Supporting Information

Probing the longest λ_{max} of azo compounds in near infrared absorption via integrating protonation, antiaromaticity and substituents: a combined DFT and machine learning study

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Table S1. NICS(1)$_{zz}$ (ppm), ΔBL (Å) values and the maximum absorption wavelengths (λ_{max}) of $S_0 \rightarrow S_1$ transition of ***Z*.AB.H$^+$**-***Z*.18.2H$^+$** and ***Z*.AB.2H$^+$**-***Z*.18.2H$^+$**.

Structures	$S_0 \rightarrow S_1$ λ_{max} (nm)	NICS(1)$_{zz}$	ΔBL_{C-C}	Structures	$S_0 \rightarrow S_1$ λ_{max} (nm)	NICS(1)$_{zz}$	ΔBL_{C-C}
***Z*.AB.H$^+$**	432.4	-26.1/-20.9	0.011/0.031	***Z*.AB.2H$^+$**	600.4	-9.9	0.039
***Z*.1.H$^+$**	431.5	-26.1/-20.5	0.056/0.086	***Z*.1.2H$^+$**	563.2	-12.7	0.081
***Z*.2.H$^+$**	453.4	-26.0/-20.6	0.059/0.085	***Z*.2.2H$^+$**	606.1	-11.4	0.086
***Z*.3.H$^+$**	455.6	-24.9/-19.8	0.079/0.104	***Z*.3.2H$^+$**	590.7	-13.1	0.097
***Z*.4.H$^+$**	467.5	-22.9/-18.4	0.072/0.095	***Z*.4.2H$^+$**	623.2	-9.3	0.096
***Z*.5.H$^+$**	488.7	-13.2/-12.4	0.127/0.134	***Z*.5.2H$^+$**	803.3	-10.1	0.133
***Z*.6.H$^+$**	549.3	-12.1/-11.2	0.124/0.129	***Z*.6.2H$^+$**	760.0	-7.7	0.120
***Z*.7.H$^+$**	565.1	-8.1/-7.2	0.127/0.127	***Z*.7.2H$^+$**	-	-	-
***Z*.8.H$^+$**	497.4	-2.4/-2.5	0.139/0.145	***Z*.8.2H$^+$**	858.9	-2.7	0.144
***Z*.9.H$^+$**	590.1	-1.3/-1.3	0.137/0.142	***Z*.9.2H$^+$**	853.8	-0.5	0.138
***Z*.10.H$^+$**	492.9	-1.2/-1.4	0.144/0.149	***Z*.10.2H$^+$**	865.4	-2.1	0.146
***Z*.11.H$^+$**	578.5	-1.3/-1.3	0.139/0.144	***Z*.11.2H$^+$**	845.5	-0.5	0.140
***Z*.12.H$^+$**	615.5	0.1/-0.3	0.149/0.143	***Z*.12.2H$^+$**	-	-	-
***Z*.13.H$^+$**	627.4	1.0/0.6	0.148/0.143	***Z*.13.2H$^+$**	-	-	-
***Z*.14.H$^+$**	616.1	10.3/9.0	0.156/0.156	***Z*.14.2H$^+$**	884.5	6.7	0.148
***Z*.15.H$^+$**	622.8	11.1/9.8	0.159/0.161	***Z*.15.2H$^+$**	873.9	6.8	0.152
***Z*.16.H$^+$**	645.7	25.0/21.9	0.172/0.176	***Z*.16.2H$^+$**	870.5	16.2	0.162
***Z*.17.H$^+$**	657.5	27.4/23.4	0.173/0.175	***Z*.17.2H$^+$**	911.1	18.4	0.158
***Z*.18.H$^+$**	672.9	29.7/24.8	0.174/0.168	***Z*.18.2H$^+$**	-	-	-

Table S2. The maximum absorption wavelengths (λ_{max}) of $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions of ***E*.AB**-***E*.18** as well as the maximum absorption wavelengths (λ_{max}) of $S_0 \rightarrow S_1$ transition of ***E*.AB.H$^+$**-***E*.18.2H$^+$** and ***E*.AB.2H$^+$**-***E*.18.2H$^+$**.

Structures	$S_0 \rightarrow S_1$ λ_{max} (nm)	$S_0 \rightarrow S_2$ λ_{max} (nm)	Structures	$S_0 \rightarrow S_1$ λ_{max} (nm)	Structures	$S_0 \rightarrow S_1$ λ_{max} (nm)
***E*.AB**	478.3	335.9	***E*.AB.H$^+$**	405.4	***E*.AB.2H$^+$**	533.6
***E*.1**	397.6	327.1	***E*.1.H$^+$**	397.6	***E*.1.2H$^+$**	503.8
***E*.2**	428.3	327.4	***E*.2.H$^+$**	396.9	***E*.2.2H$^+$**	514.2
***E*.3**	404.7	312.4	***E*.3.H$^+$**	393.7	***E*.3.2H$^+$**	510.1
***E*.4**	429.7	337.9	***E*.4.H$^+$**	416.5	***E*.4.2H$^+$**	533.4
***E*.5**	471.4	311.5	***E*.5.H$^+$**	412.2	***E*.5.H$^+$**	590.8
***E*.6**	443.3	340.9	***E*.6.H$^+$**	442.6	***E*.6.2H$^+$**	598.0
***E*.7**	436.3	366.6	***E*.7.H$^+$**	464.9	***E*.7.2H$^+$**	604.1

***E*.8**	559.8	360.1	***E*.8.H$^+$**	447.8	***E*.8.2H$^+$**	619.2
***E*.9**	508.2	362.8	***E*.9.H$^+$**	457.8	***E*.9.2H$^+$**	618.3
***E*.10**	535.1	347.1	***E*.10.H$^+$**	433.0	***E*.10.2H$^+$**	602.8
***E*.11**	493.1	352.0	***E*.11.H$^+$**	445.6	***E*.11.2H$^+$**	606.5
***E*.12**	475.9	360.2	***E*.12.H$^+$**	455.4	***E*.12.2H$^+$**	609.9
***E*.13**	490.2	367.5	***E*.13.H$^+$**	463.1	***E*.13.2H$^+$**	616.5
***E*.14**	566.5	428.0	***E*.14.H$^+$**	492.4	***E*.14.2H$^+$**	631.9
***E*.15**	565.0	441.1	***E*.15.H$^+$**	493.3	***E*.15.2H$^+$**	622.4
***E*.16**	783.2	591.7	***E*.16.H$^+$**	594.2	***E*.16.2H$^+$**	671.0
***E*.17**	824.2	596.4	***E*.17.H$^+$**	615.8	***E*.17.2H$^+$**	701.9
***E*.18**	677.7	613.4	***E*.18.H$^+$**	650.5	***E*.18.2H$^+$**	737.9

Table S3. The maximum absorption wavelengths (λ_{max}) of $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions of ***Z*.AB-*Z*.18** as well as the maximum absorption wavelengths (λ_{max}) of $S_0 \rightarrow S_1$ transition of ***Z*.AB.H$^+$-*Z*.18.2H$^+$** and ***Z*.AB.2H$^+$-*Z*.18.2H$^+$**.

Structures	$S_0 \rightarrow S_1$ λ_{max} (nm)	$S_0 \rightarrow S_2$ λ_{max} (nm)	**Structures**	$S_0 \rightarrow S_1$ λ_{max} (nm)	**Structures**	$S_0 \rightarrow S_1$ λ_{max} (nm)
***Z*.AB**	462.7	298.2	***Z*.AB.H$^+$**	432.4	***Z*.AB.2H$^+$**	600.4
***Z*.1**	456.7	342.5	***Z*.1.H$^+$**	431.5	***Z*.1.2H$^+$**	563.2
***Z*.2**	472.8	329.6	***Z*.2.H$^+$**	453.4	***Z*.2.2H$^+$**	606.1
***Z*.3**	456.4	342.9	***Z*.3.H$^+$**	455.6	***Z*.3.2H$^+$**	590.7
***Z*.4**	482.8	333.2	***Z*.4.H$^+$**	467.5	***Z*.4.2H$^+$**	623.2
***Z*.5**	420.0	296.1	***Z*.5.H$^+$**	488.7	***Z*.5.H$^+$**	803.3
***Z*.6**	453.7	341.0	***Z*.6.H$^+$**	549.3	***Z*.6.2H$^+$**	760.0
***Z*.7**	503.7	371.0	***Z*.7.H$^+$**	565.1	***Z*.7.2H$^+$**	-
***Z*.8**	452.3	337.0	***Z*.8.H$^+$**	497.4	***Z*.8.2H$^+$**	858.9
***Z*.9**	442.8	332.2	***Z*.9.H$^+$**	590.1	***Z*.9.2H$^+$**	853.8
***Z*.10**	434.5	330.0	***Z*.10.H$^+$**	492.9	***Z*.10.2H$^+$**	865.4
***Z*.11**	434.0	324.4	***Z*.11.H$^+$**	578.5	***Z*.11.2H$^+$**	845.5
***Z*.12**	463.4	351.4	***Z*.12.H$^+$**	615.5	***Z*.12.2H$^+$**	-
***Z*.13**	465.1	351.1	***Z*.13.H$^+$**	627.4	***Z*.13.2H$^+$**	-
***E*.14**	474.1	393.6	***Z*.14.H$^+$**	616.1	***Z*.14.2H$^+$**	884.5
***Z*.15**	483.8	407.9	***Z*.15.H$^+$**	622.8	***Z*.15.2H$^+$**	873.9
***Z*.16**	629.6	522.5	***Z*.16.H$^+$**	645.7	***Z*.16.2H$^+$**	870.5
***Z*.17**	616.9	514.4	***Z*.17.H$^+$**	657.5	***Z*.17.2H$^+$**	911.1
***Z*.18**	630.7	516.9	***Z*.18.H$^+$**	672.9	***Z*.18.2H$^+$**	-

Table S4. Feature selection based on variance grouping

Group	Variables	variance
0	$NICS(1)_{zz}$	149.5804
0	$\Delta BL_{C\text{-}C}$	0.0013
3	Ring A	0.2214
3	Ring B	0.2152
4	Φ1 (deg)	360.6833
4	N^4	0.0045
4	N=N (Å)	0.0016
4	N^3–C^2 (Å)	0.0022
5	Ψ (deg)	37.1969
5	C^5	0.0019
5	α (angle)	15.4128
6	C^2	0.0011
7	N^3	0.0007
8	N^4–C^5 (Å)	0.0016

Table S5. Coefficients and Significance Levels for the iterative linear Regression Model

Variable	Estimate	SE	tStat	pValue
(Intercept)	-187.88	171.39	-1.0962	0.28234
x1	6.7887	0.93901	7.2296	7.19E-08
x2	237.02	297.44	0.79685	0.43224
x3	472.27	229.8	2.0551	0.049301
x4	-30.865	16.886	-1.8278	0.07825
x5	627.03	133.22	4.7068	6.18E-05
x6	-1.2512	0.29307	-4.2693	0.000203
x7	-7.2142	0.99298	-7.2652	6.56E-08

Table S6. Performance Statistics for the iterative linear Regression Model

RMSE	R^2	Adjusted R^2	F-statistic	p-Value
21	0.943	0.943	83.4	4.69e-17

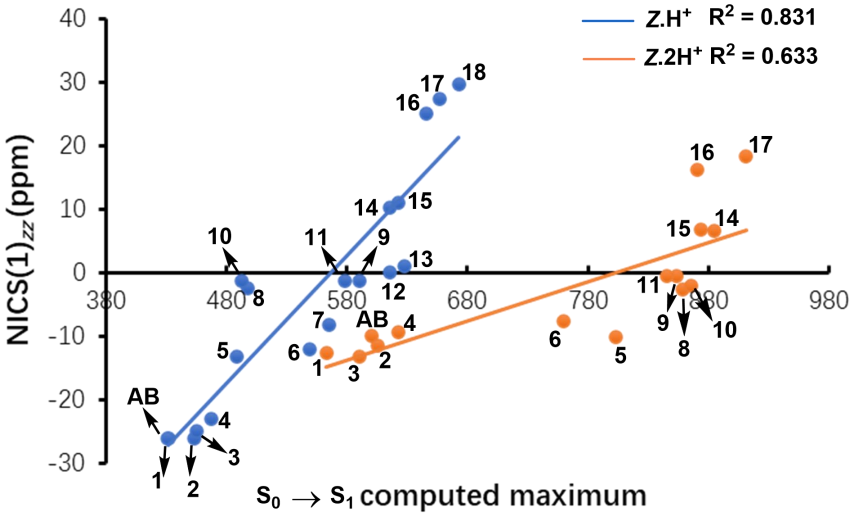


Figure S1. Correlations for NICS(1)$_{zz}$ against wavelengths associated with the maximum of absorption of $S_0 \rightarrow S_1$ bands of ***Z*.1.H$^+$-*Z*.18.H$^+$** and ***Z*.1.H$^+$-*Z*.18.2H$^+$**, respectively.

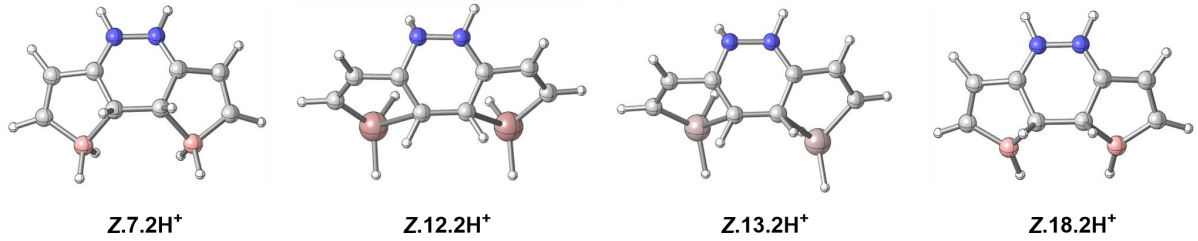


Figure S2. Structures of ***Z*.7.2H$^+$**, ***Z*.12.2H$^+$**, ***Z*.13.2H$^+$** and ***Z*.18.2H$^+$**.

Table S7. The $\Delta G_{Z\text{-}E}$ values (kcal mol^{-1}, 298.15 K) of structures **AB.H$^+$-19.H$^+$** between *E* and their corresponding *Z* isomers.

Structures	**AB.H$^+$**	**1.H$^+$**	**2.H$^+$**	**3.H$^+$**	**4.H$^+$**	**5.H$^+$**	**6.H$^+$**	**7.H$^+$**	**8.H$^+$**	**9.H$^+$**
$\Delta G_{Z\text{-}E}$	9.0	10.2	10.1	11.8	10.3	14.3	14.0	14.0	11.8	12.9
Structures	**10.H$^+$**	**11.H$^+$**	**12.H$^+$**	**13.H$^+$**	**14.H$^+$**	**15.H$^+$**	**16.H$^+$**	**17.H$^+$**	**18.H$^+$**	
$\Delta G_{Z\text{-}E}$	11.9	12.7	14.2	13.9	12.5	12.8	11.4	11.6	14.6	

Table S8. Selected geometrical parameters of *E* forms of **AB.H$^+$ ~ 18.H$^+$**.

Structures	N=N (Å)/ Mayer	N^3–C^2 (Å)/Mayer	N^4–C^5 (Å)/Mayer	Φ_1 (deg)	α (angle)	Ψ (deg)
***E*.AB.H$^+$**	1.246/1.396	1.400/1.084	1.373/1.199	0.0	123.5	180.0
***E*.1.H$^+$**	1.259/1.315	1.379/1.108	1.345/1.333	0.0	122.8	-180.0
***E*.2.H$^+$**	1.255/1.348	1.385/1.091	1.354/1.271	-0.0	122.6	180.0
***E*.3.H$^+$**	1.255/1.351	1.379/1.091	1.347/1.282	0.0	121.8	-180.0
***E*.4.H$^+$**	1.256/1.340	1.388/1.090	1.356/1.271	-0.0	122.9	180.0
***E*.5.H$^+$**	1.246/1.435	1.386/1.085	1.364/1.177	2.0	120.3	-179.8
***E*.6.H$^+$**	1.258/1.334	1.381/1.102	1.357/1.259	-0.0	122.3	-180.0
***E*.7.H$^+$**	1.268/1.262	1.385/1.109	1.357/1.332	0.0	124.1	180.0
***E*.8.H$^+$**	1.246/1.435	1.393/1.073	1.372/1.154	1.3	120.8	-178.9
***E*.9.H$^+$**	1.254/1.363	1.394/1.080	1.370/1.216	0.0	122.5	-180.0
***E*.10.H$^+$**	1.245/1.434	1.396/1.068	1.374/1.151	0.0	121.4	180.0

***E*.11.H$^+$**	1.253/1.368	1.396/1.079	1.371/1.213	0.0	122.7	180.0
***E*.12.H$^+$**	1.260/1.310	1.400/1.082	1.372/1.265	-0.0	124.3	-180.0
***E*.13.H$^+$**	1.260/1.309	1.401/1.080	1.373/1.260	0.0	124.3	180.0
***E*.14.H$^+$**	1.256/1.345	1.398/1.079	1.373/1.219	-0.0	123.2	180.0
***E*.15.H$^+$**	1.256/1.344	1.397/1.082	1.371/1.227	0.0	123.0	-180.0
***E*.16.H$^+$**	1.252/1.389	1.390/1.093	1.368/1.182	-0.0	121.4	-180.0
***E*.17.H$^+$**	1.253/1.383	1.387/1.101	1.365/1.192	0.7	120.9	-179.2
***E*.18.H$^+$**	1.270/1.265	1.370/1.151	1.348/1.300	-0.0	121.8	-180.0

Table S9. Selected geometrical parameters of *Z* forms of **AB.H$^+$** ~ **18.H$^+$**.

Structures	N=N (Å)/Mayer	N^3–C^2 (Å)/Mayer	N^4–C^5 (Å)/Mayer	Φ_1 (deg)	α (angle)	Ψ (deg)
***Z*.AB.H$^+$**	1.247/1.551	1.427/0.926	1.375/1.219	140.2	132.4	-12.2
***Z*.1.H$^+$**	1.261/1.425	1.397/1.024	1.341/1.408	151.1	134.2	-7.5
***Z*.2.H$^+$**	1.254/1.488	1.412/0.947	1.353/1.338	139.4	132.9	-9.1
***Z*.3.H$^+$**	1.253/1.499	1.405/0.966	1.347/1.352	132.0	131.9	-4.9
***Z*.4.H$^+$**	1.256/1.483	1.413/0.955	1.356/1.332	143.6	133.4	-10.5
***Z*.5.H$^+$**	1.232/1.682	1.420/0.955	1.381/1.092	134.5	130.6	-7.9
***Z*.6.H$^+$**	1.254/1.477	1.400/1.066	1.362/1.244	174.8	136.1	-11.5
***Z*.7.H$^+$**	1.271/1.351	1.399/1.092	1.357/1.331	-170.2	137.2	-16.6
***Z*.8.H$^+$**	1.228/1.717	1.434/0.911	1.390/1.032	132.0	129.9	-8.5
***Z*.9.H$^+$**	1.238/1.627	1.432/0.921	1.389/1.081	143.7	131.8	-11.4
***Z*.10.H$^+$**	1.228/1.716	1.437/0.902	1.393/1.023	132.0	130.4	-7.9
***Z*.11.H$^+$**	1.238/1.628	1.435/0.909	1.391/1.083	140.9	131.8	-10.9
***Z*.12.H$^+$**	1.260/1.433	1.419/1.038	1.376/1.185	-167.0	136.8	-18.6
***Z*.13.H$^+$**	1.258/1.444	1.421/1.026	1.378/1.169	-171.2	136.8	-18.3
***Z*.14.H$^+$**	1.237/1.633	1.440/0.897	1.394/1.053	141.2	131.2	-12.4
***Z*.15.H$^+$**	1.238/1.624	1.437/0.904	1.392/1.066	142.1	131.5	-12.2
***Z*.16.H$^+$**	1.230/1.688	1.432/0.923	1.385/1.035	142.1	130.6	-10.1
***Z*.17.H$^+$**	1.230/1.690	1.430/0.935	1.381/1.043	143.0	130.2	-10.8
***Z*.18.H$^+$**	1.269/1.403	1.384/1.120	1.345/1.262	-152.9	133.7	-17.0

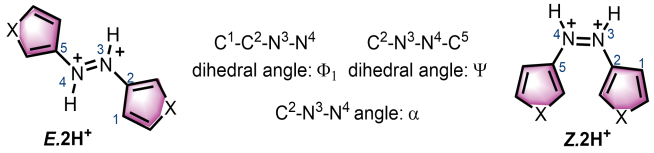


Figure S3. The dihedral angles of *E* and *Z* forms of doubly protonated heteroazo switches.

Table S10. The $\Delta G_{Z\text{-}E}$ values (kcal mol^{-1}, 298.15 K) of structures **AB.2H$^+$**-**18.2H$^+$** between *E* and their corresponding *Z* isomers.

Structures	**AB.2H$^+$**	**1.2H$^+$**	**2.2H$^+$**	**3.2H$^+$**	**4.2H$^+$**	**5.2H$^+$**	**6.2H$^+$**	**7.2H$^+$**	**8.2H$^+$**	**9.2H$^+$**
$\Delta G_{Z\text{-}E}$	6.1	7.4	8.1	9.7	6.7	14.4	10.5	-	16.0	12.4
Structures	**10.2H$^+$**	**11.2H$^+$**	**12.2H$^+$**	**13.2H$^+$**	**14.2H$^+$**	**15.2H$^+$**	**16.2H$^+$**	**17.2H$^+$**	**18.2H$^+$**	
$\Delta G_{Z\text{-}E}$	14.2	11.8	-	-	16.1	15.1	12.6	9.9	-	

Table S11. Selected geometrical parameters of *E* forms of **AB.2H$^+$-18.2H$^+$**.

Structures	N=N (Å)/Mayer	N–C (Å)/Mayer	Φ_1 (deg)	α (angle)	Ψ (deg)
***E*.AB.2H$^+$**	1.274/1.234	1.367/1.194	-0.0	127.4	180.0
***E*.1.2H$^+$**	1.283/1.188	1.349/1.222	1.9	125.8	-177.1
***E*.2.2H$^+$**	1.282/1.205	1.355/1.207	0.0	126.3	180.0
***E*.3.2H$^+$**	1.281/1.216	1.351/1.204	0.0	125.7	-180.0
***E*.4.2H$^+$**	1.284/1.189	1.357/1.206	0.0	126.4	-180.0
***E*.5.2H$^+$**	1.274/1.263	1.360/1.179	3.3	125.0	-178.6
***E*.6.2H$^+$**	1.287/1.161	1.354/1.198	-1.9	125.1	177.0
***E*.7.2H$^+$**	1.297/1.110	1.356/1.208	0.0	125.4	180.0
***E*.8.2H$^+$**	1.276/1.250	1.367/1.173	-0.0	125.4	-180.0
***E*.9.2H$^+$**	1.285/1.181	1.364/1.186	0.0	125.5	180.0
***E*.10.2H$^+$**	1.274/1.253	1.369/1.166	0.0	125.5	180.0
***E*.11.2H$^+$**	1.283/1.191	1.367/1.182	-0.0	125.7	-180.0
***E*.12.2H$^+$**	1.291/1.143	1.369/1.185	-0.0	126.2	-180.0
***E*.13.2H$^+$**	1.291/1.138	1.369/1.183	0.0	126.2	-180.0
***E*.14.2H$^+$**	1.287/1.163	1.367/1.185	0.0	126.1	180.0
***E*.15.2H$^+$**	1.287/1.169	1.367/1.187	-0.0	126.1	180.0
***E*.16.2H$^+$**	1.282/1.212	1.364/1.197	0.3	125.9	179.6
***E*.17.2H$^+$**	1.285/1.202	1.361/1.207	3.9	126.1	-175.7
***E*.18.2H$^+$**	1.301/1.102	1.345/1.256	2.2	125.2	-176.0

Table S12. Selected geometrical parameters of *Z* forms of **AB.2H$^+$-18.2H$^+$**.

Structures	N=N (Å) /Mayer	N–C (Å) /Mayer	Φ_1 (deg)	α (angle)	Ψ (deg)
***Z*AB.2H$^+$**	1.283/1.300	1.372/1.146	164.8	132.2	-19.6
***Z*.1.2H$^+$**	1.289/1.249	1.350/1.221	171.4	132.6	-11.2
***Z*.2.2H$^+$**	1.288/1.265	1.357/1.188	169.7	132.5	-15.9
***Z*.3.2H$^+$**	1.285/1.284	1.352/1.205	171.6	132.9	-10.3
***Z*.4.2H$^+$**	1.292/1.244	1.359/1.189	170.3	132.2	-19.4
***Z*.5.2H$^+$**	1.275/1.379	1.368/1.171	171.3	134.2	-11.1
***Z*.6.2H$^+$**	1.294/1.226	1.356/1.197	169.9	133.3	-14.0
***Z*.8.2H$^+$**	1.277/1.379	1.375/1.099	173.4	133.9	-15.5
***Z*.9.2H$^+$**	1.293/1.250	1.367/1.172	171.9	133.5	-20.2
***Z*.10.2H$^+$**	1.274/1.391	1.382/1.103	163.5	133.2	-18.0
***Z*.11.2H$^+$**	1.291/1.255	1.369/1.167	170.6	133.4	-21.2
***Z*.14.2H$^+$**	1.300/1.211	1.367/1.174	172.8	133.0	-25.1
***Z*.15.2H$^+$**	1.299/1.215	1.366/1.175	172.0	132.9	-24.2
***Z*.16.2H$^+$**	1.291/1.285	1.364/1.173	166.6	133.2	-22.2
***Z*.17.2H$^+$**	1.292/1.285	1.361/1.201	171.6	133.6	-19.7

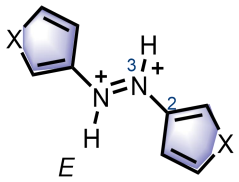


Figure S4. *E* isomer of doubly protonated heteroazo switches.

Table S13. The NPA charge analysis of 5MRs in doubly protonated ***E*.AB.2H$^+$-*E*.18.2H$^+$**.

