897	-2.38863
C	-4.02582	-1.32340	0.84844
H	-3.72089	-1.27992	1.89579
H	-4.61438	-0.42898	0.63502
H	-4.67531	-2.19278	0.71694

5_D^c

47

XYZ

Si	1.09000	0.40559	-0.13297
O	0.05242	0.29512	1.28257
Si	-1.14699	0.41724	0.08484
N	-2.02922	1.90160	0.26491

N	1.87488	1.93240	-0.40808
C	1.27288	3.02350	-1.14430
H	1.93915	3.36466	-1.94687
H	0.33229	2.70505	-1.59390
H	1.06488	3.88573	-0.49678
C	3.12453	2.30627	0.21899
H	2.98296	3.10268	0.96188
H	3.57261	1.45703	0.73538
H	3.84745	2.66731	-0.52385
C	-3.29646	2.15305	-0.37979
H	-3.20924	2.90719	-1.17356
H	-3.69361	1.24468	-0.83494
H	-4.03882	2.51495	0.34285
C	-1.46626	3.07324	0.90108
H	-2.13884	3.44311	1.68426
H	-0.51159	2.82970	1.36625
H	-1.30759	3.88760	0.18173
Si	2.72002	-1.29326	0.00264
Si	-2.64399	-1.39477	-0.12249
C	3.43102	-1.35398	1.75534
H	4.09822	-2.21326	1.86333
H	4.00062	-0.45539	2.00023
H	2.62796	-1.44901	2.48879
C	4.09257	-0.94485	-1.25154
H	4.56542	0.02242	-1.07282
H	4.86547	-1.71583	-1.19828
H	3.69430	-0.93662	-2.26848
C	1.96258	-2.98038	-0.38211
H	1.23388	-3.26723	0.37705
H	1.46345	-2.98602	-1.35322
H	2.74643	-3.74197	-0.40100
C	-4.04959	-1.16953	1.12136
H	-4.75935	-1.99812	1.05526
H	-3.65808	-1.13795	2.14009
H	-4.59485	-0.24043	0.94625
C	-1.69079	-2.97148	0.27821
H	-0.93169	-3.17414	-0.47839
H	-1.19218	-2.89322	1.24618
H	-2.37215	-3.82533	0.31119
C	-3.34231	-1.53137	-1.87555
H	-3.93592	-2.44457	-1.96829
H	-3.98668	-0.68874	-2.13365
H	-2.53888	-1.57722	-2.61354

[5_D^C-P_D^C]

50

XYZ

Si	1.14863	0.53023	-0.18232
Si	-1.21419	0.43702	-0.31991
O	-1.40595	0.79132	2.32936
N	-0.25311	0.66630	2.66240
N	0.83345	0.51804	2.35116
N	-2.29873	1.74111	-0.66315
N	2.06002	2.01068	-0.25211
C	-3.38294	2.05562	0.24252
H	-3.14887	2.92296	0.87367
H	-4.29766	2.27856	-0.31824
H	-3.59472	1.21617	0.90423
C	-1.99816	2.80276	-1.59832
H	-1.64082	3.71195	-1.09392
H	-1.23889	2.47638	-2.30721
H	-2.89828	3.06631	-2.16467
C	3.11658	2.22062	0.71630
H	3.94310	2.78043	0.26476
H	2.76998	2.77601	1.59890
H	3.51469	1.26761	1.07062
C	1.46909	3.24337	-0.72460
H	0.91613	3.77895	0.06308
H	2.25194	3.91231	-1.09685
H	0.78658	3.04208	-1.54752
Si	-2.27124	-1.66069	-0.12342
Si	2.60191	-1.33230	-0.27094
C	-2.17267	-2.51801	-1.80344
H	-1.14338	-2.56716	-2.16203
H	-2.56291	-3.53698	-1.73899
H	-2.75908	-1.97628	-2.54835
C	-4.07816	-1.49869	0.40450
H	-4.55114	-2.48406	0.41909
H	-4.16203	-1.07259	1.40623
H	-4.63877	-0.86495	-0.28520

C	-1.33736	-2.65095	1.18819
H	-1.49679	-2.21282	2.17573
H	-1.68543	-3.68633	1.21624
H	-0.26223	-2.66386	1.00061
C	1.76850	-2.62930	-1.36419
H	1.47256	-2.19073	-2.31925
H	2.45657	-3.45475	-1.56307
H	0.87498	-3.04520	-0.89628
C	2.93393	-2.04491	1.44554
H	2.00475	-2.33959	1.93735
H	3.57643	-2.92620	1.37533
H	3.42703	-1.31390	2.08924
C	4.22893	-0.81648	-1.08386
H	4.04746	-0.37343	-2.06483
H	4.76802	-0.08267	-0.48251
H	4.87683	-1.68683	-1.21705
O	0.03153	0.46769	-1.48695

$[I_E^c\text{-}4_E^c]^‡$

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XYZ

Si	1.13057	-0.71403	-0.17382
Si	-1.01751	-0.62010	-0.55798
O	-1.38040	-1.09167	2.15918
N	-0.25434	-1.21720	2.54954
N	0.87446	-1.22087	2.43261
Si	-2.42192	1.21862	-0.15762
C	-1.52040	2.36531	1.03861
H	-1.32512	1.86429	1.98782
H	-0.57055	2.71278	0.62819
H	-2.13472	3.24677	1.23918
C	-2.73789	2.10419	-1.79145
H	-1.80618	2.46245	-2.23352
H	-3.21977	1.44119	-2.51242
H	-3.39335	2.96465	-1.63335
C	-4.03242	0.58788	0.57910
H	-3.85724	0.09775	1.53735
H	-4.72330	1.42040	0.73547
H	-4.51250	-0.13104	-0.08714
Si	2.49886	1.20189	-0.15950
C	1.85823	2.43917	-1.43218
H	1.89955	2.01641	-2.43726
H	0.82247	2.72007	-1.23168
H	2.46374	3.34927	-1.41525
C	4.23918	0.63483	-0.59623
H	4.92106	1.48901	-0.59183
H	4.60645	-0.09922	0.12293
H	4.26898	0.17737	-1.58643
C	2.45648	1.96064	1.56526
H	1.44348	2.24920	1.85181
H	2.82608	1.25330	2.30943
H	3.08421	2.85492	1.59889
Cl	-2.01096	-2.35901	-1.12910
Cl	2.10920	-2.46752	-0.74881