NPA charge	***E*.AB.2H$^+$**	***E*.1.2H$^+$**	***E*.2.2H$^+$**	***E*.3.2H$^+$**	***E*.4.2H$^+$**	***E*.5.2H$^+$**	***E*.6.2H$^+$**	***E*.7.2H$^+$**
N^3	-0.132	-0.151	-0.147	-0.143	-0.155	-0.107	-0.162	-0.208
C^2	0.099	0.050	0.078	0.024	0.073	0.091	0.074	0.056
Ring	-0.613	-0.571	-0.147	-0.127	-0.117	-0.395	-0.725	-0.989
NPA charge	***E*.8.2H$^+$**	***E*.9.2H$^+$**	***E*.10.2H$^+$**	***E*.11.2H$^+$**	***E*.12.2H$^+$**	***E*.13.2H$^+$**	***E*.14.2H$^+$**	***E*.15.2H$^+$**
N^3	-0.119	-0.165	-0.119	-0.163	-0.203	-0.205	-0.181	-0.178
C^2	0.106	0.074	0.088	0.062	0.038	0.044	0.072	0.060
Ring	0.313	0.073	0.363	0.036	-0.345	-0.170	0.319	0.221
NPA charge	***E*.16.H$^+$**	***E*.17.H$^+$**	***E*.18.H$^+$**					
N^3	-0.140	-0.145	-0.200					
C^2	0.093	0.111	0.117					
Ring	0.740	0.739	-0.037					

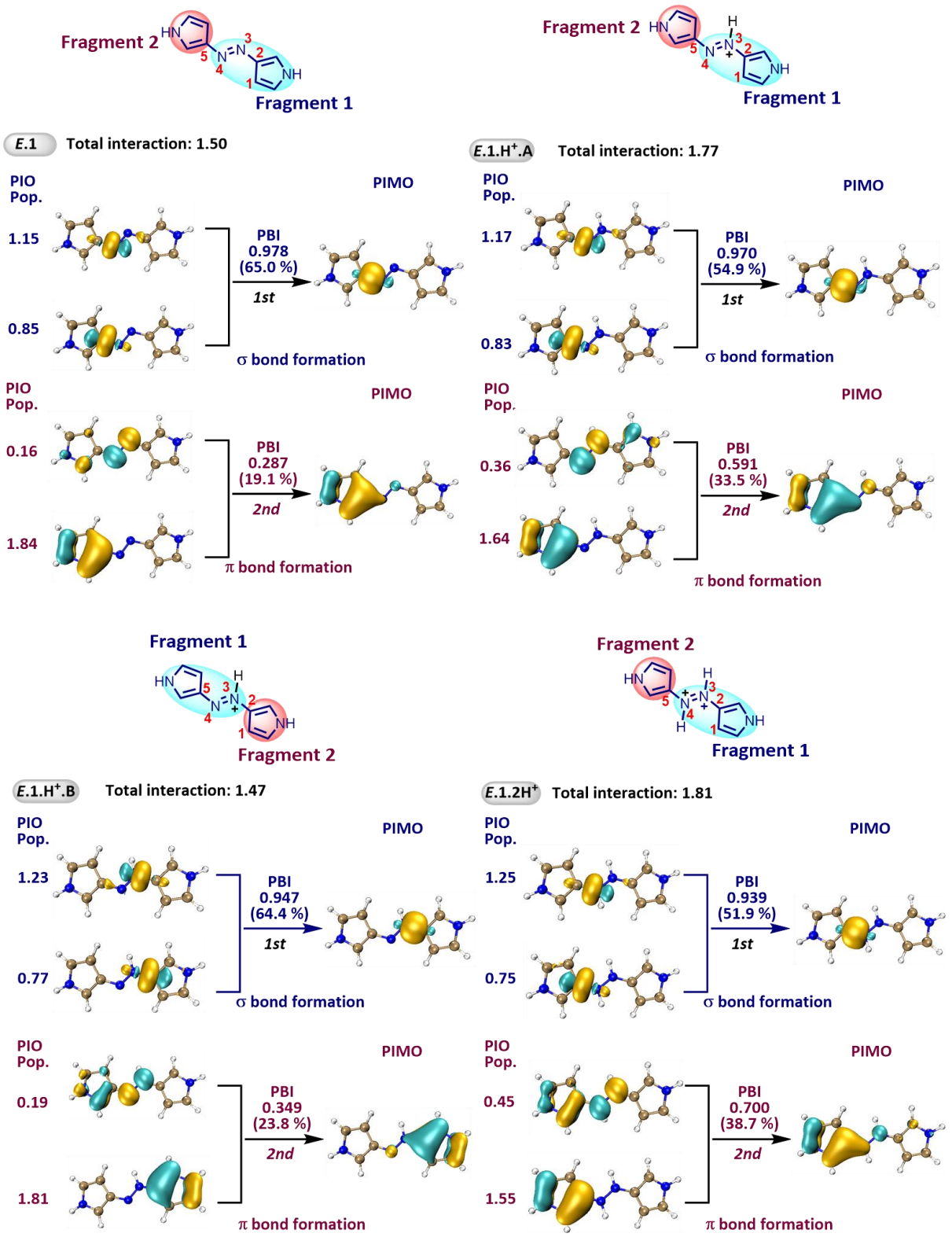


Figure S5. PIO analysis for the interaction of two fragments in ***E*.1**, ***E*.1.H$^+$.A**, ***E*.1.H$^+$.B** and ***E*.1.2H$^+$**, respectively. PIO pairs, populations (Pop), principal bond indexes (PBI) and contribution (%) of each interaction are shown in blue and red (isovalue: 0.05 a.u.), respectively.

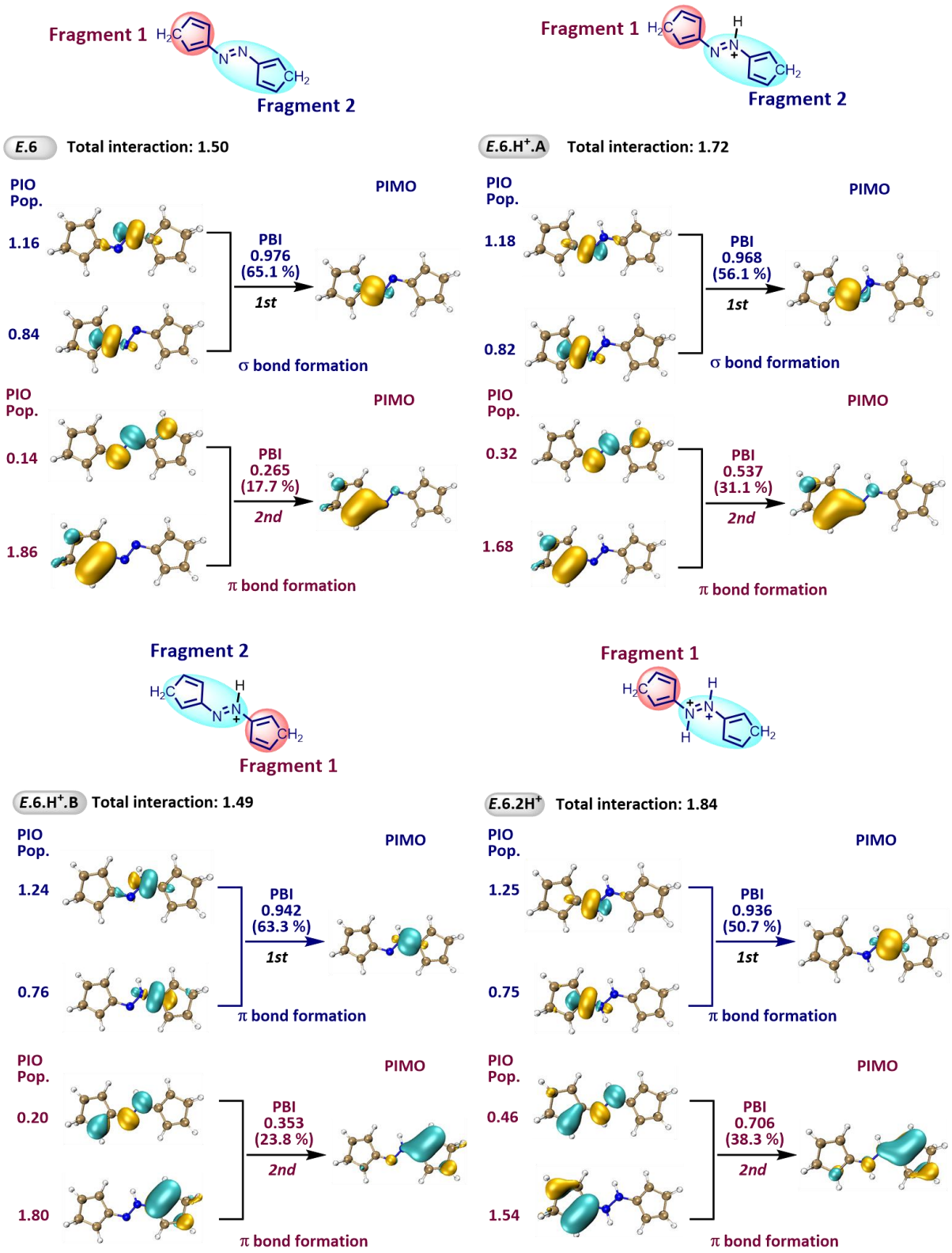


Figure S6. PIO analysis for the interaction of two fragments in ***E*.6**, ***E*.6.H$^+$.A**, ***E*.6.H$^+$.B** and ***E*.6.2H$^+$**, respectively. PIO pairs, populations (Pop), principal bond indexes (PBI) and contribution (%) of each interaction are shown in blue and red (isovalue: 0.05 a.u.), respectively.

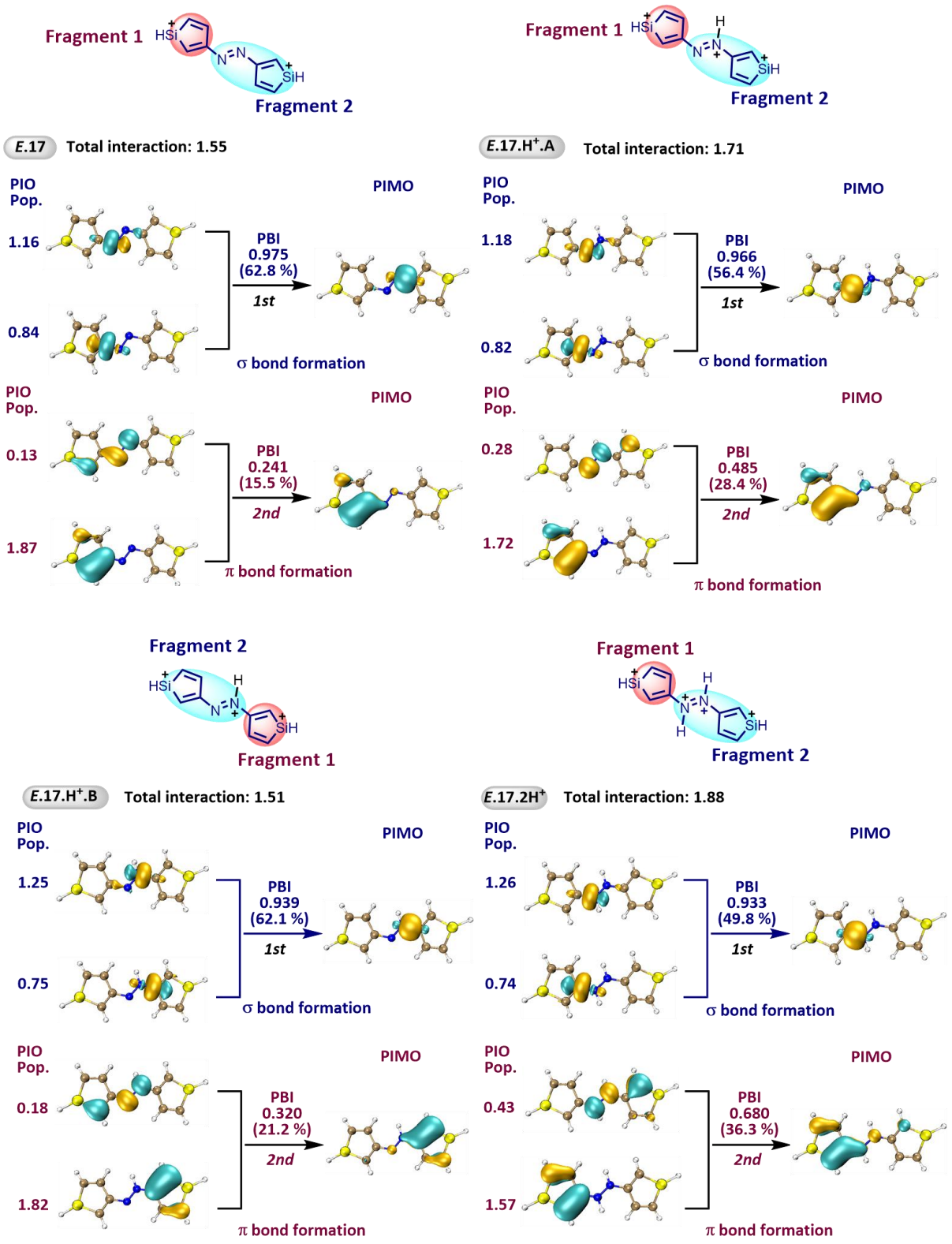
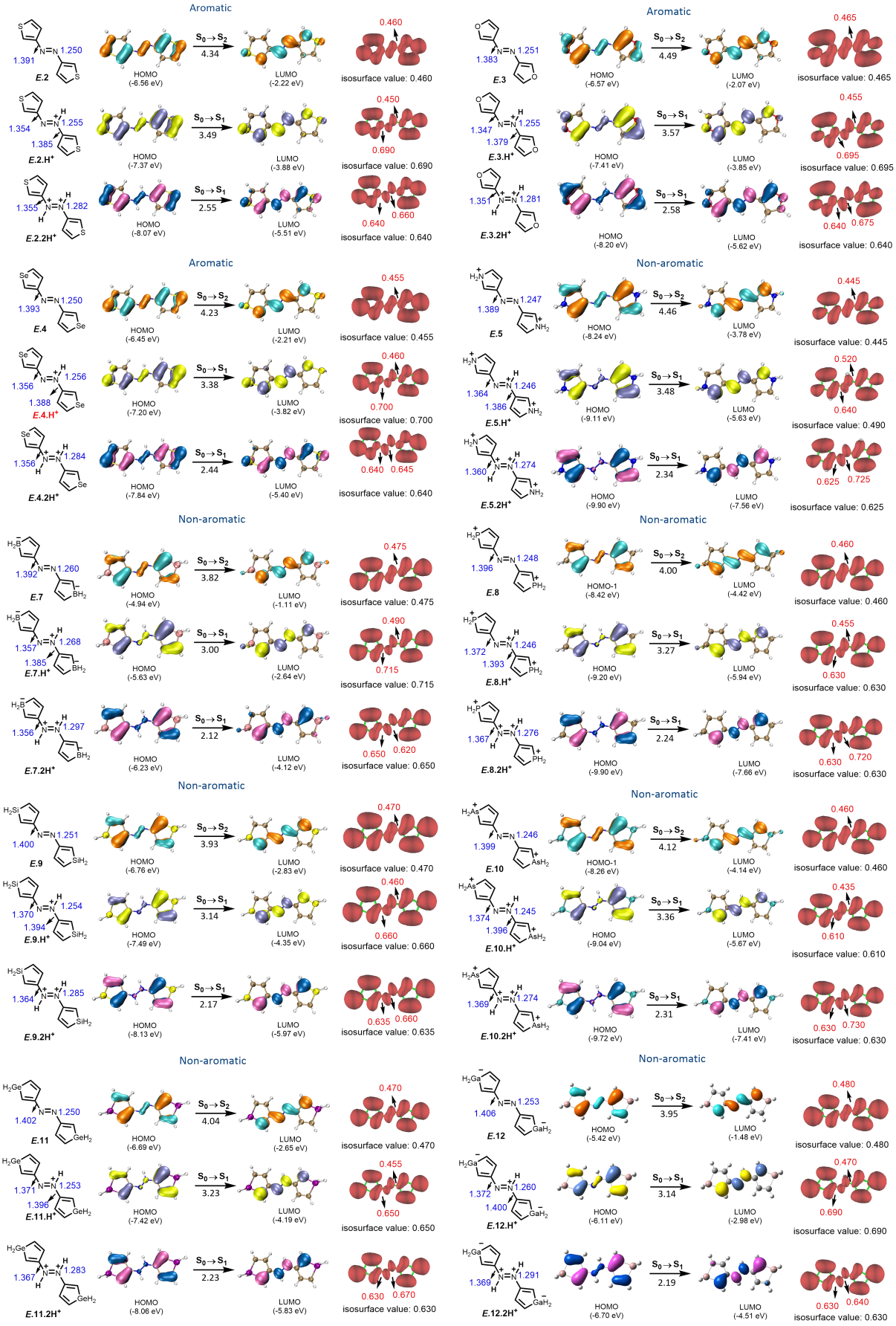


Figure S7. PIO analysis for the interaction of two fragments in ***E*.17**, ***E*.17.H$^+$.A**, ***E*.17.H$^+$.B** and ***E*.17.2H$^+$**, respectively. PIO pairs, populations (Pop), principal bond indexes (PBI) and contribution (%) of each interaction are shown in blue and red (isovalue: 0.05 a.u.), respectively.


Aromatic
1.391
1.250
E.2
HOMO
(-6.56 eV)
S0→S2
4.34
LUMO
(-2.22 eV)
0.460
isosurface value: 0.460
1.354
1.255
1.385
E.2.H+
HOMO
(-7.37 eV)
S0→S1
3.49
LUMO
(-3.88 eV)
0.450
0.690
isosurface value: 0.690
1.355
1.282
E.2.2H+
HOMO
(-8.07 eV)
S0→S1
2.55
LUMO
(-5.51 eV)
0.640
0.660
isosurface value: 0.640
Aromatic
1.393
1.250
E.4
HOMO
(-6.45 eV)
S0→S2
4.23
LUMO
(-2.21 eV)
0.455
isosurface value: 0.455
1.356
1.256
1.388
E.4.H+
HOMO
(-7.20 eV)
S0→S1
3.38
LUMO
(-3.82 eV)
0.460
0.700
isosurface value: 0.700
1.356
1.284
E.4.2H+
HOMO
(-7.84 eV)
S0→S1
2.44
LUMO
(-5.40 eV)
0.640
0.645
isosurface value: 0.640
Non-aromatic
1.392
1.260
E.7
HOMO
(-4.94 eV)
S0→S2
3.82
LUMO
(-1.11 eV)
0.475
isosurface value: 0.475
1.357
1.268
1.385
E.7.H+
HOMO
(-5.63 eV)
S0→S1
3.00
LUMO
(-2.64 eV)
0.490
0.715
isosurface value: 0.715
1.356
1.297
E.7.2H+
HOMO
(-6.23 eV)
S0→S1
2.12
LUMO
(-4.12 eV)
0.650
0.620
isosurface value: 0.650
Non-aromatic
1.400
1.251
E.9
HOMO
(-6.76 eV)
S0→S2
3.93
LUMO
(-2.83 eV)
0.470
isosurface value: 0.470
1.370
1.254
1.394
E.9.H+
HOMO
(-7.49 eV)
S0→S1
3.14
LUMO
(-4.35 eV)
0.460
0.660
isosurface value: 0.660
1.364
1.285
E.9.2H+
HOMO
(-8.13 eV)
S0→S1
2.17
LUMO
(-5.97 eV)
0.635
0.660
isosurface value: 0.635
Non-aromatic
1.402
1.250
E.11
HOMO
(-6.69 eV)
S0→S2
4.04
LUMO
(-2.65 eV)
0.470
isosurface value: 0.470
1.371
1.253
1.396
E.11.H+
HOMO
(-7.42 eV)
S0→S1
3.23
LUMO
(-4.19 eV)
0.455
0.650
isosurface value: 0.650
1.367
1.283
E.11.2H+
HOMO
(-8.06 eV)
S0→S1
2.23
LUMO
(-5.83 eV)
0.630
0.670
isosurface value: 0.630
Aromatic
1.383
1.251
E.3
HOMO
(-6.57 eV)
S0→S2
4.49
LUMO
(-2.07 eV)
0.465
isosurface value: 0.465
1.347
1.255
1.379
E.3.H+
HOMO
(-7.41 eV)
S0→S1
3.57
LUMO
(-3.85 eV)
0.455
0.695
isosurface value: 0.695
1.351
1.281
E.3.2H+
HOMO
(-8.20 eV)
S0→S1
2.58
LUMO
(-5.62 eV)
0.640
0.675
isosurface value: 0.640
Non-aromatic
1.389
1.247
E.5
HOMO
(-8.24 eV)
S0→S2
4.46
LUMO
(-3.78 eV)
0.445
isosurface value: 0.445
1.364
1.246
1.386
E.5.H+
HOMO
(-9.11 eV)
S0→S1
3.48
LUMO
(-5.63 eV)
0.520
0.640
isosurface value: 0.490
1.360
1.274
E.5.2H+
HOMO
(-9.90 eV)
S0→S1
2.34
LUMO
(-7.56 eV)
0.625
0.725
isosurface value: 0.625
Non-aromatic
1.396
1.248
E.8
HOMO-1
(-8.42 eV)
S0→S2
4.00
LUMO
(-4.42 eV)
0.460
isosurface value: 0.460
1.372
1.246
1.393
E.8.H+
HOMO
(-9.20 eV)
S0→S1
3.27
LUMO
(-5.94 eV)
0.455
0.630
isosurface value: 0.630
1.367
1.276
E.8.2H+
HOMO
(-9.90 eV)
S0→S1
2.24
LUMO
(-7.66 eV)
0.630
0.720
isosurface value: 0.630
Non-aromatic
1.399
1.246
E.10
HOMO-1
(-8.26 eV)
S0→S2
4.12
LUMO
(-4.14 eV)
0.460
isosurface value: 0.460
1.374
1.245
1.396
E.10.H+
HOMO
(-9.04 eV)
S0→S1
3.36
LUMO
(-5.67 eV)
0.435
0.610
isosurface value: 0.610
1.369
1.274
E.10.2H+
HOMO
(-9.72 eV)
S0→S1
2.31
LUMO
(-7.41 eV)
0.630
0.730
isosurface value: 0.630
Non-aromatic
1.406
1.253
E.12
HOMO
(-5.42 eV)
S0→S2
3.95
LUMO
(-1.48 eV)
0.480
isosurface value: 0.480
1.372
1.260
1.400
E.12.H+
HOMO
(-6.11 eV)
S0→S1
3.14
LUMO
(-2.98 eV)
0.470
0.690
isosurface value: 0.690
1.369
1.291
E.12.2H+
HOMO
(-6.70 eV)
S0→S1
2.19
LUMO
(-4.51 eV)
0.630
0.640
isosurface value: 0.630

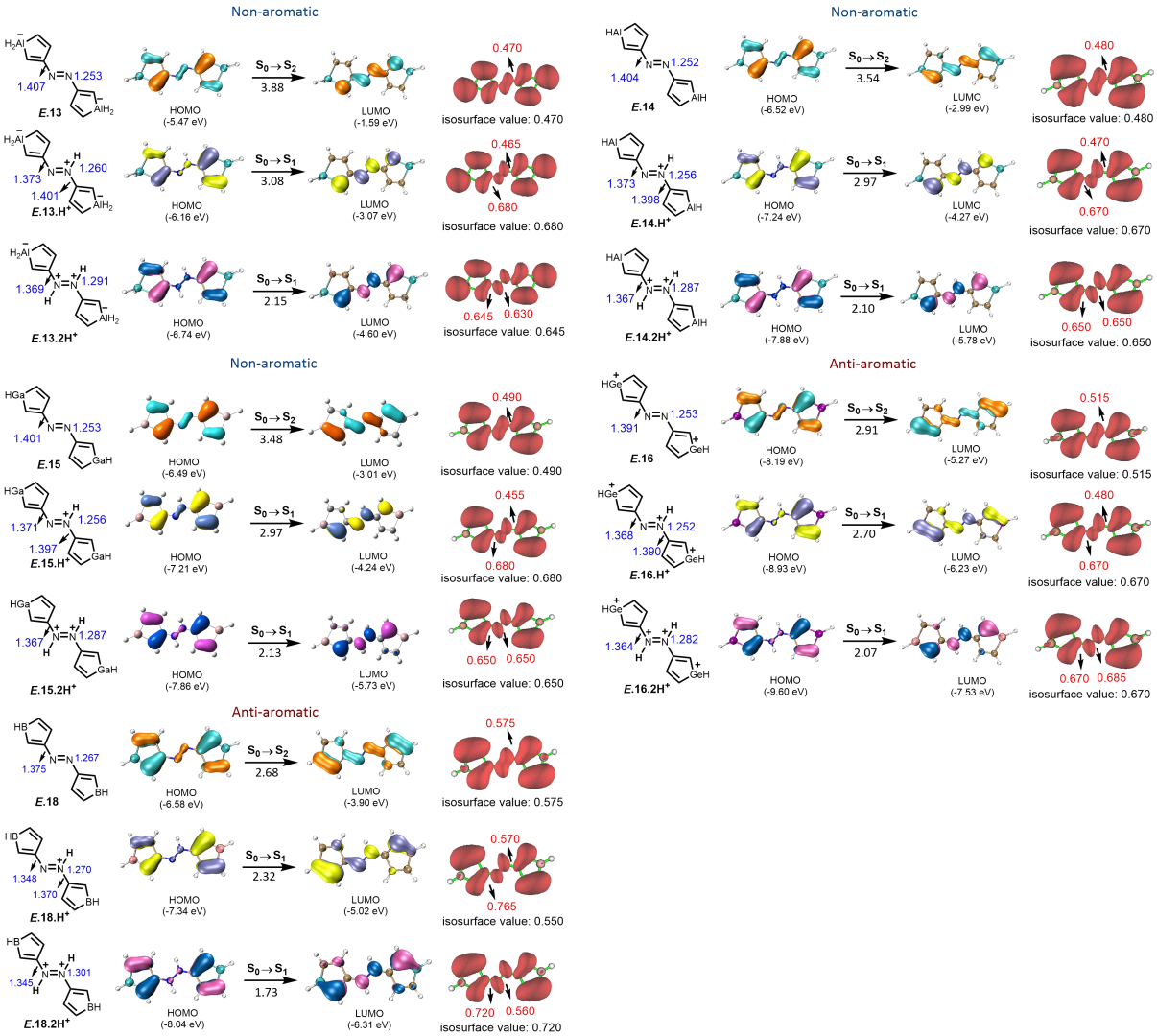


Figure S8. The key molecular orbitals of ***E*.2-*E*.5**, ***E*.7-*E*.16** and ***E*.18** as well as their corresponding singly and doubly protonated structures. The bond length (Å) is signed in blue. The ELF_{π} plots of these structures and their corresponding ELF_{π} bifurcation values ($BV(ELF_{\pi})$) (in red) of different CN bonds.

Table S14. TD-PBE0/def2-TZVP//PBE0-D3/def2-TZVP first $S_0 \rightarrow S_1$ transitions in the UV-Vis absorption spectra of *E* forms of **AB.H$^+$-18.H$^+$**.

Structures	Transition	*E*, eV	*λ*, nm	*f*	Contribution[a]	Assignment
***E*.AB.H$^+$**	$S_0 \rightarrow S_1$	3.07	404.3	0.859	H → L (94%)	π → π*
***E*.1.H$^+$**	$S_0 \rightarrow S_1$	3.12	397.6	0.610	H → L (92%)	π → π*
***E*.2.H$^+$**	$S_0 \rightarrow S_1$	3.12	396.9	0.918	H → L (97%)	π → π*
***E*.3.H$^+$**	$S_0 \rightarrow S_1$	3.15	393.7	0.440	H → L (92%)	π → π*
***E*.4.H$^+$**	$S_0 \rightarrow S_1$	2.98	416.5	0.928	H → L (89%)	π → π*
***E*.5.H$^+$**	$S_0 \rightarrow S_1$	3.01	412.2	0.305	H → L (95%)	π → π*
***E*.6.H$^+$**	$S_0 \rightarrow S_1$	2.81	442.6	0.415	H → L (96%)	π → π*
***E*.7.H$^+$**	$S_0 \rightarrow S_1$	2.67	464.9	0.558	H → L (96%)	π → π*
***E*.8.H$^+$**	$S_0 \rightarrow S_1$	2.77	447.8	0.315	H → L (97%)	π → π*
***E*.9.H$^+$**	$S_0 \rightarrow S_1$	2.71	457.8	0.410	H → L (97%)	π → π*
***E*.10.H$^+$**	$S_0 \rightarrow S_1$	2.86	433.0	0.349	H → L (97%)	π → π*
***E*.11.H$^+$**	$S_0 \rightarrow S_1$	2.78	445.6	0.439	H → L (97%)	π → π*
***E*.12.H$^+$**	$S_0 \rightarrow S_1$	2.72	455.4	0.537	H → L (97%)	π → π*
***E*.13.H$^+$**	$S_0 \rightarrow S_1$	2.68	463.1	0.507	H → L (98%)	π → π*
***E*.14.H$^+$**	$S_0 \rightarrow S_1$	2.52	492.4	0.342	H → L (98%)	π → π*
***E*.15.H$^+$**	$S_0 \rightarrow S_1$	2.51	493.3	0.350	H → L (98%)	π → π*
***E*.16.H$^+$**	$S_0 \rightarrow S_1$	2.09	594.2	0.178	H → L (94%)	π → π*
***E*.17.H$^+$**	$S_0 \rightarrow S_1$	2.01	615.8	0.174	H → L (94%)	π → π*
***E*.18.H$^+$**	$S_0 \rightarrow S_1$	1.91	650.5	0.225	H → L (97%)	π → π*

[a] > 10%, H = HOMO, L = LUMO.

Table S15. TD-PBE0/def2-TZVP//PBE0-D3/def2-TZVP first $S_0 \rightarrow S_1$ transitions in the UV-Vis absorption spectra of *Z* forms of **AB.H$^+$-18.H$^+$**.

Structures	Transition	*E*, eV	*λ*, nm	*f*	Contribution[a]	Assignment
***Z*.AB.H$^+$**	$S_0 \rightarrow S_1$	2.87	432.4	0.188	H → L (91%)	π → π*
***Z*.1.H$^+$**	$S_0 \rightarrow S_1$	2.87	431.5	0.137	H → L (97%)	π → π*
***Z*.2.H$^+$**	$S_0 \rightarrow S_1$	2.73	453.4	0.106	H → L (95%)	π → π*
***Z*.3.H$^+$**	$S_0 \rightarrow S_1$	2.72	455.6	0.061	H → L (98%)	π → π*
***Z*.4.H$^+$**	$S_0 \rightarrow S_1$	2.65	467.5	0.169	H → L (88%) H-1 → L (11%)	π → π* π → π*
***Z*.5.H$^+$**	$S_0 \rightarrow S_1$	2.54	488.7	0.056	H → L (99%)	π → π*
***Z*.6.H$^+$**	$S_0 \rightarrow S_1$	2.26	549.3	0.084	H → L (100%)	π → π*
***Z*.7.H$^+$**	$S_0 \rightarrow S_1$	2.19	565.1	0.137	H → L (98%)	π → π*
***Z*.8.H$^+$**	$S_0 \rightarrow S_1$	2.49	497.4	0.057	H → L (98%)	π → π*
***Z*.9.H$^+$**	$S_0 \rightarrow S_1$	2.10	590.1	0.064	H → L (99%)	π → π*
***Z*.10.H$^+$**	$S_0 \rightarrow S_1$	2.52	492.9	0.059	H → L (98%)	π → π*
***Z*.11.H$^+$**	$S_0 \rightarrow S_1$	2.14	578.5	0.064	H → L (99%)	π → π*
***Z*.12.H$^+$**	$S_0 \rightarrow S_1$	2.01	615.5	0.055	H → L (83%)	π → π*
***Z*.13.H$^+$**	$S_0 \rightarrow S_1$	1.98	627.4	0.063	H → L (87%)	π → π*
***Z*.14.H$^+$**	$S_0 \rightarrow S_1$	2.01	616.1	0.053	H → L (98%)	π → π*
***Z*.15.H$^+$**	$S_0 \rightarrow S_1$	1.99	622.8	0.055	H → L (98%)	π → π*
***Z*.16.H$^+$**	$S_0 \rightarrow S_1$	1.92	645.7	0.042	H → L (98%)	π → π*

***Z*.17.H$^+$**	$S_0 \rightarrow S_1$	1.89	657.5	0.042	H → L (98%)	π → π*
***Z*.18.H$^+$**	$S_0 \rightarrow S_1$	1.84	672.9	0.100	H → L (96%)	π → π*

Table S16. TD-PBE0/def2-TZVP//PBE0-D3/def2-TZVP first $S_0 \rightarrow S_1$ transitions in the UV-Vis absorption spectra of *E* forms of **AB.2H$^+$-18.2H$^+$**.

Structures	Transition	*E,* eV	*λ,* nm	*f*	Contribution[a]	Assignment
***E*.AB.2H$^+$**	$S_0 \rightarrow S_1$	2.32	533.6	0.083	H-1 → L (89%) H → L (12%)	π → π* π → π*
***E*.1.2H$^+$**	$S_0 \rightarrow S_1$	2.46	503.8	0.432	H → L (78%) H-2 → L (25%)	π → π* π → π*
***E*.2.2H$^+$**	$S_0 \rightarrow S_1$	2.41	514.2	0.126	H-2 → L (74%) H → L (26%)	π → π* π → π*
***E*.3.2H$^+$**	$S_0 \rightarrow S_1$	2.43	510.1	0.404	H → L (88%) H-2 → L (16%)	π → π* π → π*
***E*.4.2H$^+$**	$S_0 \rightarrow S_1$	2.32	533.4	0.220	H-1 → L (81%) H → L (19%)	π → π* π → π*
***E*.5.2H$^+$**	$S_0 \rightarrow S_1$	2.10	590.8	0.303	H → L (96%)	π → π*
***E*.6.2H$^+$**	$S_0 \rightarrow S_1$	2.07	598.0	0.399	H → L (97%)	π → π*
***E*.7.2H$^+$**	$S_0 \rightarrow S_1$	2.05	604.1	0.495	H → L (96%)	π → π*
***E*.8.2H$^+$**	$S_0 \rightarrow S_1$	2.00	619.2	0.347	H → L (98%)	π → π*
***E*.9.2H$^+$**	$S_0 \rightarrow S_1$	2.01	618.3	0.426	H → L (99%)	π → π*
***E*.10.2H$^+$**	$S_0 \rightarrow S_1$	2.06	602.8	0.375	H → L (98%)	π → π*
***E*.11.2H$^+$**	$S_0 \rightarrow S_1$	2.04	606.5	0.443	H → L (99%)	π → π*
***E*.12.2H$^+$**	$S_0 \rightarrow S_1$	2.03	609.9	0.441	H → L (93%)	π → π*
***E*.13.2H$^+$**	$S_0 \rightarrow S_1$	2.01	616.5	0.459	H → L (97%)	π → π*
***E*.14.2H$^+$**	$S_0 \rightarrow S_1$	1.96	631.9	0.427	H → L (100%)	π → π*
***E*.15.2H$^+$**	$S_0 \rightarrow S_1$	1.99	622.4	0.452	H → L (100%)	π → π*
***E*.16.2H$^+$**	$S_0 \rightarrow S_1$	1.85	671.0	0.319	H → L (100%)	π → π*
***E*.17.2H$^+$**	$S_0 \rightarrow S_1$	1.77	701.9	0.295	H → L (100%)	π → π*
***E*.18.2H$^+$**	$S_0 \rightarrow S_1$	1.68	737.9	0.308	H → L (100%)	π → π*

Table S17. TD-PBE0/def2-TZVP//PBE0-D3/def2-TZVP first $S_0 \rightarrow S_1$ transitions in the UV-Vis absorption spectra of *Z* forms of **AB.2H$^+$-18.2H$^+$**.

Structures	Transition	*E,* eV	*λ,* nm	*f*	Contribution[a]	Assignment
***Z*.AB.2H$^+$**	$S_0 \rightarrow S_1$	2.06	600.4	0.043	H-1 → L (77%) H → L (23%)	π → π* π → π*
***Z*.1.2H$^+$**	$S_0 \rightarrow S_1$	2.20	563.2	0.126	H-2 → L (18%) H → L (84%)	π → π* π → π*
***Z*.2.2H$^+$**	$S_0 \rightarrow S_1$	2.05	606.1	0.088	H-2 → L (39%) H → L (63%)	π → π* π → π*
***Z*.3.2H$^+$**	$S_0 \rightarrow S_1$	2.10	590.7	0.111	H → L (93%)	π → π*
***Z*.4.2H$^+$**	$S_0 \rightarrow S_1$	1.99	623.2	0.100	H → L (46%) H-1 → L (55%)	π → π* π → π*
***Z*.5.2H$^+$**	$S_0 \rightarrow S_1$	1.54	803.3	0.079	H → L (100%)	π → π*
***Z*.6.2H$^+$**	$S_0 \rightarrow S_1$	1.63	760.0	0.127	H → L (100%)	π → π*
***Z*.8.2H$^+$**	$S_0 \rightarrow S_1$	1.44	858.9	0.104	H → L (100%)	π → π*

***Z*.9.2H$^+$**	$S_0 \rightarrow S_1$	1.45	853.8	0.135	H → L (100%)	π → π*
***Z*.10.2H$^+$**	$S_0 \rightarrow S_1$	1.43	865.4	0.106	H → L (100%)	π → π*
***Z*.11.2H$^+$**	$S_0 \rightarrow S_1$	1.47	845.5	0.130	H → L (100%)	π → π*
***Z*.14.2H$^+$**	$S_0 \rightarrow S_1$	1.40	884.5	0.142	H → L (100%)	π → π*
***Z*.15.2H$^+$**	$S_0 \rightarrow S_1$	1.42	873.9	0.129	H → L (96%)	π → π*
***Z*.16.2H$^+$**	$S_0 \rightarrow S_1$	1.42	870.5	0.150	H → L (100%)	π → π*
***Z*.17.2H$^+$**	$S_0 \rightarrow S_1$	1.36	911.1	0.144	H → L (100%)	π → π*

Table S18. TD-PBE0/def2-TZVP//PBE0-D3/def2-TZVP first $S_0 \rightarrow S_1$ transitions in the UV-Vis absorption spectra of *E* forms of **17.H$^+$-11a.H$^+$**.

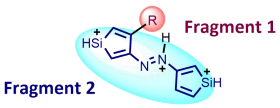
Structures	Transition	*E*, eV	*λ*, nm	*f*	Contribution[a]	Assignment
***E*.17.H$^+$**	$S_0 \rightarrow S_1$	2.01	615.8	0.174	H → L (94%)	π → π*
***E*.1a.H$^+$**	$S_0 \rightarrow S_1$	1.97	630.2	0.134	H → L (93%)	π → π*
***E*.2a.H$^+$**	$S_0 \rightarrow S_1$	1.94	639.9	0.139	H → L (93%)	π → π*
***E*.3a.H$^+$**	$S_0 \rightarrow S_1$	1.94	639.0	0.157	H → L (95%)	π → π*
***E*.4a.H$^+$**	$S_0 \rightarrow S_1$	1.91	648.3	0.159	H → L (95%)	π → π*
***E*.5a.H$^+$**	$S_0 \rightarrow S_1$	1.86	668.2	0.198	H → L (97%)	π → π*
***E*.6a.H$^+$**	$S_0 \rightarrow S_1$	1.74	712.7	0.187	H → L (99%)	π → π*
***E*.7a.H$^+$**	$S_0 \rightarrow S_1$	2.02	613.4	0.173	H → L (94%)	π → π*
***E*.8a.H$^+$**	$S_0 \rightarrow S_1$	1.93	642.0	0.144	H → L (94%)	π → π*
***E*.9a.H$^+$**	$S_0 \rightarrow S_1$	1.91	650.5	0.122	H → L (93%)	π → π*
***E*.10a.H$^+$**	$S_0 \rightarrow S_1$	1.83	677.3	0.097	H → L (92%)	π → π*
***E*.11a.H$^+$**	$S_0 \rightarrow S_1$	1.63	759.4	0.061	H → L (93%)	π → π*

Table S19. TD-PBE0/def2-TZVP//PBE0-D3/def2-TZVP first $S_0 \rightarrow S_1$ transitions in the UV-Vis absorption spectra of *Z* forms of **17.H$^+$-11a.H$^+$**.

Structures	Transition	*E*, eV	*λ*, nm	*f*	Contribution[a]	Assignment
***Z*.17.H$^+$**	$S_0 \rightarrow S_1$	1.89	657.5	0.042	H → L (98%)	π → π*
***Z*.1a.H$^+$**	$S_0 \rightarrow S_1$	1.80	690.1	0.042	H → L (97%)	π → π*
***Z*.2a.H$^+$**	$S_0 \rightarrow S_1$	1.80	690.3	0.046	H → L (97%)	π → π*
***Z*.3a.H$^+$**	$S_0 \rightarrow S_1$	1.76	705.5	0.063	H → L (97%)	π → π*
***Z*.4a.H$^+$**	$S_0 \rightarrow S_1$	1.68	738.2	0.077	H → L (97%)	π → π*
***Z*.5a.H$^+$**	$S_0 \rightarrow S_1$	1.57	790.0	0.161	H → L (97%)	π → π*
***Z*.6a.H$^+$**	$S_0 \rightarrow S_1$	1.47	843.1	0.179	H → L (99%)	π → π*
***Z*.7a.H$^+$**	$S_0 \rightarrow S_1$	1.91	648.2	0.048	H → L (98%)	π → π*
***Z*.8a.H$^+$**	$S_0 \rightarrow S_1$	1.87	662.8	0.042	H → L (97%)	π → π*
***Z*.9a.H$^+$**	$S_0 \rightarrow S_1$	1.73	718.0	0.044	H → L (98%)	π → π*
***Z*.10a.H$^+$**	$S_0 \rightarrow S_1$	1.65	750.0	0.035	H → L (97%)	π → π*
***Z*.11a.H$^+$**	$S_0 \rightarrow S_1$	1.32	936.8	0.007	H → L (92%)	π → π*

Table S20. Selected geometrical parameters of *E* and *Z* isomers of **1a.H$^+$-11a.H$^+$** as well as their corresponding $\Delta G_{Z\text{-}E}$ values (kcal mol^{-1}, 298.15 K).

Structures	N=N (Å)	N2–C3 (Å)	N4–C5 (Å)	Φ_1 (deg)	Φ_2 (deg)	α (angle)	Ψ (deg)	$\Delta G_{Z\text{-}E}$ (kcal/mol)
***E*.1a.H$^+$**	1.252	1.389	1.367	1.3	-178.1	120.6	179.2	8.6
***Z*.1a.H$^+$**	1.232	1.428	1.380	146.5	-39.6	130.5	-12.2	
***E*.2a.H$^+$**	1.254	1.387	1.364	-0.2	179.3	120.6	-179.1	7.6
***Z*.2a.H$^+$**	1.233	1.430	1.379	141.9	-44.5	130.2	-12.8	
***E*.3a.H$^+$**	1.256	1.385	1.359	0.0	-180.0	120.6	180.0	13.5
***Z*.3a.H$^+$**	1.236	1.429	1.373	141.5	-45.1	130.8	-13.3	
***E*.4a.H$^+$**	1.257	1.385	1.358	0.0	180.0	120.5	-179.8	15.8
***Z*.4a.H$^+$**	1.238	1.426	1.371	147.7	-39.3	131.6	-13.5	
***E*.5a.H$^+$**	1.264	1.385	1.347	0.7	-179.9	120.7	-178.7	5.5
***Z*.5a.H$^+$**	1.262	1.398	1.339	166.4	-20.0	134.0	-18.5	
***E*.6a.H$^+$**	1.268	1.382	1.343	0.1	180.0	121.1	179.3	5.9
***Z*.6a.H$^+$**	1.267	1.394	1.337	178.4	-7.0	133.6	-21.6	
***E*.7a.H$^+$**	1.253	1.387	1.361	0.1	179.8	120.3	-179.5	13.2
***Z*.7a.H$^+$**	1.231	1.431	1.379	139.6	-46.6	130.3	-11.8	
***E*.8a.H$^+$**	1.251	1.387	1.366	0.2	179.8	120.4	-179.3	9.7
***Z*.8a.H$^+$**	1.229	1.428	1.381	144.7	-41.3	130.7	-11.1	
***E*.9a.H$^+$**	1.252	1.387	1.363	-0.0	180.0	120.5	180.0	10.4
***Z*.9a.H$^+$**	1.232	1.427	1.379	146.4	-39.9	131.1	-12.3	
***E*.10a.H$^+$**	1.252	1.386	1.365	-0.2	179.8	120.7	-179.9	11.3
***Z*.10a.H$^+$**	1.233	1.427	1.379	145.9	-40.9	130.7	-13.6	
***E*.11a.H$^+$**	1.253	1.387	1.363	-0.8	179.1	120.6	179.7	8.2
***Z*.11a.H$^+$**	1.237	1.424	1.379	149.2	-37.2	130.7	-16.1	



E.2a Total interaction: 1.27

PIO Pop. 1.02 → PBI 1.000 (79.0 %) *1st* → PIMO

PIO Pop. 0.98 → PBI 1.000 (79.0 %) *1st* → PIMO

PIO Pop. 0.08 → PBI 0.150 (11.8 %) *2nd* → PIMO

PIO Pop. 1.92 → PBI 0.150 (11.8 %) *2nd* → PIMO

E.3a Total interaction: 1.48

PIO Pop. 0.67 → PBI 0.892 (60.2 %) *1st* → PIMO

PIO Pop. 1.33 → PBI 0.892 (60.2 %) *1st* → PIMO

PIO Pop. 0.26 → PBI 0.447 (30.2 %) *2nd* → PIMO

PIO Pop. 1.74 → PBI 0.447 (30.2 %) *2nd* → PIMO

PIO Pop. 0.05 → PBI 0.091 (6.1 %) *3th* → PIMO

PIO Pop. 1.95 → PBI 0.091 (6.1 %) *3th* → PIMO

E.4a Total interaction: 1.56

PIO Pop. 0.67 → PBI 0.889 (57.0 %) *1st* → PIMO

PIO Pop. 1.33 → PBI 0.889 (57.0 %) *1st* → PIMO

PIO Pop. 0.30 → PBI 0.506 (32.4 %) *2nd* → PIMO

PIO Pop. 1.70 → PBI 0.506 (32.4 %) *2nd* → PIMO

PIO Pop. 0.05 → PBI 0.099 (6.4 %) *3th* → PIMO

PIO Pop. 1.95 → PBI 0.099 (6.4 %) *3th* → PIMO

E.5a Total interaction: 1.79

PIO Pop. 0.80 → PBI 0.961 (53.7 %) *1st* → PIMO

PIO Pop. 1.20 → PBI 0.961 (53.7 %) *1st* → PIMO

PIO Pop. 0.47 → PBI 0.723 (40.5 %) *2nd* → PIMO

PIO Pop. 1.53 → PBI 0.723 (40.5 %) *2nd* → PIMO

E.7a Total interaction: 1.18

PIO Pop. 0.57 → PBI 0.814 (69.0 %) *1st* → PIMO

PIO Pop. 1.43 → PBI 0.814 (69.0 %) *1st* → PIMO

PIO Pop. 0.13 → PBI 0.242 (20.5 %) *2nd* → PIMO

PIO Pop. 1.87 → PBI 0.242 (20.5 %) *2nd* → PIMO

PIO Pop. 0.05 → PBI 0.090 (7.6 %) *3th* → PIMO

PIO Pop. 1.95 → PBI 0.090 (7.6 %) *3th* → PIMO

E.8a Total interaction: 1.37

PIO Pop. 1.02 → PBI 1.000 (73.0 %) *1st* → PIMO

PIO Pop. 0.98 → PBI 1.000 (73.0 %) *1st* → PIMO

PIO Pop. 0.07 → PBI 0.139 (10.1 %) *2nd* → PIMO

PIO Pop. 1.93 → PBI 0.139 (10.1 %) *2nd* → PIMO

PIO Pop. 1.95 → PBI 0.106 (7.7 %) *3th* → PIMO

PIO Pop. 0.05 → PBI 0.106 (7.7 %) *3th* → PIMO

E.9a Total interaction: 1.51

PIO Pop. 0.94 → PBI 0.996 (65.9 %) *1st* → PIMO

PIO Pop. 1.06 → PBI 0.996 (65.9 %) *1st* → PIMO

PIO Pop. 0.19 → PBI 0.337 (22.2 %) *2nd* → PIMO

PIO Pop. 1.81 → PBI 0.337 (22.2 %) *2nd* → PIMO

PIO Pop. 0.07 → PBI 0.136 (9.0 %) *3th* → PIMO

PIO Pop. 1.93 → PBI 0.136 (9.0 %) *3th* → PIMO

E.10a Total interaction: 1.54

PIO Pop. 1.02 → PBI 1.000 (64.9 %) *1st* → PIMO

PIO Pop. 0.98 → PBI 1.000 (64.9 %) *1st* → PIMO

PIO Pop. 0.19 → PBI 0.350 (22.7 %) *2nd* → PIMO

PIO Pop. 1.80 → PBI 0.350 (22.7 %) *2nd* → PIMO

PIO Pop 0.08 → PBI 0.154 (10.0 %) *3th* → PIMO

PIO Pop 1.92 → PBI 0.154 (10.0 %) *3th* → PIMO

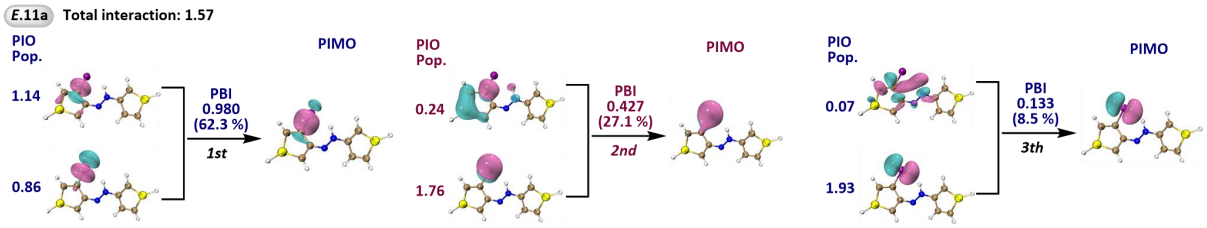


Figure S9. PIO analysis for the interaction of two fragments in ***E*.2a.H$^+$-*E*.5a.H$^+$** and ***E*.7a.H$^+$-*E*.11a.H$^+$**, respectively. PIO pairs, populations (Pop), principal bond indexes (PBI) and contribution (%) of each interaction are shown in blue and red (isovalue: 0.05 a.u.), respectively.

Table S21. TD-PBE0/def2-TZVP//PBE0-D3/def2-TZVP first $S_0 \rightarrow S_1$ transitions in the UV-Vis absorption spectra of *E* forms of **17.2H$^+$-11a.2H$^+$**.

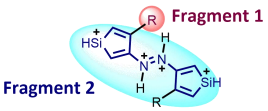
Structures	Transition	*E*, eV	*λ*, nm	*f*	Contribution[a]	Assignment
***E*.17.2H$^+$**	$S_0 \rightarrow S_1$	1.77	701.9	0.295	H → L (100%)	π → π*
***E*.1a.2H$^+$**	$S_0 \rightarrow S_1$	1.61	771.4	0.187	H → L (98%)	π → π*
***E*.2a.2H$^+$**	$S_0 \rightarrow S_1$	1.56	794.3	0.219	H → L (100%)	π → π*
***E*.3a.2H$^+$**	$S_0 \rightarrow S_1$	1.53	810.9	0.252	H → L (100%)	π → π*
***E*.4a.2H$^+$**	$S_0 \rightarrow S_1$	1.46	847.1	0.246	H → L (100%)	π → π*
***E*.5a.2H$^+$**	$S_0 \rightarrow S_1$	1.46	849.8	0.351	H → L (100%)	π → π*
***E*.6a.2H$^+$**	$S_0 \rightarrow S_1$	1.26	980.7	0.290	H → L (100%)	π → π*
***E*.7a.2H$^+$**	$S_0 \rightarrow S_1$	1.73	717.9	0.287	H → L (100%)	π → π*
***E*.8a.2H$^+$**	$S_0 \rightarrow S_1$	1.64	758.3	0.178	H → L (98%)	π → π*
***E*.9a.2H$^+$**	$S_0 \rightarrow S_1$	1.48	836.6	0.184	H → L (100%)	π → π*
***E*.10a.2H$^+$**	$S_0 \rightarrow S_1$	1.34	921.9	0.150	H → L (100%)	π → π*
***E*.11a.2H$^+$**	$S_0 \rightarrow S_1$	1.08	1153.1	0.130	H → L (100%)	π → π*

Table S22. TD-PBE0/def2-TZVP//PBE0-D3/def2-TZVP first $S_0 \rightarrow S_1$ transitions in the UV-Vis absorption spectra of *E* forms of **17.2H$^+$-11a.2H$^+$**.