5_E^c

31

XYZ

Si	1.11189	0.65214	0.04104
O	-0.00114	0.56077	-1.26455
Si	2.75667	-1.02775	0.05778
C	3.64114	-0.97856	1.72061
H	2.95254	-1.17640	2.54419
H	4.43014	-1.73391	1.75071
H	4.10070	-0.00275	1.88840
C	3.95093	-0.66136	-1.35258
H	3.43513	-0.65834	-2.31441
H	4.42595	0.31205	-1.21945
H	4.73478	-1.42212	-1.38881
C	1.88964	-2.67956	-0.21103
H	1.16772	-2.88926	0.58011
H	1.35949	-2.68647	-1.16546
H	2.62075	-3.49149	-0.22482
Si	-1.10978	0.65197	0.04496
Si	-2.75635	-1.02710	0.06210
C	-1.90248	-2.69436	0.27555
H	-1.17335	-2.87126	-0.51692
H	-1.38446	-2.75477	1.23485
H	-2.64005	-3.49991	0.24161
C	-3.63593	-0.93228	-1.60169

H	-2.93298	-1.08024	-2.42340
H	-4.40697	-1.70405	-1.66724
H	-4.11455	0.03936	-1.73610
C	-3.94568	-0.69020	1.48299
H	-4.74127	-1.43921	1.49274
H	-3.43625	-0.72707	2.44774
H	-4.40622	0.29385	1.38001
Cl	-2.06873	2.50969	0.12351
Cl	2.06864	2.50997	0.13809

[5_E^c-P_E^c]

34

XYZ

Si	1.18197	-0.54853	-0.22866
Si	-1.16569	-0.54495	-0.31507
O	-1.27955	-0.95479	2.13198
N	-0.13559	-0.96001	2.51424
N	0.96410	-0.86234	2.22644
Si	-2.75511	1.17434	-0.13204
C	-3.15379	1.74741	-1.88141
H	-2.25037	2.06762	-2.40348
H	-3.61170	0.94458	-2.46216
H	-3.85122	2.58845	-1.85671
C	-4.27377	0.49093	0.74206
H	-4.70379	-0.34297	0.18466
H	-4.02321	0.13536	1.74281
H	-5.03637	1.26799	0.83638
C	-1.96473	2.56251	0.86967
H	-1.06534	2.94474	0.38382
H	-2.66541	3.39384	0.97939
H	-1.69358	2.21829	1.86973
Si	2.82521	1.12293	-0.09902
C	3.63874	1.21564	-1.79568
H	4.13182	0.27406	-2.04393
H	2.90169	1.42667	-2.57258
H	4.39066	2.00861	-1.81371
C	4.06985	0.66552	1.23536
H	4.86307	1.41548	1.28604
H	3.59405	0.60286	2.21516
H	4.52963	-0.30115	1.02172
C	1.94473	2.74150	0.30563
H	1.23799	3.00461	-0.48417
H	1.39774	2.67681	1.24842
H	2.66824	3.55569	0.39278
Cl	-2.05095	-2.37602	-0.76896
Cl	2.07892	-2.40288	-0.58864
O	0.04650	-0.20496	-1.46153

[I_F^c-4_F^c]‡

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a_1c_2c.log Energy: -1042929.6821297

Si	-1.08509	0.79243	-0.77446
Si	1.08835	0.79141	-0.76689
O	1.13426	2.11793	1.65066
N	-0.03617	2.19050	1.88918
N	-1.13923	2.01746	1.69118
Si	2.35537	-1.02366	0.01260
C	2.34306	-1.11358	1.89838
H	2.76343	-0.20447	2.33115
H	1.32852	-1.22604	2.28466
H	2.93446	-1.96665	2.24171
C	1.68796	-2.64046	-0.70421
H	0.64452	-2.80058	-0.42668
H	1.74271	-2.63357	-1.79443
H	2.26867	-3.49062	-0.33656
C	4.12966	-0.76091	-0.58679
H	4.54479	0.17045	-0.19613
H	4.76860	-1.58107	-0.24949
H	4.18027	-0.72150	-1.67687
Si	-2.37637	-0.99277	0.01411
C	-2.56735	-2.34312	-1.29434
H	-3.03593	-1.95070	-2.19919
H	-1.59669	-2.75665	-1.57510
H	-3.19033	-3.15822	-0.91627
C	-4.07721	-0.28859	0.44268
H	-4.73167	-1.07550	0.82633
H	-3.99461	0.48820	1.20536
H	-4.55761	0.14911	-0.43507
C	-1.59757	-1.73454	1.56705
H	-0.61467	-2.16169	1.36232

H	-1.48353	-0.97676	2.34426
H	-2.23191	-2.53353	1.95968
C	2.05560	2.20398	-1.58122
H	2.79145	2.61303	-0.88744
H	2.58323	1.84709	-2.46758
H	1.38556	3.00951	-1.88381
C	-2.03938	2.20246	-1.61318
H	-1.37000	3.02037	-1.88260
H	-2.53177	1.85242	-2.52214
H	-2.80380	2.59309	-0.93924