Structures	Transition	*E*, eV	*λ*, nm	*f*	Contribution[a]	Assignment
***Z*.17.2H$^+$**	$S_0 \rightarrow S_1$	1.36	911.1	0.144	H → L (100%)	π → π*
***Z*.1a.2H$^+$**	$S_0 \rightarrow S_1$	1.23	1009.1	0.151	H → L (100%)	π → π*
***Z*.2a.2H$^+$**	$S_0 \rightarrow S_1$	1.26	981.2	0.178	H → L (100%)	π → π*
***Z*.3a.2H$^+$**	$S_0 \rightarrow S_1$	1.32	941.2	0.234	H → L (100%)	π → π*
***Z*.4a.2H$^+$**	$S_0 \rightarrow S_1$	1.32	939.4	0.283	H → L (100%)	π → π*
***Z*.5a.2H$^+$**	$S_0 \rightarrow S_1$	1.14	1083.4	0.246	H → L (100%)	π → π*
***Z*.6a.2H$^+$**	$S_0 \rightarrow S_1$	0.80	1550.2	0.162	H → L (100%)	π → π*
***Z*.7a.2H$^+$**	$S_0 \rightarrow S_1$	1.39	889.0	0.189	H → L (100%)	π → π*
***Z*.8a.2H$^+$**	$S_0 \rightarrow S_1$	1.32	942.9	0.164	H → L (100%)	π → π*
***Z*.9a.2H$^+$**	$S_0 \rightarrow S_1$	1.27	975.3	0.197	H → L (100%)	π → π*
***Z*.10a.2H$^+$**	$S_0 \rightarrow S_1$	1.17	1059.2	0.190	H → L (100%)	π → π*
***Z*.11a.2H$^+$**	$S_0 \rightarrow S_1$	0.89	1386.5	0.095	H → L (85%) H-2 → L (25%)	π → π* σ → π*

Table S23. Selected geometrical parameters of *E* and *Z* isomers of **1a.2H$^+$-11a.2H$^+$** as well as their corresponding $\Delta G_{Z\text{-}E}$ values (kcal mol^{-1}, 298.15 K).

Structures	N=N (Å)	N–C (Å)	Φ_1 (deg)	Φ_2 (deg)	α (angle)	Ψ (deg)	$\Delta G_{Z\text{-}E}$ (kcal/mol)
***E*.1a.2H$^+$**	1.278	1.365	1.9	-177.3	127.0	-178.5	5.7
***Z*.1a.2H$^+$**	1.293	1.360	173.1	-13.7	134.0	-22.6	
***E*.2a.2H$^+$**	1.284	1.362	2.3	-178.0	128.3	-178.0	4.8
***Z*.2a.2H$^+$**	1.300	1.356	169.4	-16.7	132.9	-24.9	
***E*.3a.2H$^+$**	1.287	1.357	-0.0	180.0	126.6	-180.0	10.7
***Z*.3a.2H$^+$**	1.298	1.351	172.6	-13.2	132.9	-20.3	
***E*.4a.2H$^+$**	1.287	1.355	0.9	-179.1	126.2	-179.9	11.3
***Z*.4a.2H$^+$**	1.298	1.349	178.2	-7.2	133.1	-21.9	
***E*.5a.2H$^+$**	1.317	1.354	-23.7	153.9	124.9	168.3	2.2
***Z*.5a.2H$^+$**	1.316	1.350	174.6	-11.4	130.6	-31.9	
***E*.6a.2H$^+$**	1.310	1.354	-12.1	156.9	126.5	178.6	4.4
***Z*.6a.2H$^+$**	1.332	1.347	170.4	-4.7	129.3	-46.5	
***E*.7a.2H$^+$**	1.285	1.359	-1.3	178.9	126.8	177.8	11.2
***Z*.7a.2H$^+$**	1.293	1.356	171.0	-15.5	133.0	-18.5	
***E*.8a.2H$^+$**	1.280	1.365	-1.1	179.1	127.6	178.3	10.7
***Z*.8a.2H$^+$**	1.291	1.361	165.0	-22.2	133.1	-20.2	
***E*.9a.2H$^+$**	1.280	1.360	0.7	-179.2	128.1	179.7	8.1
***Z*.9a.2H$^+$**	1.294	1.354	167.7	-18.5	133.1	-21.4	
***E*.10a.2H$^+$**	1.280	1.361	2.9	-176.0	128.3	176.2	5.3
***Z*.10a.2H$^+$**	1.297	1.352	174.0	-11.7	133.3	-25.3	
***E*.11a.2H$^+$**	1.284	1.361	1.0	-179.0	129.2	-179.3	1.2
***Z*.11a.2H$^+$**	1.304	1.351	173.3	-11.6	131.3	-32.9	



E.1a.2H$^+$ Total interaction: 1.01

PIO Pop. 1.47 / 0.53 → PBI 0.778 (76.8 %) *1st* → PIMO

PIO Pop. 0.07 / 1.93 → PBI 0.128 (12.7 %) *2nd* → PIMO

E.2a.2H$^+$ Total interaction: 1.28

PIO Pop. 1.03 / 0.97 → PBI 0.999 (78.2 %) *1st* → PIMO

PIO Pop. 0.08 / 1.92 → PBI 0.154 (12.0 %) *2nd* → PIMO

E.3a.2H$^+$ Total interaction: 1.50

PIO Pop. 0.68 / 1.32 → PBI 0.896 (59.7 %) *1st* → PIMO

PIO Pop. 0.26 / 1.74 → PBI 0.451 (30.1 %) *2nd* → PIMO

E.4a.2H$^+$ Total interaction: 1.59

PIO Pop. 0.67 / 1.33 → PBI 0.893 (56.3 %) *1st* → PIMO

PIO Pop. 0.30 / 1.70 → PBI 0.513 (32.4 %) *2nd* → PIMO

E.5a.2H$^+$ Total interaction: 1.83

PIO Pop. 0.81 / 1.19 → PBI 0.964 (52.8 %) *1st* → PIMO

PIO Pop. 0.51 / 1.49 → PBI 0.758 (41.5 %) *2nd* → PIMO

E.6a.2H$^+$ Total interaction: 1.95

PIO Pop. 0.79 / 1.21 → PBI 0.956 (49.0 %) *1st* → PIMO

PIO Pop. 0.62 / 1.38 → PBI 0.855 (43.8 %) *2nd* → PIMO

E.7a.2H$^+$ Total interaction: 1.20

PIO Pop. 0.58 / 1.42 → PBI 0.821 (68.4 %) *1st* → PIMO

PIO Pop. 0.13 / 1.87 → PBI 0.245 (20.5 %) *2nd* → PIMO

PIO Pop. 0.05 / 1.95 → PBI 0.099 (8.3 %) *3rd* → PIMO

E.8a.2H$^+$ Total interaction: 1.39

PIO Pop. 1.03 / 0.97 → PBI 0.999 (71.8 %) *1st* → PIMO

PIO Pop. 0.08 / 1.92 → PBI 0.153 (11.0 %) *2nd* → PIMO

PIO Pop. 1.95 / 0.05 → PBI 0.102 (7.3 %) *3rd* → PIMO

E.9a.2H$^+$ Total interaction: 1.57

PIO Pop. 0.96 / 1.04 → PBI 0.998 (63.7 %) *1st* → PIMO

PIO Pop. 0.20 / 1.80 → PBI 0.358 (22.8 %) *2nd* → PIMO

PIO Pop. 0.09 / 1.91 → PBI 0.167 (10.7 %) *3rd* → PIMO

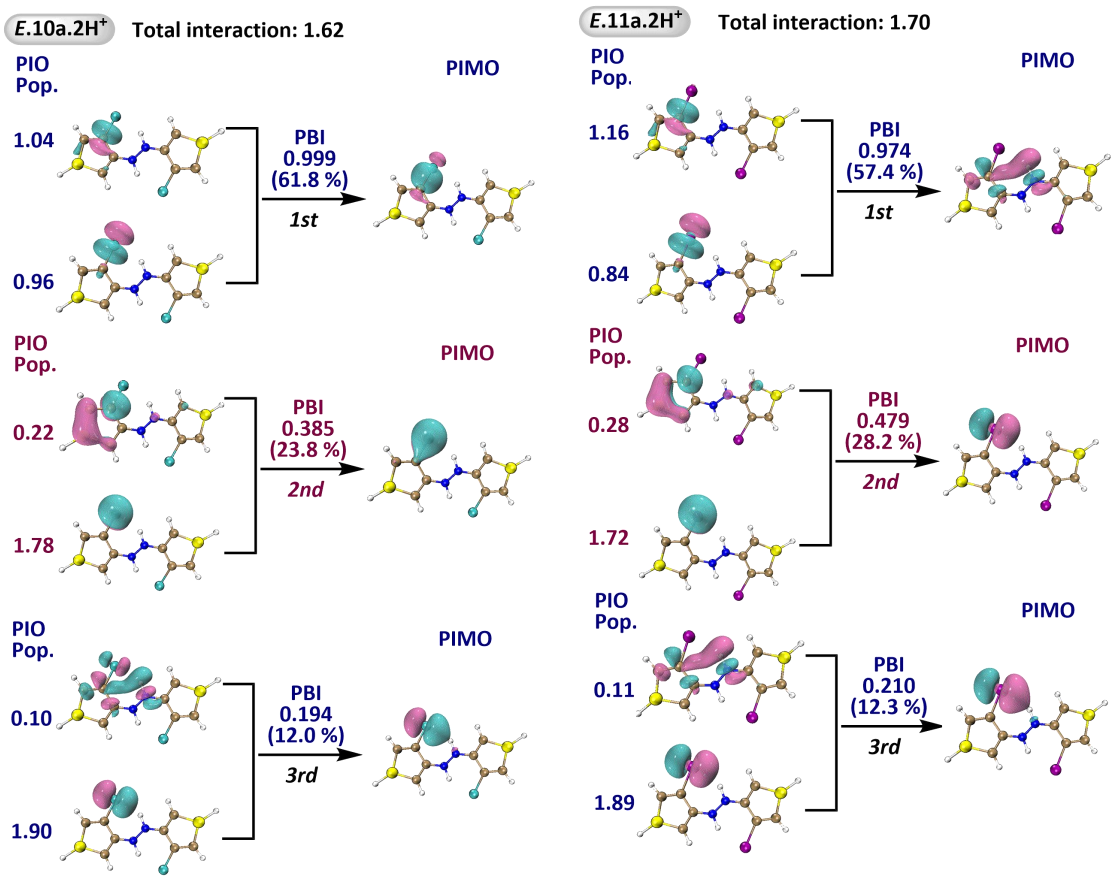


Figure S10. PIO analysis for the interaction of two fragments in ***E*.1a.2H$^+$-*E*.11a.2H$^+$**, respectively. PIO pairs, populations (Pop), principal bond indexes (PBI) and contribution (%) of each interaction are shown in blue and red (isovalue: 0.05 a.u.), respectively.

Table 24. The H-bond (Å), HOMO and LUMO energies of models ***E*.1a.H$^+$–*E*.11a.H$^+$** as well as ***E*.1a.2H$^+$–*E*.11a.2H$^+$**.

Structures	***E*.1a.H$^+$**	***E*.2a.H$^+$**	***E*.3a.H$^+$**	***E*.4a.H$^+$**	***E*.5a.H$^+$**	***E*.6a.H$^+$**
H-bond (Å)	2.518	2.288	1.944	1.933	2.470	2.522
LUMO (eV)	-6.43 (π*)	-6.37 (π*)	-6.29 (π*)	-6.25 (π*)	-6.11 (π*)	-6.02 (π*)
HOMO (eV)	-9.05 (π)	-8.96 (π)	-8.86 (π)	-8.80 (π)	-8.54 (π)	-8.32 (π)
Structures	***E*.7a.H$^+$**	***E*.8a.H$^+$**	***E*.9a.H$^+$**	***E*.10a.H$^+$**	***E*.11a.H$^+$**	
H-bond (Å)	2.027	2.312	2.238	2.303	2.536	
LUMO (eV)	-6.51 (π*)	-6.71 (π*)	-6.46 (π*)	-6.45 (π*)	-6.39 (π*)	
HOMO (eV)	-9.12 (π)	-9.23 (π)	-9.02 (π)	-8.97 (π)	-8.76 (π)	
Structures	***E*.1a.2H$^+$**	***E*.2a.2H$^+$**	***E*.3a.2H$^+$**	***E*.4a.2H$^+$**	***E*.5a.2H$^+$**	***E*.6a.2H$^+$**
H-bond (Å)	2.439	2.226	1.873	1.844	2.610	2.573
LUMO (eV)	-7.61 (π*)	-7.61 (π*)	-7.45 (π*)	-7.35 (π*)	-7.16 (π*)	-6.92 (π*)
HOMO (eV)	-9.59 (π)	-9.46 (π)	-9.26 (π)	-9.13 (π)	-8.67 (π)	-8.34 (π)
Structures	***E*.7a.2H$^+$**	***E*.8a.2H$^+$**	***E*.9a.2H$^+$**	***E*.10a.2H$^+$**	***E*.11a.2H$^+$**	
H-bond (Å)	1.963	2.200	2.172	2.238	2.411	
LUMO (eV)	-7.88 (π*)	-8.10 (π*)	-7.71 (π*)	-7.65 (π*)	-7.50 (π*)	
HOMO (eV)	-9.85 (π)	-10.11 (π)	-9.58 (π)	-9.44 (π)	-9.04 (π)	

Comparison of TD-DFT calculated results with different functionals.

***E*.17e.2H$^+$**

PBE0-D3/def2-TZVP

Excited State	1:	0.9856 eV	1257.98 nm	f=0.1145
88 -> 89		0.72719		
88 <- 89		-0.23322		
Excited State	2:	1.4722 eV	842.15 nm	f=0.0001
87 -> 89		-0.16527		
88 -> 90		0.68447		
Excited State	3:	1.6358 eV	757.96 nm	f=0.0003
87 -> 89		0.68712		
88 -> 90		0.16252		
Excited State	4:	1.7078 eV	725.98 nm	f=0.0005
86 -> 89		0.70380		
Excited State	5:	1.9202 eV	645.70 nm	f=0.0000
85 -> 89		0.69790		

ωB97X-D/def2-TZVP

Excited State	1:	1.0057 eV	1232.80 nm	f=0.1146
87 -> 90		-0.14490		
88 -> 89		0.68975		
88 <- 89		-0.12725		
Excited State	2:	1.5583 eV	795.62 nm	f=0.0003
83 -> 89		-0.10119		
87 -> 89		0.54067		
88 -> 90		-0.44119		
Excited State	3:	2.0171 eV	614.65 nm	f=0.0000
85 -> 90		-0.10998		
87 -> 89		0.45251		
87 -> 91		0.14369		
88 -> 90		0.49793		
Excited State	4:	2.0374 eV	608.53 nm	f=0.0009
86 -> 89		0.69843		
Excited State	5:	2.2722 eV	545.66 nm	f=0.0000
84 -> 89		0.69350		
86 -> 90		0.12573		

CAM-B3LYP/def2-TZVP

Excited State	1:	1.0101 eV	1227.44 nm	f=0.1160
87 -> 90		-0.13281		
88 -> 89		0.69578		
88 -> 91		-0.10102		
88 <- 89		-0.14445		

Excited State	2:	1.5645 eV	792.49 nm	f=0.0003
87 -> 89		0.52155		
88 -> 90		-0.46557		
Excited State	3:	1.9301 eV	642.37 nm	f=0.0000
85 -> 90		-0.10019		
87 -> 89		0.47615		
87 -> 91		0.10992		
88 -> 90		0.49288		
Excited State	4:	2.0337 eV	609.65 nm	f=0.0008
86 -> 89		0.69935		
Excited State	5:	2.2602 eV	548.55 nm	f=0.0000
84 -> 89		0.69428		
86 -> 90		0.12454		

Cartesian Coordinates of Models Described in the Text.

***E*.AB.H$^+$**

N	-0.44485700	0.48762800	-0.01293800
C	-1.77937600	0.17000200	-0.01453700
C	-2.62503800	1.28758500	0.04209100
C	-3.99438800	1.11510100	0.06139100
H	-4.64969600	1.97516300	0.11222000
C	-4.52232500	-0.16729400	0.01005000
H	-5.59654300	-0.30864100	0.01972600
C	-3.68512500	-1.28413600	-0.06125300
H	-4.11415200	-2.27689600	-0.11301700
C	-2.31960800	-1.12816400	-0.07327400
N	0.42201400	-0.40929700	0.03446500
C	1.80008900	-0.16374000	0.01830800
C	2.63866800	-1.27503300	0.06264500
C	4.00709800	-1.08001000	0.04433000
H	4.67203200	-1.93360800	0.07689600
C	4.52067000	0.20821400	-0.01613400
H	5.59312500	0.35965700	-0.03096500
C	3.66758500	1.30916700	-0.05856100
H	4.07792800	2.31016900	-0.10465200
C	2.29949700	1.13551800	-0.04297100
H	-2.17429400	2.27157900	0.07872000
H	-1.69767100	-2.01397200	-0.14533900
H	2.22734900	-2.27839900	0.10778400
H	1.62236700	1.97858400	-0.07538500
H	0.15297000	-1.39522100	0.09081500

PBE0-D3/def2-TZVP：

Zero-point correction= 0.205583 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.167568

Sum of electronic and zero-point Energies= -572.493794

Sum of electronic and thermal Energies= -572.482909

Sum of electronic and thermal Enthalpies= -572.481965

Sum of electronic and thermal Free Energies= -572.531809.

PBE0-D3/def2-TZVP Electronic Energy = -572.699377 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -572.732978964 a.u.

***Z*.AB.H$^+$**

N	-0.54441900	1.76113400	-0.02368900
C	-1.49898400	0.70217100	-0.07401400
C	-2.59825400	0.79157200	0.76800600
C	-3.56660300	-0.19720800	0.70283500
H	-4.42205100	-0.15249200	1.36502900

C	-3.44122000	-1.23262400	-0.21205300
H	-4.20403400	-1.99990800	-0.26551100
C	-2.34922900	-1.28424800	-1.07301100
H	-2.26827200	-2.07944700	-1.80351500
C	-1.36528200	-0.31667700	-1.01025700
N	0.70178100	1.77238900	-0.07233800
C	1.50679500	0.66296600	0.04159600
C	1.18325000	-0.54047000	0.69543700
C	2.14936900	-1.51233200	0.81445700
H	1.92121100	-2.43008700	1.34169400
C	3.41595500	-1.32477300	0.25854400
H	4.15710400	-2.11068300	0.34340000
C	3.74199600	-0.13478400	-0.37818100
H	4.73255700	0.01351600	-0.78852700
C	2.80290300	0.87342600	-0.45478100
H	-2.68376000	1.61031500	1.47270400
H	-0.51784300	-0.34301900	-1.68310800
H	0.21029000	-0.69254600	1.13947200
H	3.03351000	1.82905500	-0.90885700
H	-0.94442500	2.69852700	-0.01205600

PBE0-D3/def2-TZVP：

Zero-point correction= 0.205678 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.167566

Sum of electronic and zero-point Energies= -572.508680

Sum of electronic and thermal Energies= -572.497881

Sum of electronic and thermal Enthalpies= -572.496937

Sum of electronic and thermal Free Energies= -572.546792

PBE0-D3/def2-TZVP Electronic Energy = -572.714358 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -572.718664817 a.u.

***E*.1.H$^+$**

N	-0.45319400	0.49314300	-0.00000600
N	0.42090500	-0.41266300	-0.00001500
N	-3.91605000	0.53854400	0.00003000
C	-1.75319300	0.14948500	0.00002400
C	-2.43038000	-1.11740700	0.00001100
C	-3.75744100	-0.83240900	0.00004000
C	-2.73410500	1.14871800	0.00010200
H	-2.62194700	2.22079800	0.00014500
C	2.74679600	-1.12918900	-0.00004700
C	1.77343000	-0.14453200	-0.00001600
C	2.40719400	1.12354600	0.00001400
C	3.74896800	0.86596200	-0.00004700

N	3.93154100	-0.49008700	-0.00009600
H	4.82673900	-0.95045200	-0.00007100
H	2.66397300	-2.20397300	-0.00006900
H	1.92873400	2.08834800	0.00004700
H	4.59045100	1.53888400	-0.00006800
H	-4.61475700	-1.48523000	-0.00000800
H	-2.00785700	-2.10958100	-0.00004800
H	-4.80599500	1.01152000	0.00019600
H	0.15062200	-1.39790400	0.00000100

PBE0-D3/def2-TZVP：

Zero-point correction= 0.170982 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.134732

Sum of electronic and zero-point Energies= -528.494189

Sum of electronic and thermal Energies= -528.484578

Sum of electronic and thermal Enthalpies= -528.483633

Sum of electronic and thermal Free Energies= -528.530438

PBE0-D3/def2-TZVP Electronic Energy = -528.665170 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -528.669767120 a.u.

***Z*.1.H$^+$**

C	1.56095400	0.46664000	-0.04223900
C	1.47714200	-0.86031100	0.42826300
C	2.92930000	0.72854100	-0.37621500
C	-1.56081800	0.46645000	0.04238600
C	-2.92919000	0.72860700	0.37623200
C	-3.60560900	-0.41173900	0.11133700
H	-3.32566100	1.64950500	0.77241500
C	-1.47718900	-0.86063300	-0.42779100
C	3.60547900	-0.41205900	-0.11168400
H	3.32600200	1.64937700	-0.77224800
H	0.66196400	-1.43287600	0.83391800
H	4.64590000	-0.66112700	-0.23458700
H	-0.66210900	-1.43346500	-0.83328100
H	-4.64614900	-0.66053300	0.23376200
N	0.64193100	1.45484500	-0.05752000
N	-0.64170800	1.45468800	0.05749500
N	-2.70869700	-1.34119000	-0.38020600
N	2.70847300	-1.34128300	0.38011800
H	-2.95575200	-2.27853600	-0.66457700
H	2.95533900	-2.27874500	0.66427300
H	1.02086600	2.39205700	-0.17783800
H	-1.02081300	2.39194000	0.17722300

PBE0-D3/def2-TZVP：

Zero-point correction= 0.171513 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.135457

Sum of electronic and zero-point Energies= -528.478066

Sum of electronic and thermal Energies= -528.468660

Sum of electronic and thermal Enthalpies= -528.467716

Sum of electronic and thermal Free Energies= -528.514121

PBE0-D3/def2-TZVP Electronic Energy = -528.649579 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -528.654178107 a.u.

***E*.2.H$^+$**

N	0.46295600	0.46418900	-0.00000300
N	-0.43398100	-0.41377100	-0.00000300
C	1.76312400	0.08625300	0.00001000
C	2.34478100	-1.22519900	0.00001500
C	3.69414400	-1.16122500	0.00002500
C	2.72103600	1.09369400	0.00002000
H	2.52832500	2.15610000	0.00001900
C	-2.74340800	-1.08761000	-0.00003500
C	-1.78395600	-0.10261500	-0.00000200
C	-2.30739600	1.21685400	0.00003300
C	-3.66402600	1.19431600	0.00003900
H	-2.59727100	-2.15798400	-0.00006400
H	-1.70305400	2.11171100	0.00007000
H	-4.33967100	2.03616900	0.00007600
H	4.39747900	-1.98033600	0.00003000
H	1.80658300	-2.16318600	0.00001200
S	-4.28625200	-0.40268900	-0.00006800
S	4.27107800	0.46306700	0.00002200
H	-0.19822800	-1.40826500	0.00000500

PBE0-D3/def2-TZVP：

Zero-point correction= 0.138119 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.100675

Sum of electronic and zero-point Energies= -1214.009164

Sum of electronic and thermal Energies= -1213.999087

Sum of electronic and thermal Enthalpies= -1213.998143

Sum of electronic and thermal Free Energies= -1214.046608

PBE0-D3/def2-TZVP Electronic Energy = -1214.147284 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1214.15034707 a.u.

***Z*.2.H$^+$**

C	1.49066100	0.77702300	0.00324400
C	1.55379600	-0.30574600	0.84222800

C	2.58384000	0.87211500	-0.89635000
C	-1.53540300	0.73446900	0.11774000
C	-2.92976000	0.97973000	0.35369600
C	-3.69003600	-0.11254100	0.12570000
H	-3.30434400	1.94173000	0.67416100
C	-1.30225900	-0.58161900	-0.29839900
S	-2.72947800	-1.43678300	-0.39958200
C	3.43868800	-0.17317500	-0.73779800
S	2.93095600	-1.22434200	0.50794400
H	2.70615600	1.66184400	-1.62502700
H	0.87952900	-0.57854100	1.63947300
H	4.34050200	-0.38286100	-1.29234900
H	-0.37137400	-1.05463000	-0.56353400
H	-4.75853900	-0.22575600	0.22382900
N	0.53214600	1.80969000	0.08853500
N	-0.71667600	1.80803700	0.20667100
H	0.91897400	2.75058900	0.08286200

PBE0-D3/def2-TZVP：

Zero-point correction= 0.138219 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.100388

Sum of electronic and zero-point Energies= -1213.992759

Sum of electronic and thermal Energies= -1213.982735

Sum of electronic and thermal Enthalpies= -1213.981791

Sum of electronic and thermal Free Energies= -1214.030590

PBE0-D3/def2-TZVP Electronic Energy = -1214.130978 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1214.13399954 a.u.

***E*.3.H$^+$**

N	0.44113000	0.46845600	0.00001000
N	-0.42002800	-0.44451200	-0.00000900
C	1.74731900	0.13851900	0.00000600
C	2.46569600	-1.11112700	0.00000400
C	3.76226400	-0.76341300	-0.00003300
C	2.70319900	1.13628600	0.00004100
H	2.61485800	2.21145100	0.00006700
C	-2.75623600	-1.11599300	-0.00004600
C	-1.77135400	-0.16843100	-0.00001300
C	-2.40126500	1.11020200	0.00000000
C	-3.72139000	0.83759300	0.00001600
H	-2.74165100	-2.19399900	-0.00006800
H	-1.92715200	2.07688800	0.00001100
H	-4.60102300	1.45881900	0.00004100
H	4.67955600	-1.32745100	-0.00006100

H	2.08686600	-2.12048200	0.00000100
O	-3.94082800	-0.50663400	0.00000300
O	3.90567300	0.60354800	0.00001800
H	-0.14732600	-1.42996900	-0.00003100

PBE0-D3/def2-TZVP：

Zero-point correction= 0.144910 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.108789

Sum of electronic and zero-point Energies= -568.181575

Sum of electronic and thermal Energies= -568.172265

Sum of electronic and thermal Enthalpies= -568.171321

Sum of electronic and thermal Free Energies= -568.217696

PBE0-D3/def2-TZVP Electronic Energy = -568.326485 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -568.329469221 a.u.

***Z*.3.H$^+$**

C	-1.47450000	0.54415900	-0.06329800
C	-1.63907700	-0.51748000	-0.90101500
C	-2.56428700	0.53544400	0.85899700
C	1.51528600	0.48483600	-0.08733300
C	2.94739300	0.65349100	-0.07737800
C	3.46078400	-0.55668100	0.17449800
H	3.47592700	1.58006900	-0.22920100
C	1.29458200	-0.87087800	0.15352100
C	-3.28472700	-0.55687500	0.52971700
H	-2.75139100	1.23293800	1.65893700
H	-1.10399300	-0.86692700	-1.76874600
H	-4.17225600	-1.00672300	0.94150400
H	0.41178200	-1.48249800	0.22410500
H	4.45744800	-0.94747700	0.28432700
N	-0.52885500	1.57811400	-0.16593600
N	0.72259800	1.56580500	-0.21584600
O	-2.73123300	-1.19057000	-0.53568100
O	2.44462100	-1.47599900	0.31459300
H	-0.91354300	2.51962400	-0.19599500

PBE0-D3/def2-TZVP：

Zero-point correction= 0.145261 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.108992

Sum of electronic and zero-point Energies= -568.162573

Sum of electronic and thermal Energies= -568.153401

Sum of electronic and thermal Enthalpies= -568.152457

Sum of electronic and thermal Free Energies= -568.198842

PBE0-D3/def2-TZVP Electronic Energy = -568.307834 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -568.310798932 a.u.

***E*.4.H$^+$**

N	0.48433100	0.43960500	0.00000700
N	-0.44937400	-0.40055000	0.00000100
C	1.76988600	0.00980200	0.00001800
C	2.27184300	-1.33935500	0.00001800
C	3.61606700	-1.41277900	0.00003400
C	2.74933300	0.99097400	0.00003500
H	2.56432500	2.05483800	0.00003900
C	-2.76410100	-1.00098700	-0.00001900
C	-1.78896400	-0.03874000	-0.00001000
C	-2.23574800	1.31486800	-0.00001000
C	-3.58257700	1.42553000	-0.00001700
H	-2.62401700	-2.07220700	-0.00001900
H	-1.55935300	2.15806500	-0.00000100
H	-4.16323400	2.33557800	-0.00001700
H	4.22473200	-2.30443500	0.00003800
H	1.65612000	-2.23009900	0.00000900
Se	-4.42621400	-0.23224600	-0.00004700
Se	4.41730500	0.27614500	0.00003600
H	-0.25477900	-1.40358500	0.00000700

PBE0-D3/def2-TZVP：

Zero-point correction= 0.135380 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.095812

Sum of electronic and zero-point Energies= -5220.401722

Sum of electronic and thermal Energies= -5220.390984

Sum of electronic and thermal Enthalpies= -5220.390040

Sum of electronic and thermal Free Energies= -5220.441290

PBE0-D3/def2-TZVP Electronic Energy = -5220.537102 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -5220.54016762 a.u.

***Z*.4.H$^+$**

C	1.48698100	1.13717500	-0.08658100
C	1.53764300	0.04102100	0.72717700
C	2.56382200	1.28261700	-1.00933500
C	-1.54678800	1.12675400	0.19128700
C	-2.90766300	1.41023200	0.56935800
C	-3.76214000	0.38254800	0.41312300
H	-3.19253600	2.38345300	0.94725200
C	-1.35049500	-0.16814400	-0.28495400
C	3.46084200	0.27051000	-0.95333800
H	2.64030400	2.11314100	-1.69972500

H	0.85263900	-0.23094900	1.51530100
H	4.34313700	0.14220900	-1.56169400
H	-0.43907700	-0.61468000	-0.64625500
H	-4.81816100	0.35156200	0.63253300
N	0.53481700	2.17458600	0.03059900
N	-0.70541000	2.18989500	0.22567600
Se	3.01486800	-0.97300800	0.34623700
Se	-2.89763900	-1.10652700	-0.29836400
H	0.92885400	3.11180500	-0.00943100

PBE0-D3/def2-TZVP：

Zero-point correction= 0.135503 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.095620

Sum of electronic and zero-point Energies= -5220.385026

Sum of electronic and thermal Energies= -5220.374366

Sum of electronic and thermal Enthalpies= -5220.373422

Sum of electronic and thermal Free Energies= -5220.424909

PBE0-D3/def2-TZVP Electronic Energy = -5220.520529 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -5220.52352809 a.u.

***E*.5.H$^+$**

N	-0.41693400	-0.47982400	0.00047400
N	0.41797400	0.44488300	-0.02444700
C	-1.77330300	-0.19674700	0.00116800
C	-2.35537700	1.13325500	-0.06641100
C	-3.67386300	0.98788600	-0.04210500
C	-2.72568700	-1.13762000	0.06712300
H	-2.70144100	-2.21470500	0.12796700
C	2.62970400	1.15078000	0.04842200
C	1.74556200	0.13359800	-0.02785400
C	2.46071700	-1.14309100	-0.08381500
C	3.75818100	-0.87877900	-0.03308100
H	2.49399200	2.21998900	0.10777600
H	2.03957100	-2.13381300	-0.16171600
H	4.63301400	-1.50787500	-0.05060200
H	-4.48952300	1.69146200	-0.07191700
H	-1.80752600	2.06002500	-0.12487700
N	-3.99295200	-0.43969800	0.04433200
N	3.95080300	0.57261400	0.06543100
H	-4.57256900	-0.74698500	-0.75172600
H	-4.54756500	-0.65105500	0.88820200
H	4.53311200	0.93946100	-0.70404500
H	4.45276700	0.82975300	0.93133800
H	-0.14167400	-1.46778100	0.02838000

PBE0-D3/def2-TZVP：

Zero-point correction= 0.196455 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.160160

Sum of electronic and zero-point Energies= -529.178874

Sum of electronic and thermal Energies= -529.168966

Sum of electronic and thermal Enthalpies= -529.168022

Sum of electronic and thermal Free Energies= -529.215169

PBE0-D3/def2-TZVP Electronic Energy = -529.375329 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -529.381292217 a.u.

***Z*.5.H$^+$**

C	-1.46181400	0.56204000	-0.03556200
C	-1.46734800	-0.35765400	-1.00185000
C	-2.59388100	0.39327500	0.86256600
C	1.45472900	0.55486400	0.01578300
C	2.68192100	0.47607800	-0.77145600
C	3.33746200	-0.61226600	-0.39231900
H	2.97007200	1.17389300	-1.54191000
C	1.39724700	-0.46332500	0.89126900
C	-3.27627600	-0.66473300	0.44084000
H	-2.81554500	1.00798700	1.72119300
H	-0.84364100	-0.53833800	-1.86304700
H	-4.15952600	-1.16099400	0.80756500
H	0.72591300	-0.71160500	1.69822800
H	4.25714600	-1.06752400	-0.72078300
N	-0.56248000	1.65789800	0.04559600
N	0.66843100	1.68966400	0.00345500
N	-2.62194000	-1.19548600	-0.75451100
N	2.59220000	-1.25441100	0.69040700
H	3.15556400	-1.30079200	1.55357500
H	2.35182600	-2.23182400	0.46455200
H	-2.34662400	-2.18188300	-0.63275800
H	-3.26078000	-1.18463800	-1.56493900
H	-1.00011300	2.58238900	0.12806400

PBE0-D3/def2-TZVP：

Zero-point correction= 0.196692 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.160696

Sum of electronic and zero-point Energies= -529.156448

Sum of electronic and thermal Energies= -529.146672

Sum of electronic and thermal Enthalpies= -529.145728

Sum of electronic and thermal Free Energies= -529.192444

PBE0-D3/def2-TZVP Electronic Energy = -529.353140 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -529.359042475 a.u.

***E*.6.H$^+$**

N	-0.41102000	-0.41657400	-0.00000300
N	0.43348500	0.51528500	0.00000000
C	-1.77145900	-0.17910300	-0.00000600
C	-2.39529600	1.13505900	0.00000000
C	-3.72211300	0.94375800	-0.00000300
C	-2.69938400	-1.16334000	-0.00001600
H	-2.51806100	-2.22908400	-0.00002200
C	2.68967300	1.17459200	0.00000900
C	1.74938200	0.18448400	0.00000200
C	2.41131400	-1.12488000	-0.00000100
C	3.73309000	-0.91210000	0.00000400
H	2.48183600	2.23523600	0.00001100
H	1.93029100	-2.09344000	-0.00000600
H	4.50027700	-1.67343200	0.00000200
H	-4.47800200	1.71614300	0.00000100
H	-1.85850700	2.07172000	0.00000700
H	-4.62726600	-0.81855200	-0.87249400
H	-4.62727800	-0.81856800	0.87244700
H	4.61450000	0.87268900	-0.87056500
H	4.61444400	0.87265600	0.87066400
C	-4.03328100	-0.51637200	-0.00001600
C	4.02586700	0.55281200	0.00002300
H	-0.11624500	-1.39579600	-0.00000200

PBE0-D3/def2-TZVP：

Zero-point correction= 0.189643 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.153083

Sum of electronic and zero-point Energies= -496.325220

Sum of electronic and thermal Energies= -496.315042

Sum of electronic and thermal Enthalpies= -496.314098

Sum of electronic and thermal Free Energies= -496.361780

PBE0-D3/def2-TZVP Electronic Energy = -496.514863 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -496.519041559 a.u.

***Z*.6.H$^+$**

C	1.54324300	0.49802900	-0.02775500
C	1.50653000	-0.72234200	0.58980100
C	2.89052500	0.73079600	-0.55690400
C	-1.53557300	0.43264300	0.04325900
C	-2.92782900	0.75407700	0.35334600
C	-3.67224800	-0.32305700	0.07905400

H	-3.26400900	1.70473300	0.74599000
C	-1.43629000	-0.83875100	-0.41315500
C	3.64439300	-0.33948000	-0.28572700
H	3.17431800	1.62673300	-1.09063100
H	0.68655200	-1.15681800	1.14138600
H	4.67674800	-0.49000200	-0.56664400
H	-0.55572000	-1.37082100	-0.73290100
H	-4.74070200	-0.41554200	0.20855100
N	0.66349800	1.53768000	0.00854500
N	-0.58259000	1.45483200	0.11834000
H	-3.07548600	-1.72241800	-1.45764900
H	-2.85795800	-2.33013200	0.16126400
H	2.78665600	-2.32073800	0.01074500
H	3.26414500	-1.52946800	1.48521600
C	2.84563600	-1.33221700	0.48848200
C	-2.80070600	-1.41273900	-0.43984500
H	-1.00699700	2.37512700	0.22315400

PBE0-D3/def2-TZVP：

Zero-point correction= 0.189492 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.152364

Sum of electronic and zero-point Energies= -496.302382

Sum of electronic and thermal Energies= -496.292206

Sum of electronic and thermal Enthalpies= -496.291262

Sum of electronic and thermal Free Energies= -496.339510

PBE0-D3/def2-TZVP Electronic Energy = -496.491874 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -496.496052660 a.u.

***E*.7.H$^+$**

N	-0.44158400	0.56707400	0.00001500
N	0.40375800	-0.37779500	-0.00000100
C	-1.75844500	0.23884100	-0.00002400
C	-2.37275300	-1.09913900	0.00014700
C	-3.71596600	-0.98791400	0.00003900
C	-2.71477700	1.22936000	-0.00038800
H	-2.40325200	2.27051700	-0.00048600
C	2.66146600	-1.22353800	-0.00030800
C	1.77640500	-0.19079600	-0.00007100
C	2.41614900	1.12182100	0.00013300
C	3.75628800	0.96520500	0.00004300
H	2.32414800	-2.25759500	-0.00045400
H	1.85111500	2.04738400	0.00046300
H	4.41420800	1.83191500	0.00028300
H	-4.34259400	-1.87741400	0.00012000

H	-1.81834000	-2.03427100	0.00052400
H	-4.80441200	0.90145700	0.98360400
H	-4.80640000	0.90184100	-0.98210900
H	4.78018600	-0.94696300	0.98746500
H	4.78172200	-0.94743800	-0.98630400
B	-4.14765700	0.55946300	-0.00005100
B	4.13037200	-0.59748400	-0.00006600
H	0.08462100	-1.34731300	-0.00003700

PBE0-D3/def2-TZVP：

Zero-point correction= 0.173294 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.136344

Sum of electronic and zero-point Energies= -470.104188

Sum of electronic and thermal Energies= -470.093154

Sum of electronic and thermal Enthalpies= -470.092210

Sum of electronic and thermal Free Energies= -470.141138

PBE0-D3/def2-TZVP Electronic Energy = -470.277482 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -470.281194070 a.u.

***Z*.7.H$^+$**

C	-1.54157200	0.34692900	0.10686000
C	-1.44035000	-0.97416900	-0.21815600
C	-2.94443900	0.78271900	0.19835100
C	1.55720800	0.47087400	0.00762000
C	2.86959500	0.74768600	-0.59996200
C	3.71206200	-0.28495400	-0.41782600
H	3.05567100	1.67252700	-1.13953400
C	1.55974300	-0.76208100	0.63261900
C	-3.77663700	-0.23146700	-0.09609900
H	-3.21490200	1.80364400	0.46377600
H	-0.49766300	-1.49722500	-0.29027900
H	-4.85491400	-0.09089200	-0.08272000
H	0.71553600	-1.09830600	1.22288400
H	4.71560800	-0.26902900	-0.83726100
N	-0.58900700	1.36315800	0.23829100
N	0.66641100	1.49103200	0.08490000
H	3.51483400	-1.60233100	1.56242900
H	2.90698700	-2.52870400	-0.05662500
H	-3.13590600	-2.49957000	0.30439100
H	-3.07550100	-1.95240700	-1.58573800
B	-2.91457900	-1.53827800	-0.43600100
B	2.99098000	-1.41393000	0.46319700
H	-1.02724200	2.27077400	0.35992000

PBE0-D3/def2-TZVP：

Zero-point correction= 0.173050 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.135520

Sum of electronic and zero-point Energies= -470.081313

Sum of electronic and thermal Energies= -470.070204

Sum of electronic and thermal Enthalpies= -470.069260

Sum of electronic and thermal Free Energies= -470.118843

PBE0-D3/def2-TZVP Electronic Energy = -470.254362 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -470.258071604 a.u.

***E*.8.H$^+$**

N	-0.42397000	-0.42833300	-0.01106100
N	0.42962300	0.47839000	0.03209500
C	-1.75628400	-0.10145300	-0.02006900
C	-2.37216300	1.24413400	-0.10442600
C	-3.70607100	1.24628300	-0.08445200
C	-2.62021500	-1.14092700	0.05583900
H	-2.35788700	-2.18773000	0.11590800
C	2.71358700	1.15435400	0.08166300
C	1.79003800	0.17968300	0.01869400
C	2.27093700	-1.20934600	-0.07514100
C	3.60089800	-1.32036700	-0.08591700
H	2.55903100	2.22257700	0.14820400
H	1.58535400	-2.04415200	-0.13126600
H	4.17708100	-2.23095600	-0.15029100
H	-4.35351100	2.10854200	-0.14163600
H	-1.80304800	2.16149300	-0.19079800
P	4.28749100	0.31540800	0.02656400
P	-4.26529800	-0.43488500	0.04791400
H	5.04261500	0.70318600	-1.08807900
H	5.03601600	0.54821000	1.18755000
H	-5.00848200	-0.89521300	-1.04759500
H	-4.95319300	-0.72953600	1.23286700
H	0.17918900	1.47117500	0.08358800

PBE0-D3/def2-TZVP：

Zero-point correction= 0.174939 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.137033

Sum of electronic and zero-point Energies= -1102.222206

Sum of electronic and thermal Energies= -1102.210854

Sum of electronic and thermal Enthalpies= -1102.209909

Sum of electronic and thermal Free Energies= -1102.260112

PBE0-D3/def2-TZVP Electronic Energy = -1102.397145 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1102.40118700 a.u.

***Z*.8.H$^+$**

C	-1.44300700	0.78005800	0.03896200
C	-1.45049600	-0.12546000	-0.95589000
C	-2.52404400	0.68499500	1.04356400
C	1.46242400	0.78112300	-0.00771600
C	2.50613100	0.67027100	-1.04289200
C	3.33817400	-0.35767600	-0.86151600
H	2.55798700	1.36109900	-1.87469500
C	1.46987800	-0.10833000	0.98888300
C	-3.36049000	-0.33632100	0.85115200
H	-2.58585500	1.38894200	1.86322700
H	-0.80585300	-0.17903200	-1.82063200
H	-4.20141300	-0.61439900	1.46836700
H	0.83293100	-0.16085300	1.85954500
H	4.16140100	-0.64946700	-1.49593900
N	-0.66054100	1.92892500	0.04152600
N	0.56405600	1.89854800	-0.04855000
H	3.80306200	-1.15726600	1.64894200
H	2.41963900	-2.51248500	0.43479800
H	-2.47600900	-2.50525600	-0.45609100
H	-3.80750600	-1.10477000	-1.66396000
P	-2.85997400	-1.16956000	-0.63432900
P	2.84546800	-1.19136900	0.62748100
H	1.00317600	2.82314200	-0.13895600

PBE0-D3/def2-TZVP：

Zero-point correction= 0.174978 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.136645

Sum of electronic and zero-point Energies= -1102.203052

Sum of electronic and thermal Energies= -1102.191634

Sum of electronic and thermal Enthalpies= -1102.190690

Sum of electronic and thermal Free Energies= -1102.241385

PBE0-D3/def2-TZVP Electronic Energy = -1102.378030 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1102.38198143 a.u.

***E*.9.H$^+$**

N	-0.42310400	-0.42571700	0.00000800
N	0.43563000	0.48786900	-0.00001800
C	-1.79275800	-0.16587800	0.00002100
C	-2.29041700	1.22195800	0.00000100
C	-3.62409000	1.34298700	0.00002300
C	-2.68528500	-1.17585200	0.00005300
H	-2.39688900	-2.21956600	0.00006900

C	2.65525300	1.17504400	-0.00006200
C	1.76270300	0.14866800	-0.00003200
C	2.32312300	-1.22429900	-0.00001700
C	3.65925200	-1.30552600	-0.00003400
H	2.31289200	2.20183800	-0.00007400
H	1.69100200	-2.10726300	0.00000800
H	4.16769900	-2.26105800	-0.00002500
H	-4.10648800	2.31170500	0.00000600
H	-1.58903400	2.04767300	-0.00002700
Si	-4.37621400	-0.36465100	0.00009100
Si	4.37478600	0.41737900	-0.00007400
H	-5.15235800	-0.69640200	-1.21873200
H	-5.15219600	-0.69632500	1.21904200
H	5.13098500	0.77773400	-1.22219900
H	5.13101800	0.77777600	1.22201900
H	-0.15100900	-1.41198300	0.00002100

PBE0-D3/def2-TZVP：

Zero-point correction= 0.168380 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.129666

Sum of electronic and zero-point Energies= -998.938927

Sum of electronic and thermal Energies= -998.926915

Sum of electronic and thermal Enthalpies= -998.925971

Sum of electronic and thermal Free Energies= -998.977641

PBE0-D3/def2-TZVP Electronic Energy = -999.107307 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -999.111079078 a.u.

***Z*.9.H$^+$**

C	1.41395700	-0.26084200	0.89950700
C	1.48166300	0.72769600	-0.00086200
C	2.63898400	0.79427700	-0.91485500
H	2.70550800	1.59083400	-1.65001500
C	3.53441600	-0.18989700	-0.76884500
C	-1.42751500	-0.20877600	-0.89730600
C	-1.47415900	0.74864100	0.05440200
C	-2.63738800	0.76370400	0.96961000
H	-2.70154800	1.53534800	1.72987800
C	-3.52406600	-0.22276800	0.79304000
H	0.61766300	-0.36283100	1.62388900
H	4.41442200	-0.25937400	-1.39430700
H	-0.64801700	-0.26345300	-1.64564500
H	-4.39735000	-0.32501800	1.42375100
Si	2.95220100	-1.29895800	0.61337900
Si	-2.97052700	-1.24947000	-0.66019900

H	-2.62419400	-2.65665900	-0.34307200
H	-3.87835500	-1.18566800	-1.83043200
H	2.60900800	-2.67750500	0.18874900
H	3.83585900	-1.31546300	1.80301200
N	-0.66661900	1.87901800	0.06440700
N	0.56481800	1.82671600	-0.05012400
H	1.00082300	2.74543400	-0.15846300

PBE0-D3/def2-TZVP：

Zero-point correction= 0.167927 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.128748

Sum of electronic and zero-point Energies= -998.918001

Sum of electronic and thermal Energies= -998.905903

Sum of electronic and thermal Enthalpies= -998.904958

Sum of electronic and thermal Free Energies= -998.957180

PBE0-D3/def2-TZVP Electronic Energy = -999.085928 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -999.089585737 a.u.

***E*.10.H$^+$**

N	0.44191800	-0.46015300	0.00010100
N	-0.44509300	0.41382400	0.00006000
C	1.79590200	-0.12144600	0.00007500
C	2.21627800	1.28949400	0.00000200
C	3.53017500	1.50155700	-0.00003300
C	2.72743900	-1.08686900	0.00011300
H	2.57864600	-2.15750800	0.00015200
C	-2.65543400	1.05060900	-0.00000500
C	-1.76531700	0.03344000	0.00000800
C	-2.29843500	-1.34792100	-0.00004800
C	-3.62283600	-1.47272100	-0.00010100
H	-2.41500400	2.10412100	0.00002200
H	-1.65978000	-2.22329100	-0.00004700
H	-4.19246500	-2.38941000	-0.00014400
H	4.03906400	2.45304800	-0.00009000
H	1.48175700	2.08425600	-0.00002400
As	4.40239100	-0.18516200	0.00005400
As	-4.39259900	0.26307400	-0.00008900
H	5.19690300	-0.48135500	1.22478500
H	5.19695600	-0.48152100	-1.22460000
H	-5.15921500	0.61486000	1.22791600
H	-5.15915000	0.61493400	-1.22811300
H	0.22475300	-1.46178500	0.00011800

PBE0-D3/def2-TZVP:

Zero-point correction= 0.169614 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.129137

Sum of electronic and zero-point Energies= -4890.925208

Sum of electronic and thermal Energies= -4890.912924

Sum of electronic and thermal Enthalpies= -4890.911980

Sum of electronic and thermal Free Energies= -4890.965686

PBE0-D3/def2-TZVP Electronic Energy = -4891.094823 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4891.09887153 a.u.

***Z*.10.H$^+$**

C	1.46888600	1.11568900	-0.11857900
C	1.54238800	0.22890500	0.87426200
C	2.42488200	1.04611200	-1.23939600
C	-1.44288200	1.10958600	0.14841500
C	-2.43638900	1.05354500	1.24316800
C	-3.32153500	0.06224800	1.18221300
H	-2.40193400	1.78128500	2.04465000
C	-1.51443300	0.20379600	-0.83976400
C	3.30417200	0.04802100	-1.18844300
H	2.38227300	1.76135900	-2.05233800
H	0.96435000	0.17422500	1.78503900
H	4.06790500	-0.19071300	-1.91239700
H	-0.93077600	0.14671500	-1.74634800
H	-4.10252000	-0.16392500	1.89170500
N	0.55947500	2.22838700	-0.08716800
N	-0.65585400	2.25791200	0.08907000
As	2.98094200	-0.93105900	0.40485700
As	-2.99262900	-0.91468100	-0.40960500
H	2.51492600	-2.33125600	0.19640500
H	4.08112500	-0.87884200	1.40720000
H	-4.07998800	-0.82460400	-1.42400600
H	-2.57276800	-2.33139900	-0.21560500
H	0.98719500	3.15506600	-0.20218800

PBE0-D3/def2-TZVP:

Zero-point correction= 0.169199 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.128749

Sum of electronic and zero-point Energies= -4890.906356

Sum of electronic and thermal Energies= -4890.894063

Sum of electronic and thermal Enthalpies= -4890.893119

Sum of electronic and thermal Free Energies= -4890.946806

PBE0-D3/def2-TZVP Electronic Energy = -4891.075555 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4891.07948446 a.u.

***E*.11.H$^+$**

N	-0.45657500	0.46264700	0.00002400
N	0.43964300	-0.41309200	0.00000700
C	-1.77093000	0.07134000	0.00002100
C	-2.26637900	-1.32493700	-0.00005300
C	-3.59167000	-1.49169600	-0.00006200
C	-2.69119000	1.07080300	0.00008000
H	-2.37983500	2.10744400	0.00011500
C	2.71904700	-1.08451800	-0.00003400
C	1.80060300	-0.10069000	-0.00001700
C	2.23436700	1.30717000	-0.00002500
C	3.55479600	1.51198400	-0.00005500
H	2.46206700	-2.13645200	-0.00003500
H	1.49021400	2.09475500	-0.00000600
H	3.98378100	2.50526200	-0.00006100
H	-4.04673700	-2.47344200	-0.00011300
H	-1.58798800	-2.17290300	-0.00009800
Ge	-4.46474500	0.24657400	0.00008300
Ge	4.46537400	-0.20743900	-0.00006400
H	-5.24912900	0.57795700	1.26979600
H	-5.24933800	0.57819100	-1.26943300
H	5.26707800	-0.51348400	1.26674600
H	5.26705900	-0.51351100	-1.26688000
H	0.20935900	-1.40975700	0.00000500

PBE0-D3/def2-TZVP:

Zero-point correction= 0.165382 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.124689

Sum of electronic and zero-point Energies= -4573.648910

Sum of electronic and thermal Energies= -4573.636256

Sum of electronic and thermal Enthalpies= -4573.635312

Sum of electronic and thermal Free Energies= -4573.689603

PBE0-D3/def2-TZVP Electronic Energy = -4573.814292 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4573.81813147 a.u.

***Z*.11.H$^+$**

C	1.47484000	1.09514300	-0.11998100
C	1.49797500	0.14684900	0.82124900
C	2.51644800	1.13753300	-1.16372500
C	-1.47058700	1.10763900	0.16729700
C	-2.57487500	1.15762900	1.15044100
C	-3.48194900	0.18033400	1.08288400
H	-2.58472800	1.95865600	1.88271400
C	-1.46188000	0.12520700	-0.75705700

C	3.43777000	0.17168300	-1.11297500
H	2.48426300	1.91379900	-1.92271100
H	0.78044600	0.07842800	1.62723300
H	4.23611500	0.09284000	-1.83858900
H	-0.72188800	0.05242700	-1.54283200
H	-4.31198000	0.11085400	1.77324600
N	0.55131900	2.19297600	-0.10482600
N	-0.66817800	2.24178400	0.10178400
H	2.64005100	-2.40232500	0.05056500
H	4.09721900	-0.94088800	1.52558700
H	-4.04362300	-0.93783200	-1.56862200
H	-2.65266900	-2.41246500	-0.04814200
Ge	-3.04080700	-0.97732500	-0.41369400
Ge	3.05001000	-0.97271000	0.41137800
H	0.97386100	3.11222100	-0.25182000

PBE0-D3/def2-TZVP:

Zero-point correction= 0.164701 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.123191

Sum of electronic and zero-point Energies= -4573.628060

Sum of electronic and thermal Energies= -4573.615263

Sum of electronic and thermal Enthalpies= -4573.614319

Sum of electronic and thermal Free Energies= -4573.669570

PBE0-D3/def2-TZVP Electronic Energy = -4573.792761 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4573.79646636 a.u.

***E*.12.H$^+$**

N	0.43788700	-0.35986400	-0.00000800
N	-0.46881600	0.51500200	-0.00002800
C	1.80864400	-0.07561600	-0.00000300
C	2.25658300	1.32822000	-0.00003400
C	3.58185300	1.54103000	-0.00010100
C	2.70204100	-1.08900300	0.00002000
H	2.32778600	-2.11150400	-0.00000600
C	-2.72413500	1.10011300	-0.00001500
C	-1.78055100	0.11184000	-0.00001000
C	-2.23474100	-1.29921800	0.00002700
C	-3.55686500	-1.52806200	0.00003600
H	-2.34334100	2.11889100	-0.00005300
H	-1.51184500	-2.11520900	0.00004000
H	-3.88891200	-2.56448400	0.00005900
H	3.92846000	2.57267100	-0.00009000
H	1.49969500	2.10818600	0.00001000
H	5.38355400	-0.56236600	1.32505700

H	5.38358800	-0.56265500	-1.32502400
H	-5.38825400	0.54480200	1.32673600
H	-5.38840700	0.54483400	-1.32652700
Ga	4.54470200	-0.23450000	-0.00003300
Ga	-4.55450200	0.22671100	0.00005000
H	0.20100900	-1.35348700	0.00001800

PBE0-D3/def2-TZVP:

Zero-point correction= 0.156750 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.114897

Sum of electronic and zero-point Energies= -4269.631650

Sum of electronic and thermal Energies= -4269.617985

Sum of electronic and thermal Enthalpies= -4269.617041

Sum of electronic and thermal Free Energies= -4269.673503

PBE0-D3/def2-TZVP Electronic Energy = -4269.788400 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4269.79237613 a.u.

***Z*.12.H$^+$**

C	1.54928400	0.97451100	-0.25269600
C	1.39826400	-0.33130800	0.05524700
C	2.91914100	1.52200500	-0.43554000
C	-1.53139100	1.07523600	0.08674300
C	-2.63971300	1.34721300	1.03307800
C	-3.65404500	0.47333200	1.08648900
H	-2.54955900	2.23625200	1.65684500
C	-1.60948000	-0.02168200	-0.71806900
C	3.96165400	0.70539100	-0.24629800
H	3.01361000	2.57455800	-0.71453700
H	0.41347200	-0.77494900	0.11156600
H	4.96086600	1.11526700	-0.37461800
H	-0.83521300	-0.16882600	-1.46594800
H	-4.44646800	0.65464400	1.80973900
N	0.57018100	1.99660300	-0.34853100
N	-0.65580600	2.12226400	-0.08669500
H	3.53555000	-2.28244000	-0.80110100
H	3.59003200	-1.59091400	1.75602600
H	-4.38061400	-0.95701300	-1.52051600
H	-3.11072600	-2.45014900	0.26579100
Ga	3.26302200	-1.11457000	0.26284400
Ga	-3.35820100	-0.96799200	-0.28868500
H	0.99667300	2.90273200	-0.52929300

PBE0-D3/def2-TZVP:

Zero-point correction= 0.156370 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.113924

Sum of electronic and zero-point Energies= -4269.608451

Sum of electronic and thermal Energies= -4269.594725

Sum of electronic and thermal Enthalpies= -4269.593781

Sum of electronic and thermal Free Energies= -4269.650897

PBE0-D3/def2-TZVP Electronic Energy = -4269.764821 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4269.76875430 a.u.

***E*.13.H$^+$**

N	0.42111800	-0.38015100	0.00002900
N	-0.44627700	0.53366600	-0.00001700
C	1.80364900	-0.15636500	0.00002500
C	2.30876400	1.23077300	-0.00002300
C	3.64303800	1.39545700	-0.00004800
C	2.65244600	-1.20863000	0.00006200
H	2.22142100	-2.20891100	0.00008800
C	-2.67615600	1.21705000	-0.00008300
C	-1.77556400	0.18863800	-0.00001600
C	-2.28873500	-1.20479700	0.00004600
C	-3.62058100	-1.38498600	0.00001900
H	-2.23954000	2.21346300	-0.00012900
H	-1.59518100	-2.04675700	0.00011700
H	-3.97232000	-2.41545000	0.00007000
H	4.00868900	2.42104300	-0.00007700
H	1.57860000	2.03661500	-0.00003100
Al	-4.52431100	0.40398500	-0.00006800
Al	4.50652400	-0.41474600	0.00005200
H	-5.35925700	0.76543600	1.34591800
H	-5.35928800	0.76535800	-1.34605300
H	5.35062500	-0.78268400	1.34227600
H	5.35077100	-0.78288700	-1.34201800
H	0.14165900	-1.36276500	0.00006800

PBE0-D3/def2-TZVP:

Zero-point correction= 0.156994 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.117121

Sum of electronic and zero-point Energies= -905.096296

Sum of electronic and thermal Energies= -905.083028

Sum of electronic and thermal Enthalpies= -905.082084

Sum of electronic and thermal Free Energies= -905.136168

PBE0-D3/def2-TZVP Electronic Energy = -905.253289 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -905.257056312 a.u.

***Z*.13.H$^+$**

C	-1.54483500	0.68654500	0.02262500
C	-1.59572700	-0.39719300	-0.80190400
C	-2.69915900	0.97198000	0.91197200
C	1.55523700	0.56708700	-0.16402900
C	2.93315300	1.09106000	-0.36722500
C	3.97036500	0.27286900	-0.14267400
H	3.03393800	2.12986800	-0.69452800
C	1.37964100	-0.72197300	0.19613500
C	-3.73991600	0.12436900	0.89861900
H	-2.61779800	1.85307200	1.54941600
H	-0.76759200	-0.55114100	-1.48899600
H	-4.55791000	0.33788700	1.58446400
H	0.37909300	-1.12637100	0.27864800
H	4.96574300	0.68444300	-0.29672600
N	-0.64876800	1.72699900	-0.09709600
N	0.58657500	1.59857800	-0.29647700
Al	-3.38873200	-1.27615200	-0.48465800
Al	3.23067100	-1.49468500	0.43271800
H	3.54534700	-1.91980500	1.97163200
H	3.50874800	-2.73176600	-0.58822300
H	-3.22612000	-2.80432400	0.04940100
H	-4.35072800	-1.20086800	-1.79358500
H	1.02485800	2.50238200	-0.46237900

PBE0-D3/def2-TZVP:

Zero-point correction= 0.156382 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.115625

Sum of electronic and zero-point Energies= -905.073252

Sum of electronic and thermal Energies= -905.059822

Sum of electronic and thermal Enthalpies= -905.058878

Sum of electronic and thermal Free Energies= -905.114009

PBE0-D3/def2-TZVP Electronic Energy = -905.229634 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -905.233344691 a.u.

***E*.14.H$^+$**

N	-0.41749200	-0.42522600	0.00001800
N	0.42404900	0.50676600	-0.00001800
C	-1.79844100	-0.20859600	0.00002100
C	-2.30222600	1.19268500	0.00000600
C	-3.62911100	1.38108400	0.00002600
C	-2.64161800	-1.25882800	0.00004600
H	-2.25753100	-2.27318600	0.00007300
C	2.61739200	1.25933800	-0.00007100

C	1.76289700	0.20182900	-0.00001100
C	2.32355600	-1.18562600	0.00006300
C	3.65485500	-1.34321100	0.00007100
H	2.18807700	2.25455500	-0.00011300
H	1.65561400	-2.04504800	0.00011200
H	4.06098000	-2.34812800	0.00013100
H	-4.01480500	2.39382900	0.00002800
H	-1.56677100	1.99122400	-0.00001600
Al	-4.41957000	-0.40308100	-0.00000200
Al	4.42708900	0.44599800	-0.00006000
H	-5.87071600	-1.00876300	-0.00017100
H	5.86349300	1.07986500	-0.00019700
H	-0.12580400	-1.40510100	0.00004900

PBE0-D3/def2-TZVP:

Zero-point correction= 0.146023 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.106672

Sum of electronic and zero-point Energies= -903.619327

Sum of electronic and thermal Energies= -903.606868

Sum of electronic and thermal Enthalpies= -903.605923

Sum of electronic and thermal Free Energies= -903.658677

PBE0-D3/def2-TZVP Electronic Energy = -903.765350 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -903.768948663 a.u.

***Z*.14.H$^+$**

C	-1.47755500	0.64437600	-0.05816600
C	-1.38183200	-0.30734200	-0.99029700
C	-2.62501300	0.71652000	0.89211400
C	1.46401300	0.66590700	-0.00996400
C	2.59277100	0.64288200	-0.99061000
C	3.54347600	-0.28816500	-0.84447300
H	2.56515100	1.38105000	-1.78912600
C	1.41645000	-0.20451600	1.01845000
C	-3.57692700	-0.22026800	0.80111500
H	-2.62178000	1.51775000	1.62937900
H	-0.56006100	-0.32647300	-1.69513600
H	-4.40866200	-0.19926500	1.49493100
H	0.62567900	-0.14476300	1.75674600
H	4.35118800	-0.33618100	-1.56520600
N	-0.56729700	1.75737500	0.01683000
N	0.66613700	1.80757000	-0.06465700
Al	-3.01827800	-1.37205400	-0.67362500
Al	3.05951900	-1.26811600	0.77054200
H	3.67341500	-2.44292300	1.61795400

H	-3.57649800	-2.65330700	-1.39409500
H	-1.00873100	2.67533200	0.11040900

PBE0-D3/def2-TZVP:

Zero-point correction= 0.145564 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.105557

Sum of electronic and zero-point Energies= -903.598952

Sum of electronic and thermal Energies= -903.586382

Sum of electronic and thermal Enthalpies= -903.585438

Sum of electronic and thermal Free Energies= -903.638960

PBE0-D3/def2-TZVP Electronic Energy = -903.744516 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -903.747968437 a.u.

***E*.15.H$^+$**

N	-0.43749600	-0.41735500	0.00009600
N	0.44669600	0.47510700	0.00001400
C	-1.80502100	-0.13418300	0.00002400
C	-2.24339500	1.28874300	-0.00016000
C	-3.55756400	1.53061300	-0.00023800
C	-2.69938000	-1.13773600	0.00011200
H	-2.38543800	-2.17547500	0.00023800
C	2.66894300	1.12607100	0.00000100
C	1.76846400	0.11042800	0.00003200
C	2.27030600	-1.29903000	0.00007300
C	3.59106300	-1.50521600	0.00009900
H	2.30202600	2.14576100	-0.00002700
H	1.57239000	-2.13314800	0.00008800
H	3.98388600	-2.51479300	0.00014100
H	-3.92626900	2.54907800	-0.00037600
H	-1.47750000	2.05712700	-0.00022500
H	-5.91646100	-0.76300800	0.00000800
H	5.90329700	0.83471600	-0.00001600
Ga	-4.47122300	-0.21575000	-0.00004600
Ga	4.47480200	0.25210700	0.00003100
H	-0.19178900	-1.40971700	0.00020200

PBE0-D3/def2-TZVP:

Zero-point correction= 0.145813 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.104820

Sum of electronic and zero-point Energies= -4268.162718

Sum of electronic and thermal Energies= -4268.149997

Sum of electronic and thermal Enthalpies= -4268.149053

Sum of electronic and thermal Free Energies= -4268.203711

PBE0-D3/def2-TZVP Electronic Energy = -4268.308531 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4268.31206560 a.u.

***Z*.15.H$^+$**

C	-1.46319900	1.03431300	0.15272500
C	-1.50188100	0.13782800	-0.84995700
C	-2.51400700	1.03449500	1.21709600
C	1.47845100	1.02397200	-0.08377000
C	2.54417600	1.10670600	-1.12460000
C	3.50517300	0.18083400	-1.10485200
H	2.47752500	1.90223300	-1.86396100
C	1.47636800	0.07083300	0.84841700
C	-3.46430900	0.09895900	1.16254400
H	-2.43342100	1.78873500	1.99572700
H	-0.78330600	0.15966200	-1.66011000
H	-4.22549900	0.04138500	1.93084100
H	0.72511300	0.02202700	1.62619200
H	4.28946700	0.18297500	-1.85140300
N	-0.66507400	2.17394700	0.11784700
N	0.55650300	2.12635100	-0.07980500
H	3.71509700	-2.25784400	1.09634100
H	-3.76833900	-2.14319300	-1.22472200
Ga	-3.12813200	-0.95911400	-0.46375400
Ga	3.10933500	-1.00770500	0.41859100
H	0.98143600	3.04565900	-0.22077800

PBE0-D3/def2-TZVP:

Zero-point correction= 0.145253 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.103592

Sum of electronic and zero-point Energies= -4268.141841

Sum of electronic and thermal Energies= -4268.128998

Sum of electronic and thermal Enthalpies= -4268.128054

Sum of electronic and thermal Free Energies= -4268.183502

PBE0-D3/def2-TZVP Electronic Energy = -4268.287094 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4268.29048513 a.u.

***E*.16.H$^+$**

N	-0.43070600	0.42281700	-0.00019600
N	0.44074200	-0.47573300	-0.00018500
C	-1.75485600	0.08018400	-0.00009400
C	-2.31090000	-1.31919600	0.00005100
C	-3.63791600	-1.47161900	0.00008700
C	-2.62898700	1.10987300	-0.00011300
H	-2.34115100	2.15168300	-0.00024900
C	2.71537500	-1.14702900	-0.00008400

C	1.79670400	-0.17042600	-0.00012600
C	2.22554900	1.26602500	-0.00011000
C	3.53664400	1.51137200	-0.00006200
H	2.52461600	-2.21120200	-0.00009900
H	1.46740500	2.03999200	-0.00012800
H	3.98773700	2.49168400	-0.00004300
H	-4.15119100	-2.42126100	0.00016000
H	-1.65733700	-2.18529900	0.00013700
H	-5.75835900	0.89244600	0.00054700
H	5.80779700	-0.70681100	0.00015200
Ge	4.38823300	-0.18765000	0.00000300
Ge	-4.38201400	0.27001400	0.00015500
H	0.20156900	-1.47157000	-0.00016400

PBE0-D3/def2-TZVP:

Zero-point correction= 0.149620 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.109257

Sum of electronic and zero-point Energies= -4571.982649

Sum of electronic and thermal Energies= -4571.970437

Sum of electronic and thermal Enthalpies= -4571.969493

Sum of electronic and thermal Free Energies= -4572.023012

PBE0-D3/def2-TZVP Electronic Energy = -4572.132269 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4572.13567245 a.u.

***Z*.16.H$^+$**

C	1.48559800	1.03338100	-0.06162400
C	1.45570900	0.04265100	0.82536300
C	2.59803700	1.12588600	-1.06723400
C	-1.44830300	1.02146200	0.13671600
C	-2.47779500	0.98453300	1.23862600
C	-3.42465700	0.05081000	1.16272100
H	-2.39289200	1.70312100	2.04629800
C	-1.53101300	0.15450800	-0.88400300
C	3.52950900	0.17345700	-1.04150700
H	2.59775800	1.94313000	-1.78150100
H	0.74617900	-0.10629000	1.62560500
H	4.37166900	0.10077400	-1.71227200
H	-0.90589400	0.13179500	-1.76434100
H	-4.20344000	-0.11210100	1.89196100
N	0.56722900	2.13224400	-0.04910700
N	-0.65195800	2.15476900	0.11525200
H	-3.72859000	-2.03301300	-1.21118100
H	3.58154800	-2.23779300	1.03214500
Ge	3.04013900	-0.98423800	0.38323900

Ge	-3.08964700	-0.89016700	-0.45456600
H	0.98849700	3.06212700	-0.16163200

PBE0-D3/def2-TZVP:

Zero-point correction= 0.148791 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.108001

Sum of electronic and zero-point Energies= -4571.964192

Sum of electronic and thermal Energies= -4571.951829

Sum of electronic and thermal Enthalpies= -4571.950885

Sum of electronic and thermal Free Energies= -4572.004982

PBE0-D3/def2-TZVP Electronic Energy = -4572.112983 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4572.11626180 a.u.

***E*.17.H$^+$**

N	0.40590400	-0.43544200	0.01170500
N	-0.42594600	0.50080600	-0.02846700
C	1.74279800	-0.15891500	0.02122600
C	2.38819900	1.20497000	0.08332200
C	3.72892100	1.24967300	0.06459400
C	2.57507000	-1.22484700	-0.03366000
H	2.23763500	-2.25113000	-0.07487900
C	-2.69023200	1.23877300	-0.06901400
C	-1.78910000	0.24288100	-0.02125400
C	-2.27826000	-1.17655100	0.05049600
C	-3.60683100	-1.34389800	0.06256300
H	-2.47162900	2.29668300	-0.11758800
H	-1.55837100	-1.98548000	0.08846100
H	-4.09774400	-2.30393200	0.11245600
H	4.30215900	2.16361300	0.11013000
H	1.79638600	2.11212900	0.14875700
Si	4.27374800	-0.46797400	-0.04319400
Si	-4.29269800	0.33157000	-0.01803300
H	-5.65321000	0.87347500	-0.03708700
H	5.57522600	-1.13205300	-0.13313300
H	-0.14824900	1.48628200	-0.07224300

PBE0-D3/def2-TZVP:

Zero-point correction= 0.151717 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.113242

Sum of electronic and zero-point Energies= -997.248068

Sum of electronic and thermal Energies= -997.236376

Sum of electronic and thermal Enthalpies= -997.235432

Sum of electronic and thermal Free Energies= -997.286544

PBE0-D3/def2-TZVP Electronic Energy = -997.399786 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -997.403326872 a.u.

***Z*.17.H$^+$**

C	-1.37711300	-0.35172200	-0.91551000
C	-1.48445600	0.66451300	-0.05952900
C	-2.69056600	0.75038800	0.83775400
H	-2.77670400	1.57355900	1.53972200
C	-3.58959600	-0.23325600	0.72079300
C	1.49015700	-0.15578000	1.04137400
C	1.44994800	0.67224300	-0.01890200
C	2.55550800	0.59162000	-1.04699500
H	2.52602600	1.26382000	-1.89713400
C	3.49480300	-0.33516700	-0.83310400
H	-0.60039000	-0.51149800	-1.64911400
H	-4.48999400	-0.31147700	1.31079200
H	0.81482000	-0.14543700	1.88447300
H	4.32540600	-0.52745700	-1.49537500
Si	-2.92663000	-1.30929200	-0.57561000
Si	3.02618100	-1.11324200	0.73737700
H	-3.38778400	-2.54116000	-1.21955600
H	3.62668100	-2.16670700	1.55931500
N	0.64879900	1.79546100	-0.08615700
N	-0.57900400	1.77088900	-0.01486200
H	-1.01245000	2.70034300	0.05398300

PBE0-D3/def2-TZVP:

Zero-point correction= 0.151645 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.112810

Sum of electronic and zero-point Energies= -997.229282

Sum of electronic and thermal Energies= -997.217549

Sum of electronic and thermal Enthalpies= -997.216604

Sum of electronic and thermal Free Energies= -997.268117

PBE0-D3/def2-TZVP Electronic Energy = -997.380927 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -997.384376091 a.u.

***E*.18.H$^+$**

N	0.40252000	0.53022500	-0.00000500
N	-0.40145500	-0.45286600	0.00000100
C	1.72532800	0.26893500	0.00000900
C	2.43135200	-1.06583800	-0.00002100
C	3.76224200	-0.90374400	0.00007600
C	2.61640800	1.29563800	0.00012300
H	2.29981800	2.33051200	0.00018200
C	-2.65093400	-1.28588900	-0.00004700

C	-1.75987800	-0.27485100	-0.00002600
C	-2.39619600	1.08287100	-0.00005500
C	-3.72910700	0.96228900	-0.00009200
H	-2.38002300	-2.33349400	-0.00003000
H	-1.80645100	1.99054000	-0.00006500
H	-4.39324300	1.81620500	-0.00012700
H	4.44724400	-1.74125600	0.00012600
H	1.92145700	-2.02365200	-0.00004000
B	-4.06494400	-0.57034500	-0.00010800
B	4.06332900	0.62501800	0.00008400
H	5.10828100	1.18821500	0.00054000
H	-5.12854100	-1.10114300	-0.00028000
H	-0.06321400	-1.41727500	0.00003100

PBE0-D3/def2-TZVP:

Zero-point correction= 0.158391 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.120244

Sum of electronic and zero-point Energies= -468.576783

Sum of electronic and thermal Energies= -468.565793

Sum of electronic and thermal Enthalpies= -468.564849

Sum of electronic and thermal Free Energies= -468.614930

PBE0-D3/def2-TZVP Electronic Energy = -468.735174 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -468.738498385 a.u.

***Z*.18.H$^+$**

C	1.48859600	0.43658400	0.09309200
C	1.61141800	-0.71385200	0.81140300
C	2.71184200	0.67348100	-0.75649700
C	-1.51254600	0.29432800	0.19704200
C	-2.93934700	0.69949500	-0.08346400
C	-3.69763400	-0.35855900	-0.38373100
H	-3.24748600	1.74023200	-0.05379400
C	-1.35480100	-1.04547700	0.13238300
C	3.59159900	-0.33030200	-0.64374300
H	2.78773400	1.55940600	-1.37680100
H	0.95569000	-0.98133800	1.62800200
H	4.50822800	-0.36995700	-1.21689500
H	-0.48625700	-1.60274800	0.43710900
H	-4.74392000	-0.27597100	-0.64380700
N	0.63017900	1.45954800	0.25393700
N	-0.62127800	1.33017900	0.41757200
B	3.00967500	-1.34730000	0.37773000
B	-2.74495800	-1.59271300	-0.41255700
H	-2.94244700	-2.68596100	-0.83555500

H	3.45580000	-2.37854700	0.76349800
H	-1.06800400	2.23267300	0.57290300

PBE0-D3/def2-TZVP:

Zero-point correction= 0.158316 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.120853

Sum of electronic and zero-point Energies= -468.554208

Sum of electronic and thermal Energies= -468.543324

Sum of electronic and thermal Enthalpies= -468.542380

Sum of electronic and thermal Free Energies= -468.591670

PBE0-D3/def2-TZVP Electronic Energy = -468.712523 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -468.715882377 a.u.

***E*.AB.2H$^+$**

N	-0.48281600	-0.42156700	-0.10555500
C	-1.82359600	-0.15650200	-0.04616500
C	-2.66809600	-1.28545300	-0.10918400
C	-4.02781200	-1.10033300	-0.04702000
H	-4.69153500	-1.95374200	-0.09203300
C	-4.54282600	0.18780600	0.07806700
H	-5.61526100	0.33180200	0.13409400
C	-3.69641700	1.30442300	0.14362600
H	-4.11917000	2.29524800	0.24820700
C	-2.33611300	1.14759300	0.08650900
N	0.48285000	0.42158400	-0.10538900
C	1.82359100	0.15653000	-0.04603700
C	2.66811200	1.28545500	-0.10910100
C	4.02782100	1.10032000	-0.04705600
H	4.69156200	1.95371400	-0.09213300
C	4.54281300	-0.18784000	0.07796100
H	5.61524700	-0.33188500	0.13386400
C	3.69639900	-1.30443000	0.14361800
H	4.11914900	-2.29526200	0.24813900
C	2.33608100	-1.14758200	0.08665300
H	-2.25165000	-2.28394300	-0.19772100
H	-1.70127600	2.02393200	0.15516500
H	2.25167200	2.28394800	-0.19760800
H	1.70123500	-2.02388300	0.15546500
H	0.20027300	1.39873400	-0.14497000
H	-0.20022500	-1.39870400	-0.14507900

PBE0-D3/def2-TZVP：

Zero-point correction= 0.219141 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.181964

Sum of electronic and zero-point Energies= -572.776541

Sum of electronic and thermal Energies= -572.765652

Sum of electronic and thermal Enthalpies= -572.764708

Sum of electronic and thermal Free Energies= -572.813717

PBE0-D3/def2-TZVP Electronic Energy = -572.995681 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -573.110280047 a.u.

***Z*.AB.2H$^+$**

N	0.63793600	1.59742000	-0.06697600
C	1.57185200	0.59537300	0.00930500
C	2.83417600	0.92741800	-0.52354800
C	3.85867900	0.01695500	-0.43058800
H	4.82680700	0.24963900	-0.85330900
C	3.64509400	-1.19479000	0.21975900
H	4.45400300	-1.91076700	0.29847400
C	2.40254300	-1.49795900	0.78814300
H	2.26464100	-2.42881700	1.32217900
C	1.35325800	-0.62305600	0.67655600
N	-0.63790400	1.59745800	0.06683700
C	-1.57190400	0.59549200	-0.00944900
C	-1.35342000	-0.62278300	-0.67701200
C	-2.40266700	-1.49777300	-0.78836300
H	-2.26485700	-2.42853500	-1.32259000
C	-3.64504600	-1.19479200	-0.21951900
H	-4.45391900	-1.91083000	-0.29805200
C	-3.85853800	0.01687900	0.43102000
H	-4.82656000	0.24944300	0.85404900
C	-2.83407800	0.92739700	0.52381500
H	2.98502900	1.88366700	-1.01100100
H	0.40356300	-0.85653600	1.13500400
H	-0.40389400	-0.85607500	-1.13592000
H	-2.98484100	1.88357900	1.01143000
H	1.01210900	2.53542100	-0.21335700
H	-1.01199300	2.53549600	0.21335000

PBE0-D3/def2-TZVP：

Zero-point correction= 0.219148 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.181772

Sum of electronic and zero-point Energies= -572.876041

Sum of electronic and thermal Energies= -572.865187

Sum of electronic and thermal Enthalpies= -572.864243

Sum of electronic and thermal Free Energies= -572.913416

PBE0-D3/def2-TZVP Electronic Energy = -573.095189 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -573.100376483 a.u.

***E*.1.2H$^+$**

N	-0.47970300	0.42629300	-0.03604200
N	0.47970200	-0.42629000	-0.03606700
N	-3.94443200	0.51841400	-0.01483900
C	-1.79619600	0.13235000	-0.00818800
C	-2.44796900	-1.13119300	0.06263300
C	-3.77610900	-0.85132800	0.05600900
C	-2.77640100	1.14048800	-0.05397900
H	-2.67439800	2.21299400	-0.10985500
C	2.77639900	-1.14048600	-0.05408600
C	1.79619500	-0.13234900	-0.00823600
C	2.44797200	1.13119100	0.06261000
C	3.77611100	0.85132600	0.05594200
N	3.94443100	-0.51841500	-0.01495400
H	4.83907600	-0.98577300	-0.03215500
H	2.67439300	-2.21299100	-0.10999300
H	2.01009800	2.11432900	0.11812700
H	4.62747300	1.50991300	0.09913000
H	-4.62746900	-1.50991800	0.09919700
H	-2.01009300	-2.11433200	0.11810600
H	-4.83907700	0.98577200	-0.03200000
H	0.20006200	-1.40451600	-0.05675900
H	-0.20006300	1.40452000	-0.05671200

PBE0-D3/def2-TZVP：

Zero-point correction= 0.185348 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.149663

Sum of electronic and zero-point Energies= -528.871650

Sum of electronic and thermal Energies= -528.862100

Sum of electronic and thermal Enthalpies= -528.861156

Sum of electronic and thermal Free Energies= -528.907335

PBE0-D3/def2-TZVP Electronic Energy = -529.056998 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -529.062408838 a.u.

***Z*.1.2H$^+$**

C	1.56095400	0.46664000	-0.04223900
C	1.47714200	-0.86031100	0.42826300
C	2.92930000	0.72854100	-0.37621500
C	-1.56081800	0.46645000	0.04238600
C	-2.92919000	0.72860700	0.37623200
C	-3.60560900	-0.41173900	0.11133700
H	-3.32566100	1.64950500	0.77241500
C	-1.47718900	-0.86063300	-0.42779100

C	3.60547900	-0.41205900	-0.11168400
H	3.32600200	1.64937700	-0.77224800
H	0.66196400	-1.43287600	0.83391800
H	4.64590000	-0.66112700	-0.23458700
H	-0.66210900	-1.43346500	-0.83328100
H	-4.64614900	-0.66053300	0.23376200
N	0.64193100	1.45484500	-0.05752000
N	-0.64170800	1.45468800	0.05749500
N	-2.70869700	-1.34119000	-0.38020600
N	2.70847300	-1.34128300	0.38011800
H	-2.95575200	-2.27853600	-0.66457700
H	2.95533900	-2.27874500	0.66427300
H	1.02086600	2.39205700	-0.17783800
H	-1.02081300	2.39194000	0.17722300

PBE0-D3/def2-TZVP：

Zero-point correction= 0.185247 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.149606

Sum of electronic and zero-point Energies= -528.859842

Sum of electronic and thermal Energies= -528.850387

Sum of electronic and thermal Enthalpies= -528.849443

Sum of electronic and thermal Free Energies= -528.895483

PBE0-D3/def2-TZVP Electronic Energy = -529.045090 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -529.050517346 a.u.

***E*.2.2H$^+$**

N	-0.49425500	-0.40777500	0.00000600
N	0.49417500	0.40839800	-0.00001000
C	-1.80802700	-0.07612200	0.00001200
C	-2.35960300	1.23859900	0.00000200
C	-3.70827200	1.18153000	0.00001500
C	-2.76943700	-1.08914700	0.00003500
H	-2.59724400	-2.15662500	0.00004600
C	2.76929000	1.08900700	-0.00001200
C	1.80799300	0.07594900	-0.00000500
C	2.35945000	-1.23870600	0.00001700
C	3.70819900	-1.18126600	0.00002900
H	2.59746600	2.15652900	-0.00002200
H	1.80719400	-2.16760000	0.00003800
H	4.40317900	-2.00747500	0.00005100
H	-4.40375600	2.00727600	0.00001300
H	-1.80659800	2.16704000	-0.00001000
S	4.30234900	0.43995900	-0.00006200
S	-4.30218000	-0.44015800	0.00002200

H	0.25096700	1.39684800	-0.00002400
H	-0.25090500	-1.39623800	0.00001900

PBE0-D3/def2-TZVP：

Zero-point correction= 0.151640 (Hartree/Particle)

Thermal correction to Energy= 0.161969

Thermal correction to Enthalpy= 0.162914

Thermal correction to Gibbs Free Energy= 0.113490

Sum of electronic and zero-point Energies= -1214.375568

Sum of electronic and thermal Energies= -1214.365238

Sum of electronic and thermal Enthalpies= -1214.364294

Sum of electronic and thermal Free Energies= -1214.413717

PBE0-D3/def2-TZVP Electronic Energy = -1214.527208 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1214.53116249 a.u.

***Z*.2.2H$^+$**

C	-1.56542600	0.69965200	0.08398200
C	-1.45508000	-0.57908400	-0.46726700
C	-2.88939100	1.00004000	0.54503000
C	1.56543500	0.69978400	-0.08373800
C	2.88913900	0.99996200	-0.54559700
C	3.72213300	-0.03954300	-0.34228600
H	3.17249100	1.93591700	-1.00740800
C	1.45532700	-0.57877400	0.46800500
S	2.92317500	-1.35739200	0.42612100
C	-3.72233100	-0.03946400	0.34151100
S	-2.92305400	-1.35754500	-0.42611300
H	-3.17291600	1.93613500	1.00644400
H	-0.60535900	-1.04568700	-0.93957700
H	-4.76736300	-0.11878300	0.59888500
H	0.60579900	-1.04493600	0.94111100
H	4.76701000	-0.11902800	-0.60023100
N	-0.63755500	1.69017400	0.09122800
N	0.63751200	1.69026200	-0.09086500
H	-1.00486900	2.62838300	0.24492400
H	1.00471500	2.62849000	-0.24465600

PBE0-D3/def2-TZVP：

Zero-point correction= 0.151807 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.115001

Sum of electronic and zero-point Energies= -1214.363999

Sum of electronic and thermal Energies= -1214.353997

Sum of electronic and thermal Enthalpies= -1214.353053

Sum of electronic and thermal Free Energies= -1214.400805

PBE0-D3/def2-TZVP Electronic Energy = -1214.515806 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1214.51973454 a.u.

***E*.3.2H$^+$**

N	0.47810200	-0.42600800	-0.00000900
N	-0.47793500	0.42595300	0.00001400
C	1.79605100	-0.13094200	0.00000200
C	2.47556900	1.12470700	0.00004100
C	3.77879800	0.79936600	-0.00001200
C	2.76785100	-1.12761400	-0.00000900
H	2.70244900	-2.20593300	-0.00002700
C	-2.76767300	1.12761900	0.00001900
C	-1.79607300	0.13076600	0.00000300
C	-2.47563200	-1.12467000	-0.00003400
C	-3.77895000	-0.79897900	-0.00001200
H	-2.70232100	2.20593400	0.00004300
H	-2.07253100	-2.12426800	-0.00006000
H	-4.68391800	-1.38236200	-0.00001800
H	4.68419200	1.38205500	-0.00002400
H	2.07196300	2.12410600	0.00007400
O	-3.94706400	0.56664800	0.00002200
O	3.94699500	-0.56673900	-0.00002400
H	-0.20259900	1.40709500	0.00004100
H	0.20250800	-1.40703900	-0.00003500

PBE0-D3/def2-TZVP：

Zero-point correction= 0.158701 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.122730

Sum of electronic and zero-point Energies= -568.542402

Sum of electronic and thermal Energies= -568.532986

Sum of electronic and thermal Enthalpies= -568.532042

Sum of electronic and thermal Free Energies= -568.578373

PBE0-D3/def2-TZVP Electronic Energy = -568.701103 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -568.704938468 a.u.

***Z*.3.2H$^+$**

C	1.56524200	0.45482100	-0.03850500
C	1.49799100	-0.86787300	0.40558300
C	2.94138500	0.71203200	-0.35444500
C	-1.56515100	0.45458700	0.03873700
C	-2.94151000	0.71214700	0.35356500
C	-3.58114300	-0.43433500	0.09372700
H	-3.35997000	1.62966400	0.73419900
C	-1.49778500	-0.86832600	-0.40469600

C	3.58099600	-0.43450300	-0.09476800
H	3.35976000	1.62929800	-0.73576300
H	0.71166300	-1.48717200	0.80378700
H	4.60374800	-0.75729000	-0.18586000
H	-0.71129800	-1.48822000	-0.80166400
H	-4.60409200	-0.75675400	0.18391500
N	0.64012400	1.44025200	-0.05193400
N	-0.64012600	1.44011000	0.05257100
O	2.69621200	-1.37899700	0.37738700
O	-2.69617900	-1.37917900	-0.37724100
H	1.02144100	2.38114500	-0.15683300
H	-1.02165400	2.38091400	0.15741300

PBE0-D3/def2-TZVP：

Zero-point correction= 0.158755 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.122775

Sum of electronic and zero-point Energies= -568.526976

Sum of electronic and thermal Energies= -568.517736

Sum of electronic and thermal Enthalpies= -568.516792

Sum of electronic and thermal Free Energies= -568.562957

PBE0-D3/def2-TZVP Electronic Energy = -568.685732 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -568.689591152 a.u.

***E*.4.2H$^+$**

N	-0.51082400	-0.38792700	0.00000400
N	0.51089600	0.38905100	-0.00000700
C	-1.81233900	-0.00573200	0.00001300
C	-2.28225500	1.34584700	0.00001300
C	-3.62539000	1.42587000	0.00002300
C	-2.79420300	-0.99176500	0.00002300
H	-2.63164800	-2.06052400	0.00002300
C	2.79461600	0.99196800	-0.00003100
C	1.81234700	0.00637600	-0.00001700
C	2.28166600	-1.34536700	-0.00001700
C	3.62480600	-1.42597500	-0.00003000
H	2.63249000	2.06079200	-0.00003300
H	1.65240100	-2.22563100	-0.00000800
H	4.22432800	-2.32370300	-0.00003300
H	-4.22547700	2.32322200	0.00002500
H	-1.65313400	2.22618500	0.00000400
Se	4.44392700	0.25787700	-0.00003500
Se	-4.44379200	-0.25837000	0.00004100
H	0.30671500	1.38559300	-0.00000800
H	-0.30627300	-1.38437500	0.00000500

PBE0-D3/def2-TZVP：

Zero-point correction= 0.148977 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.109255

Sum of electronic and zero-point Energies= -5220.770977

Sum of electronic and thermal Energies= -5220.760065

Sum of electronic and thermal Enthalpies= -5220.759120

Sum of electronic and thermal Free Energies= -5220.810699

PBE0-D3/def2-TZVP Electronic Energy = -5220.919954 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -5220.92392587 a.u.

***Z*.4.2H$^+$**

C	-1.55941900	1.08073800	0.16747500
C	-1.46172100	-0.17722900	-0.41849900
C	-2.84634000	1.39782800	0.72908900
C	1.55950400	1.08064500	-0.16769700
C	2.84677500	1.39801800	-0.72833400
C	3.74723400	0.41090000	-0.59410400
H	3.05925800	2.34073700	-1.21670100
C	1.46146500	-0.17755900	0.41775900
C	-3.74683600	0.41071000	0.59512200
H	-3.05851700	2.34030700	1.21805700
H	-0.62198000	-0.60860100	-0.93920800
H	-4.76845800	0.39631900	0.94260500
H	0.62131000	-0.60907700	0.93766400
H	4.76911200	0.39665100	-0.94083600
N	-0.63097300	2.07253000	0.13779200
N	0.63107300	2.07242700	-0.13830900
Se	-3.03219600	-1.05621300	-0.31325400
Se	3.03203100	-1.05642300	0.31319100
H	-0.98092000	3.00724800	0.34031300
H	0.98114500	3.00705600	-0.34102100

PBE0-D3/def2-TZVP：

Zero-point correction= 0.148688 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.108978

Sum of electronic and zero-point Energies= -5220.760389

Sum of electronic and thermal Energies= -5220.749568

Sum of electronic and thermal Enthalpies= -5220.748624

Sum of electronic and thermal Free Energies= -5220.800100

PBE0-D3/def2-TZVP Electronic Energy = -5220.909077 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -5220.91298278 a.u.

***E*.5.2H$^+$**

N	0.46910800	0.43108100	-0.00014700
N	-0.46909500	-0.43089100	-0.00014800
C	1.79773700	0.13879200	-0.01412200
C	2.45616400	-1.15115000	-0.09606900
C	3.76369200	-0.92609400	-0.05308300
C	2.71578300	1.13997100	0.07124500
H	2.62317000	2.21619100	0.14470900
C	-2.71557100	-1.13995000	0.07119800
C	-1.79768400	-0.13861100	-0.01414900
C	-2.45635900	1.15121600	-0.09607400
C	-3.76383100	0.92591500	-0.05315300
H	-2.62280400	-2.21618200	0.14448800
H	-2.00015100	2.12569200	-0.18141900
H	-4.61451100	1.58815200	-0.08822900
H	4.61428000	-1.58844700	-0.08810800
H	1.99967000	-2.12546600	-0.18162400
N	4.00916600	0.51551900	0.06271700
N	-4.00912300	-0.51573100	0.06276200
H	4.59741100	0.87678500	-0.70994700
H	4.53266800	0.74721300	0.92750900
H	-4.59754000	-0.87726700	-0.70959900
H	-4.53224300	-0.74727800	0.92783200
H	0.18998000	1.41545100	0.02162500
H	-0.18990900	-1.41522100	0.02172300

PBE0-D3/def2-TZVP：

Zero-point correction= 0.210018 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.174494

Sum of electronic and zero-point Energies= -529.495518

Sum of electronic and thermal Energies= -529.485755

Sum of electronic and thermal Enthalpies= -529.484811

Sum of electronic and thermal Free Energies= -529.531042

PBE0-D3/def2-TZVP Electronic Energy = -529.705536 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -529.712380579 a.u.

***Z*.5.2H$^+$**

C	1.59162100	0.45885700	-0.05085800
C	1.50193500	-0.81465200	0.42579600
C	2.97294800	0.76556600	-0.39680300
C	-1.58706300	0.47453300	0.01945500
C	-2.92686300	0.75366600	0.51617800
C	-3.67699300	-0.30888700	0.26622400
H	-3.23494300	1.65570200	1.02386400
C	-1.54925500	-0.75788900	-0.55813300

C	3.70416100	-0.30466000	-0.12720100
H	3.32131100	1.69789300	-0.81569600
H	0.69994100	-1.42928600	0.80558500
H	4.75433100	-0.52159900	-0.23958300
H	-0.80005700	-1.30640600	-1.11140700
H	-4.70631900	-0.54506700	0.48442800
N	0.64106900	1.44156000	-0.09126700
N	-0.62937200	1.45365200	0.01297700
N	2.83547300	-1.34708200	0.42353900
N	-2.86812800	-1.31127000	-0.43090400
H	-3.25945800	-1.54415200	-1.36202100
H	-2.83970800	-2.21393100	0.07835400
H	2.88165200	-2.22813700	-0.11991900
H	3.11957100	-1.61671000	1.38379000
H	1.03032600	2.38748600	-0.19633700
H	-1.00287900	2.40699300	0.10058200

PBE0-D3/def2-TZVP：

Zero-point correction= 0.209630 (Hartree/Particle)

Thermal correction to Energy= 0.219466

Thermal correction to Enthalpy= 0.220410

Thermal correction to Gibbs Free Energy= 0.173448

Sum of electronic and zero-point Energies= -529.471894

Sum of electronic and thermal Energies= -529.462058

Sum of electronic and thermal Enthalpies= -529.461114

Sum of electronic and thermal Free Energies= -529.508076

PBE0-D3/def2-TZVP Electronic Energy = -529.681524 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -529.688317351 a.u.

***E*.6.2H$^+$**

N	0.47043900	-0.43875900	0.04340500
N	-0.47043900	0.43875900	0.04338900
C	1.79517900	-0.15958200	0.01397800
C	2.43413000	1.13856600	-0.06072700
C	3.75880900	0.92371700	-0.06427500
C	2.73270700	-1.16494300	0.05257800
H	2.53736400	-2.22796600	0.10481100
C	-2.73270700	1.16494400	0.05251400
C	-1.79518000	0.15958200	0.01395200
C	-2.43413000	-1.13856700	-0.06072700
C	-3.75880900	-0.92371900	-0.06430000
H	-2.53736300	2.22796800	0.10472200
H	-1.94451000	-2.10000300	-0.11276800
H	-4.52003500	-1.68845400	-0.11751100

H	4.52003600	1.68845200	-0.11749600
H	1.94451100	2.10000000	-0.11280000
H	4.65389200	-0.81160400	0.89205400
H	4.64501000	-0.90304300	-0.84446700
H	-4.65390100	0.81162400	0.89197500
H	-4.64499700	0.90302000	-0.84455400
C	4.05918900	-0.53539200	0.00959800
C	-4.05919100	0.53539300	0.00953200
H	0.17515200	-1.41263500	0.06788400
H	-0.17515200	1.41263500	0.06784900

PBE0-D3/def2-TZVP：

Zero-point correction= 0.203316 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.167149

Sum of electronic and zero-point Energies= -496.694820

Sum of electronic and thermal Energies= -496.684600

Sum of electronic and thermal Enthalpies= -496.683656

Sum of electronic and thermal Free Energies= -496.730987

PBE0-D3/def2-TZVP Electronic Energy = -496.898136 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -496.903197488 a.u.

***Z*.6.2H$^+$**

C	1.58303500	0.45445500	-0.03203900
C	1.52138100	-0.83752900	0.45251300
C	2.94648300	0.76655800	-0.43560300
C	-1.58535500	0.43954600	0.07157300
C	-2.97850200	0.77061900	0.34072600
C	-3.71800300	-0.31015300	0.07072000
H	-3.31849600	1.73117400	0.70188100
C	-1.49035300	-0.87814800	-0.33581600
C	3.70098100	-0.31231400	-0.19896000
H	3.25344600	1.70880400	-0.86690100
H	0.67691500	-1.35406300	0.87981000
H	4.75505200	-0.41112300	-0.41252200
H	-0.61242000	-1.44006300	-0.60892100
H	-4.78951700	-0.39155600	0.17830000
N	0.63916700	1.42769400	-0.03314000
N	-0.64742500	1.41727400	0.10704600
H	-3.07485500	-1.74080200	-1.43417300
H	-2.93316100	-2.34683700	0.18573500
H	2.88576600	-2.33617800	-0.17617600
H	3.20436300	-1.69580500	1.40580500
C	2.87535100	-1.39836100	0.39881800
C	-2.84962900	-1.42293200	-0.40418900

H	-1.02118900	2.35849000	0.22193300
H	0.99956100	2.37273600	-0.15856700

PBE0-D3/def2-TZVP：

Zero-point correction= 0.202333 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.164387

Sum of electronic and zero-point Energies= -496.676260

Sum of electronic and thermal Energies= -496.665895

Sum of electronic and thermal Enthalpies= -496.664951

Sum of electronic and thermal Free Energies= -496.714206

PBE0-D3/def2-TZVP Electronic Energy = -496.878593 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -496.883659324 a.u.

***E*.7.2H$^+$**

N	0.46724900	-0.44944300	-0.00000200
N	-0.46725600	0.44966200	0.00001500
C	1.80006200	-0.19758300	-0.00007800
C	2.41178700	1.11920700	-0.00013400
C	3.75587700	0.97833400	-0.00020400
C	2.72748800	-1.22382500	-0.00015800
H	2.41470200	-2.26419800	-0.00009400
C	-2.72764500	1.22377600	-0.00007700
C	-1.80008700	0.19772000	-0.00003500
C	-2.41159000	-1.11916900	-0.00008800
C	-3.75570300	-0.97842000	-0.00015700
H	-2.41477500	2.26416600	-0.00002300
H	-1.86332900	-2.05597100	-0.00011100
H	-4.39706800	-1.85543900	-0.00021100
H	4.39735400	1.85524000	-0.00025500
H	1.86327400	2.05588200	-0.00015900
H	4.80814400	-0.93516800	0.97908000
H	4.80971900	-0.93582300	-0.97711400
H	-4.80826100	0.93450900	0.97926200
H	-4.80945500	0.93504700	-0.97769800
B	4.16133900	-0.57346000	0.00030200
B	-4.16160000	0.57340500	0.00025800
H	-0.14549600	1.41187700	0.00002000
H	0.14540700	-1.41161100	-0.00000400

PBE0-D3/def2-TZVP：

Zero-point correction= 0.185975 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.147322

Sum of electronic and zero-point Energies= -470.515853

Sum of electronic and thermal Energies= -470.504217

Sum of electronic and thermal Enthalpies= -470.503273

Sum of electronic and thermal Free Energies= -470.554507

PBE0-D3/def2-TZVP Electronic Energy = -470.701829 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -470.706455087 a.u.

***E*.8.2H$^+$**

N	0.47549600	-0.42552000	-0.00006100
N	-0.47531100	0.42491900	-0.00009800
C	1.80796100	-0.12229100	-0.00002500
C	2.35930600	1.23949600	-0.00008800
C	3.69402600	1.28353500	-0.00002400
C	2.70878600	-1.14500700	0.00009700
H	2.51011400	-2.21066400	0.00014300
C	-2.70855500	1.14492600	-0.00000300
C	-1.80776200	0.12202700	-0.00008200
C	-2.35963100	-1.23954000	-0.00011600
C	-3.69436400	-1.28331700	-0.00007400
H	-2.50974200	2.21056200	0.00002700
H	-1.75648500	-2.13849200	-0.00016700
H	-4.30422200	-2.17520300	-0.00009300
H	4.30388100	2.17542400	-0.00005500
H	1.75589800	2.13827300	-0.00017600
P	-4.33531100	0.37676500	0.00004400
P	4.33529200	-0.37649200	0.00014400
H	-5.04532100	0.73744100	1.15476100
H	-5.04546500	0.73758600	-1.15454000
H	5.04558500	-0.73649200	1.15488500
H	5.04575500	-0.73670300	-1.15442600
H	-0.20303300	1.41066400	-0.00012600
H	0.20343200	-1.41127500	-0.00004700

PBE0-D3/def2-TZVP：

Zero-point correction= 0.187201 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.147138

Sum of electronic and zero-point Energies= -1102.540491

Sum of electronic and thermal Energies= -1102.528576

Sum of electronic and thermal Enthalpies= -1102.527632

Sum of electronic and thermal Free Energies= -1102.580553

PBE0-D3/def2-TZVP Electronic Energy = -1102.727691 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1102.73269854 a.u.

***Z*.8.2H$^+$**

C	-1.58248200	0.69250000	0.05729500
C	-1.54485900	-0.47980900	-0.62993900

C	-2.85168700	1.00085300	0.74607100
C	1.59816900	0.67069000	-0.12209100
C	2.96553000	1.04259600	-0.53850000
C	3.88780000	0.10428200	-0.32395100
H	3.18200800	2.00161200	-0.99358100
C	1.45772700	-0.58384200	0.38838600
C	-3.79738200	0.07154900	0.60057900
H	-2.97757300	1.89688800	1.34285900
H	-0.76160600	-0.88524700	-1.25633600
H	-4.78138000	0.08104800	1.04675700
H	0.57582600	-1.08727800	0.75794900
H	4.93876600	0.16904500	-0.56550900
N	-0.61960600	1.67844300	0.02341700
N	0.64423300	1.66006100	-0.15549300
H	3.47299800	-1.57928800	1.74513100
H	3.12231200	-2.47991500	-0.35000300
H	-3.04768600	-2.48416800	0.18195600
H	-3.78585100	-1.35057300	-1.68807400
P	-3.17224500	-1.22862900	-0.43220600
P	3.10869300	-1.30515300	0.41806100
H	1.02152800	2.60671600	-0.28981900
H	-0.97533800	2.63544800	0.13827300

PBE0-D3/def2-TZVP：

Zero-point correction= 0.187651 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.150006

Sum of electronic and zero-point Energies= -1102.517537

Sum of electronic and thermal Energies= -1102.506183

Sum of electronic and thermal Enthalpies= -1102.505239

Sum of electronic and thermal Free Energies= -1102.555182

PBE0-D3/def2-TZVP Electronic Energy = -1102.705188 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1102.71007226 a.u.

***E*.9.2H$^+$**

N	0.47638600	0.43111300	0.00001700
N	-0.47623400	-0.43078400	-0.00002000
C	1.80909200	0.13926100	0.00003600
C	2.33335100	-1.23100900	0.00001600
C	3.67091600	-1.32002400	0.00003600
C	2.70955500	1.16849600	0.00007500
H	2.40931800	2.20981000	0.00009200
C	-2.70929900	-1.16850600	-0.00007700
C	-1.80915900	-0.13909800	-0.00003900
C	-2.33366200	1.23114500	-0.00001900

C	-3.67123500	1.31993200	-0.00003800
H	-2.40891100	-2.20975700	-0.00009500
H	-1.68734200	2.10257300	0.00001100
H	-4.16564500	2.28254400	-0.00002600
H	4.16503300	-2.28278700	0.00002200
H	1.68688900	-2.10232900	-0.00001400
Si	4.42818700	0.38892300	0.00008900
Si	-4.42808500	-0.38917100	-0.00008400
H	5.16110600	0.74704800	-1.23296400
H	5.16104700	0.74698900	1.23319500
H	-5.16076300	-0.74721600	-1.23330400
H	-5.16079100	-0.74726600	1.23310500
H	0.19080100	1.40866500	0.00003000
H	-0.19057200	-1.40828900	-0.00003300

PBE0-D3/def2-TZVP：

Zero-point correction= 0.181144 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.142062

Sum of electronic and zero-point Energies= -999.303178

Sum of electronic and thermal Energies= -999.290850

Sum of electronic and thermal Enthalpies= -999.289906

Sum of electronic and thermal Free Energies= -999.342260

PBE0-D3/def2-TZVP Electronic Energy = -999.484323 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -999.489045643 a.u.

***Z*.9.2H$^+$**

C	1.49659100	-0.60106700	0.44086500
C	1.59232200	0.64954200	-0.11093700
C	2.91853500	1.05061500	-0.61648300
H	3.03885100	2.01013400	-1.11045700
C	3.90231100	0.16278400	-0.43648900
C	-1.49687600	-0.60064200	-0.44186100
C	-1.59231400	0.64969600	0.11061800
C	-2.91815000	1.05046600	0.61732900
H	-3.03820000	2.00980700	1.11170500
C	-3.90194700	0.16254400	0.43783300
H	0.58787100	-1.02980500	0.83904500
H	4.90716200	0.35936600	-0.78617400
H	-0.58845400	-1.02876700	-0.84139400
H	-4.90651600	0.35881100	0.78850400
Si	3.23754400	-1.33923300	0.44060000
Si	-3.23775600	-1.33894300	-0.44060800
H	-3.25046800	-2.59911900	0.33447000
H	-3.69838100	-1.51894400	-1.83450700

H	3.25044500	-2.59871200	-0.33564600
H	3.69729800	-1.52062000	1.83458700
N	-0.63628400	1.62645600	0.11462600
N	0.63632100	1.62631700	-0.11529800
H	0.98914500	2.56953000	-0.28021700
H	-0.98887200	2.56974900	0.27964500

PBE0-D3/def2-TZVP：

Zero-point correction= 0.180314 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.141263

Sum of electronic and zero-point Energies= -999.283500

Sum of electronic and thermal Energies= -999.271131

Sum of electronic and thermal Enthalpies= -999.270187

Sum of electronic and thermal Free Energies= -999.322551

PBE0-D3/def2-TZVP Electronic Energy = -999.463814 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -999.468443308 a.u.

***E*.10.2H$^+$**

N	0.49006600	0.40676600	-0.00001600
N	-0.49008500	-0.40706900	0.00001200
C	1.81382500	0.05831500	-0.00003400
C	2.29459500	-1.32872800	-0.00001900
C	3.61762800	-1.48237400	-0.00003700
C	2.73118400	1.06298700	-0.00006500
H	2.54373100	2.13000700	-0.00007400
C	-2.73130000	-1.06308100	0.00005900
C	-1.81386400	-0.05852200	0.00003100
C	-2.29441200	1.32858700	0.00002300
C	-3.61743100	1.48239000	0.00004600
H	-2.54412900	-2.13014200	0.00006600
H	-1.63237700	2.18607600	-0.00000100
H	-4.15467600	2.41922800	0.00004600
H	4.15501200	-2.41912900	-0.00003000
H	1.63270400	-2.18635100	0.00000700
As	4.45390000	0.22433900	-0.00007600
As	-4.45393800	-0.22420200	0.00007700
H	5.20533600	0.56668600	-1.24068000
H	5.20537600	0.56672700	1.24049200
H	-5.20550500	-0.56636000	-1.24049600
H	-5.20547600	-0.56634000	1.24067300
H	0.25357800	1.40124200	-0.00002400
H	-0.25355100	-1.40150500	0.00001900

PBE0-D3/def2-TZVP:

Zero-point correction= 0.183124 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.143169

Sum of electronic and zero-point Energies= -4891.246836

Sum of electronic and thermal Energies= -4891.234589

Sum of electronic and thermal Enthalpies= -4891.233645

Sum of electronic and thermal Free Energies= -4891.286792

PBE0-D3/def2-TZVP Electronic Energy = -4891.429961 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4891.43498498 a.u.

***Z*.10.2H$^+$**

C	-1.57954100	1.01246400	0.18703900
C	-1.52966200	-0.15064000	-0.51038700
C	-2.82762900	1.33806200	0.90423800
C	1.57958900	1.01279300	-0.18690800
C	2.82809200	1.33829600	-0.90367600
C	3.82138000	0.46250700	-0.78506900
H	2.90522600	2.23419000	-1.50973200
C	1.52974100	-0.15049000	0.51025400
C	-3.82106200	0.46239100	0.78556900
H	-2.90419300	2.23373100	1.51066800
H	-0.72913000	-0.55058500	-1.11763100
H	-4.79281900	0.51633300	1.25322900
H	0.72924300	-0.55032500	1.11758900
H	4.79330300	0.51662000	-1.25235200
N	-0.62227600	2.00776000	0.13690900
N	0.62207300	2.00770400	-0.13726400
As	-3.25993600	-0.96469000	-0.32915500
As	3.25981200	-0.96486400	0.32902900
H	-3.13351500	-2.29850600	0.32561800
H	-3.91281800	-1.04962300	-1.66711500
H	3.91260100	-1.05020400	1.66701400
H	3.13297400	-2.29863300	-0.32577200
H	-0.98042700	2.95582000	0.30558500
H	0.97963500	2.95591500	-0.30680000

PBE0-D3/def2-TZVP:

Zero-point correction= 0.182214 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.142719

Sum of electronic and zero-point Energies= -4891.224862

Sum of electronic and thermal Energies= -4891.212732

Sum of electronic and thermal Enthalpies= -4891.211788

Sum of electronic and thermal Free Energies= -4891.264357

PBE0-D3/def2-TZVP Electronic Energy = -4891.407076 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4891.41189850 a.u.

***E*.11.2H$^+$**

N	0.49296300	-0.41057600	0.00000900
N	-0.49306600	0.41082900	-0.00002700
C	1.81629500	-0.06878600	0.00002400
C	2.27711200	1.32297200	-0.00001200
C	3.60363200	1.49560700	0.00000100
C	2.74215200	-1.07292200	0.00007200
H	2.46876400	-2.12157000	0.00009500
C	-2.74239100	1.07280000	-0.00007900
C	-1.81601400	0.06882800	-0.00003700
C	-2.27676300	-1.32280600	-0.00000400
C	-3.60330700	-1.49551800	-0.00001500
H	-2.46900800	2.12149100	-0.00010800
H	-1.58563200	-2.15915700	0.00003000
H	-4.04459700	-2.48328900	0.00000800
H	4.04522800	2.48323000	-0.00002700
H	1.58587600	2.15923000	-0.00004700
Ge	4.51531100	-0.22558600	0.00008400
Ge	-4.51540100	0.22549800	-0.00007200
H	5.27476000	-0.55771400	1.28020400
H	5.27486300	-0.55782400	-1.27994300
H	-5.27541400	0.55767400	1.27968700
H	-5.27540200	0.55760700	-1.27985500
H	-0.24768400	1.39915600	-0.00004500
H	0.24755100	-1.39883300	0.00002500

PBE0-D3/def2-TZVP:

Zero-point correction= 0.178823 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.138223

Sum of electronic and zero-point Energies= -4574.014571

Sum of electronic and thermal Energies= -4574.001811

Sum of electronic and thermal Enthalpies= -4574.000867

Sum of electronic and thermal Free Energies= -4574.055171

PBE0-D3/def2-TZVP Electronic Energy = -4574.193394 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4574.19819774 a.u.

***Z*.11.2H$^+$**

C	-1.58678200	1.00816900	0.20086100
C	-1.50898800	-0.23510600	-0.36441400
C	-2.87758300	1.42348300	0.78017400
C	1.58588300	1.01189200	-0.19009100
C	2.86392700	1.41666500	-0.80344300
C	3.87990700	0.55917700	-0.69136100

H	2.92606700	2.36741000	-1.32554800
C	1.51904700	-0.22016300	0.40049900
C	-3.89353600	0.56786600	0.65633800
H	-2.94926300	2.38161500	1.28724800
H	-0.61399900	-0.66200300	-0.79530400
H	-4.87266700	0.78136600	1.06336500
H	0.63559700	-0.62882000	0.87124700
H	4.84955500	0.76288700	-1.12524700
N	-0.62849000	1.98521600	0.15929700
N	0.62680000	1.98770900	-0.14413100
H	-3.29899800	-2.31657000	0.49593000
H	-3.86461100	-1.17015100	-1.72023700
H	3.90431800	-1.14871100	1.70686000
H	3.27849800	-2.32059000	-0.47937500
Ge	3.32123800	-1.01124000	0.30391300
Ge	-3.31709500	-1.01708100	-0.30464800
H	-0.97239400	2.92751600	0.34515500
H	0.96589200	2.92995400	-0.33811900

PBE0-D3/def2-TZVP:

Zero-point correction= 0.177722 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.136292

Sum of electronic and zero-point Energies= -4573.995034

Sum of electronic and thermal Energies= -4573.982083

Sum of electronic and thermal Enthalpies= -4573.981139

Sum of electronic and thermal Free Energies= -4574.036464

PBE0-D3/def2-TZVP Electronic Energy = -4574.172756 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4574.17742059 a.u.

***E*.12.2H$^+$**

N	-0.49730100	0.41096800	0.00000100
N	0.49737500	-0.41179800	-0.00001300
C	-1.82416300	0.07583700	-0.00001400
C	-2.26532800	-1.32076600	-0.00005100
C	-3.59332000	-1.52815500	-0.00007600
C	-2.74830100	1.08962500	0.00000300
H	-2.38110700	2.11412800	0.00002300
C	2.74860600	-1.08978600	-0.00000300
C	1.82424200	-0.07628700	0.00000400
C	2.26492900	1.32042100	0.00003100
C	3.59285400	1.52822700	0.00004800
H	2.38190200	-2.11444200	-0.00002600
H	1.54095600	2.13351400	0.00003500
H	3.93493400	2.56027100	0.00006600

H	-3.93567400	-2.56011900	-0.00010200
H	-1.54152100	-2.13398100	-0.00005400
H	-5.39127300	0.56271200	1.33481900
H	-5.39129100	0.56282300	-1.33483700
H	5.39134600	-0.56202700	1.33499700
H	5.39142600	-0.56200300	-1.33486900
Ga	-4.59398400	0.22889600	-0.00003000
Ga	4.59406500	-0.22854000	0.00004200
H	-0.25076100	1.39622700	0.00002600
H	0.25091700	-1.39702600	-0.00003700

PBE0-D3/def2-TZVP:

Zero-point correction= 0.170121 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.128363

Sum of electronic and zero-point Energies= -4270.034005

Sum of electronic and thermal Energies= -4270.020132

Sum of electronic and thermal Enthalpies= -4270.019188

Sum of electronic and thermal Free Energies= -4270.075762

PBE0-D3/def2-TZVP Electronic Energy = -4270.204125 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4270.20907206 a.u.

***E*.13.2H$^+$**

N	-0.47957800	0.43186900	0.00001900
N	0.47971900	-0.43264200	-0.00002900
C	-1.81943200	0.15298300	0.00002000
C	-2.31764900	-1.22669600	-0.00004100
C	-3.65450100	-1.38464500	-0.00003400
C	-2.70175600	1.20383800	0.00008000
H	-2.28425300	2.20915700	0.00012100
C	2.70215700	-1.20393600	-0.00008100
C	1.81956400	-0.15335600	-0.00002900
C	2.31724500	1.22644900	0.00002500
C	3.65404300	1.38491000	0.00002200
H	2.28507300	-2.20940900	-0.00012000
H	1.62249100	2.06565200	0.00006600
H	4.01690400	2.41041000	0.00006200
H	-4.01774200	-2.41002700	-0.00008100
H	-1.62316000	-2.06608700	-0.00008800
Al	4.56602600	-0.40620000	-0.00005500
Al	-4.56594100	0.40673500	0.00007300
H	5.36000100	-0.78012900	1.35644300
H	5.36001100	-0.78002600	-1.35657400
H	-5.35980500	0.78111600	1.35648900
H	-5.35988900	0.78126300	-1.35625100

H	-0.19124100	1.40559500	0.00005700
H	0.19149000	-1.40635100	-0.00006600

PBE0-D3/def2-TZVP:

Zero-point correction= 0.170020 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.129522

Sum of electronic and zero-point Energies= -905.497901

Sum of electronic and thermal Energies= -905.484241

Sum of electronic and thermal Enthalpies= -905.483297

Sum of electronic and thermal Free Energies= -905.538400

PBE0-D3/def2-TZVP Electronic Energy = -905.667922 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -905.672664818 a.u.

***E*.14.2H$^+$**

N	-0.47009300	0.43970900	-0.00002000
N	0.47005800	-0.43959300	0.00002300
C	-1.81248600	0.18281200	-0.00001900
C	-2.34054200	-1.19910600	0.00001400
C	-3.67402000	-1.35404200	0.00001900
C	-2.66978500	1.24571800	-0.00004800
H	-2.28107000	2.25886700	-0.00007500
C	2.66974700	-1.24564700	0.00006100
C	1.81242800	-0.18270900	0.00001900
C	2.34063900	1.19908700	-0.00003400
C	3.67414800	1.35400800	-0.00004100
H	2.28107900	-2.25881000	0.00009700
H	1.66325200	2.04977600	-0.00006400
H	4.07518400	2.36050400	-0.00008000
H	-4.07520300	-2.36048700	0.00003900
H	-1.66298100	-2.04964400	0.00003000
Al	-4.49069600	0.42202900	-0.00001500
Al	4.49066000	-0.42214300	0.00002700
H	-5.91543000	1.06437400	-0.00000200
H	5.91525900	-1.06479600	0.00005500
H	-0.16848300	1.41112100	-0.00005300
H	0.16834500	-1.41097100	0.00006100

PBE0-D3/def2-TZVP:

Zero-point correction= 0.158858 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.118711

Sum of electronic and zero-point Energies= -903.990648

Sum of electronic and thermal Energies= -903.977793

Sum of electronic and thermal Enthalpies= -903.976849

Sum of electronic and thermal Free Energies= -904.030795

PBE0-D3/def2-TZVP Electronic Energy = -904.149506 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -904.154114901 a.u.

***Z*.14.2H$^+$**

C	-0.10880800	1.59291100	0.54972300
C	0.47242300	1.49184700	-0.68509300
C	-0.65742700	2.90866500	0.97459900
C	0.10880800	-1.59291100	0.54972300
C	0.65742700	-2.90866500	0.97459900
C	0.47242300	-3.97186300	0.18025000
H	1.20363400	-2.94445500	1.91590700
C	-0.47242300	-1.49184700	-0.68509300
C	-0.47242300	3.97186300	0.18025000
H	-1.20363400	2.94445500	1.91590700
H	0.83947100	0.55374500	-1.08092300
H	-0.88199100	4.92611200	0.48884200
H	-0.83947100	-0.55374500	-1.08092300
H	0.88199100	-4.92611200	0.48884200
N	-0.13203100	0.63620500	1.52539300
N	0.13203100	-0.63620500	1.52539300
Al	0.52724900	3.37694400	-1.37757000
Al	-0.52724900	-3.37694400	-1.37757000
H	-1.18723600	-3.94719800	-2.67466800
H	1.18723600	3.94719800	-2.67466800
H	-0.32780700	0.98077500	2.46463100
H	0.32780700	-0.98077500	2.46463100

PBE0-D3/def2-TZVP:

Zero-point correction= 0.158270 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.118897

Sum of electronic and zero-point Energies= -903.971366

Sum of electronic and thermal Energies= -903.958595

Sum of electronic and thermal Enthalpies= -903.957651

Sum of electronic and thermal Free Energies= -904.010740

PBE0-D3/def2-TZVP Electronic Energy = -904.129636 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -904.134133801 a.u.

***E*.15.2H$^+$**

N	0.48885800	0.41888700	0.00003700
N	-0.48875600	-0.41867500	-0.00003900
C	1.81869800	0.10434200	0.00000000
C	2.28715600	-1.29874000	-0.00011800
C	3.60955600	-1.50745300	-0.00016200
C	2.72170900	1.12575700	0.00006700

H	2.39297300	2.15963400	0.00015300
C	-2.72160900	-1.12558000	-0.00006600
C	-1.81859200	-0.10415200	-0.00000200
C	-2.28725600	1.29881700	0.00011400
C	-3.60968900	1.50743300	0.00016000
H	-2.39315900	-2.15953700	-0.00015100
H	-1.57852500	2.12227300	0.00015800
H	-3.99310300	2.52007900	0.00024500
H	3.99298600	-2.52009700	-0.00024900
H	1.57820500	-2.12199700	-0.00016400
H	5.94978300	0.82871500	-0.00001500
H	-5.94963600	-0.82921500	0.00002000
Ga	4.53506000	0.23116200	-0.00003900
Ga	-4.53507100	-0.23129600	0.00004100
H	0.23044100	1.40290500	0.00013000
H	-0.23018700	-1.40265100	-0.00013300

PBE0-D3/def2-TZVP:

Zero-point correction= 0.159224 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.118260

Sum of electronic and zero-point Energies= -4268.534055

Sum of electronic and thermal Energies= -4268.521224

Sum of electronic and thermal Enthalpies= -4268.520280

Sum of electronic and thermal Free Energies= -4268.575019

PBE0-D3/def2-TZVP Electronic Energy = -4268.693278 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4268.69782112 a.u.

***Z*.15.2H$^+$**

C	0.15300000	-1.58676800	0.93729000
C	-0.43100000	-1.50021500	-0.29450300
C	0.74554700	-2.88526600	1.35622200
C	-0.15300000	1.58676800	0.93729000
C	-0.74554700	2.88526600	1.35622200
C	-0.60387400	3.94165600	0.55057200
H	-1.28933800	2.91454800	2.29844300
C	0.43100000	1.50021500	-0.29450300
C	0.60387400	-3.94165600	0.55057200
H	1.28933800	-2.91454800	2.29844300
H	-0.82976000	-0.57907800	-0.69906200
H	1.04230900	-4.89338600	0.82257000
H	0.82976000	0.57907800	-0.69906200
H	-1.04230900	4.89338600	0.82257000
N	0.14690100	-0.63246300	1.91520200
N	-0.14690100	0.63246300	1.91520200

H	1.08524700	3.94460800	-2.30083500
H	-1.08524700	-3.94460800	-2.30083500
Ga	-0.43100000	-3.40086900	-1.02193500
Ga	0.43100000	3.40086900	-1.02193500
H	-0.34462700	0.97367700	2.85496900
H	0.34462700	-0.97367700	2.85496900

PBE0-D3/def2-TZVP:

Zero-point correction= 0.158338 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.117495

Sum of electronic and zero-point Energies= -4268.515561

Sum of electronic and thermal Energies= -4268.502602

Sum of electronic and thermal Enthalpies= -4268.501658

Sum of electronic and thermal Free Energies= -4268.556404

PBE0-D3/def2-TZVP Electronic Energy = -4268.673899 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4268.67832673 a.u.

***E*.16.2H$^+$**

N	-0.48467100	0.41943300	0.01319200
N	0.48464000	-0.41920100	0.01319900
C	-1.81190900	0.10662200	0.00929100
C	-2.31071000	-1.29839500	0.01138200
C	-3.63528200	-1.48364200	0.00399000
C	-2.71609300	1.12071300	-0.00014300
H	-2.49037700	2.18023800	-0.00285800
C	2.71597800	-1.12064600	-0.00015600
C	1.81189700	-0.10646800	0.00928800
C	2.31084200	1.29850400	0.01136900
C	3.63543300	1.48361500	0.00399800
H	2.49014700	-2.18014700	-0.00288300
H	1.63276100	2.14505200	0.01861900
H	4.11629600	2.45069500	0.00506500
H	-4.11604600	-2.45077100	0.00504700
H	-1.63252800	-2.14486100	0.01865700
H	-5.83579700	0.83906200	-0.02046100
H	5.83570400	-0.83932700	-0.02043000
Ge	4.45633700	-0.22771700	-0.00794900
Ge	-4.45636200	0.22760300	-0.00795000
H	0.22591800	-1.40706700	0.01461500
H	-0.22597800	1.40730400	0.01454600

PBE0-D3/def2-TZVP:

Zero-point correction= 0.163350 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.122459

Sum of electronic and zero-point Energies= -4572.307147

Sum of electronic and thermal Energies= -4572.294901

Sum of electronic and thermal Enthalpies= -4572.293957

Sum of electronic and thermal Free Energies= -4572.348038

PBE0-D3/def2-TZVP Electronic Energy = -4572.470497 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4572.47486642 a.u.

***Z*.16.2H$^+$**

C	1.58832400	0.96702200	-0.11641600
C	1.55394900	-0.23564800	0.51682000
C	2.86432000	1.36078800	-0.79634200
C	-1.59032600	0.93695000	0.19868100
C	-2.94533000	1.39793300	0.64687100
C	-3.98610700	0.57407500	0.49240500
H	-3.04284100	2.38248100	1.09578400
C	-1.48721200	-0.34093900	-0.25480800
C	3.90011000	0.51789800	-0.73903900
H	2.90867800	2.30724900	-1.32817100
H	0.74405000	-0.65570500	1.09603700
H	4.85590500	0.68666900	-1.21267300
H	-0.60353100	-0.87892300	-0.56488100
H	-4.99963600	0.80339200	0.78679500
N	0.62393100	1.93079400	-0.08682100
N	-0.63628400	1.91191600	0.19244100
H	-3.81328200	-2.34286500	-0.82368800
H	3.89646400	-2.27954800	0.82393200
Ge	3.36064400	-0.97747100	0.28122000
Ge	-3.33564100	-1.01409400	-0.29256800
H	0.94834700	2.88111500	-0.28874900
H	-0.99415400	2.85875500	0.35036300

PBE0-D3/def2-TZVP:

Zero-point correction= 0.161925 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.121532

Sum of electronic and zero-point Energies= -4572.287749

Sum of electronic and thermal Energies= -4572.275387

Sum of electronic and thermal Enthalpies= -4572.274443

Sum of electronic and thermal Free Energies= -4572.328142

PBE0-D3/def2-TZVP Electronic Energy = -4572.449674 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -4572.45393460 a.u.

***E*.17.2H$^+$**

N	0.47185900	-0.43594500	-0.06421500
N	-0.47185300	0.43596800	-0.06420800

C	1.80673400	-0.17383300	-0.02321100
C	2.38498700	1.19917700	0.11418900
C	3.72544100	1.28471200	0.13970600
C	2.68210200	-1.21465300	-0.09837100
C	-2.68209400	1.21467300	-0.09856600
C	-1.80673200	0.17384400	-0.02348500
C	-2.38499300	-1.19919500	0.11353300
C	-3.72545100	-1.28475600	0.13878400
Si	4.36444000	-0.40112000	-0.02725800
Si	-4.36444000	0.40112200	-0.02774700
H	-5.68080000	1.03376200	-0.11021000
H	5.68079500	-1.03374200	-0.10993900
H	0.18497500	-1.41566100	-0.09983300
H	-0.18497500	1.41569200	-0.09952800
H	2.42100100	-2.26248200	-0.18658300
H	1.76083600	2.08234100	0.19854800
H	4.25769800	2.21912900	0.24548700
H	-1.76084600	-2.08236100	0.19788500
H	-4.25771300	-2.21920300	0.24427400
H	-2.42098800	2.26252000	-0.18654600

PBE0-D3/def2-TZVP:

Zero-point correction= 0.165212 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.126871

Sum of electronic and zero-point Energies= -997.568350

Sum of electronic and thermal Energies= -997.556621

Sum of electronic and thermal Enthalpies= -997.555677

Sum of electronic and thermal Free Energies= -997.606690

PBE0-D3/def2-TZVP Electronic Energy = -997.733562 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -997.738050619 a.u.

***Z*.17.2H$^+$**

C	-1.59272800	0.58760400	0.07117700
C	-1.50359300	-0.66629400	-0.45468600
C	-2.95078200	1.00655800	0.55551800
C	1.59271100	0.58751700	-0.07134300
C	2.95092200	1.00660100	-0.55516800
C	3.96376900	0.14017800	-0.38935600
H	3.06965800	1.97392300	-1.03454400
C	1.50344700	-0.66654400	0.45411900
C	-3.96362200	0.14007500	0.38996300
H	-3.06942900	1.97383200	1.03500700
H	-0.63169700	-1.15545100	-0.86477300
H	-4.97450600	0.33402500	0.71871600

H	0.63143400	-1.15604800	0.86353800
H	4.97476300	0.33425200	-0.71769700
N	-0.63879900	1.55864000	0.09673900
N	0.63881000	1.55857600	-0.09702700
H	3.74356300	-2.59978700	0.92522800
H	-3.74375500	-2.59960000	-0.92528600
H	-0.99310200	2.50994000	0.24162600
H	0.99320400	2.50984900	-0.24185700
Si	3.26790900	-1.31289300	0.41736800
Si	-3.26797700	-1.31279400	-0.41731700

PBE0-D3/def2-TZVP:

Zero-point correction= 0.163234 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.121866

Sum of electronic and zero-point Energies= -997.549534

Sum of electronic and thermal Energies= -997.537481

Sum of electronic and thermal Enthalpies= -997.536537

Sum of electronic and thermal Free Energies= -997.590902

PBE0-D3/def2-TZVP Electronic Energy = -997.712768 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -997.717199965 a.u.

***E*.18.2H$^+$**

N	0.45481162	-0.46518618	-0.06392800
N	-0.45482259	0.46517430	-0.06413823
C	1.78225397	-0.25102290	-0.02596305
C	2.44801974	1.07801662	0.06822556
C	3.78412774	0.92757974	0.09674369
C	2.67860994	-1.28281618	-0.05941650
C	-2.67863315	1.28279913	-0.05968138
C	-1.78226268	0.25102392	-0.02594638
C	-2.44800121	-1.07799313	0.06882866
C	-3.78410944	-0.92756241	0.09752566
B	-4.11460564	0.59503646	-0.00860187
B	4.11461728	-0.59504954	-0.00903978
H	5.16056080	-1.14587004	-0.06342990
H	-5.16057649	1.14583661	-0.06270561
H	-0.11656732	1.42418315	-0.09911253
H	0.11654466	-1.42420871	-0.09842188
H	-2.39567542	2.32661181	-0.11552078
H	-1.92022907	-2.02348069	0.11569342
H	-4.45392900	-1.77312344	0.17369018
H	1.92027420	2.02353112	0.11485339
H	4.45395946	1.77316812	0.17251366
H	2.39562735	-2.32664821	-0.11478557

PBE0-D3/def2-TZVP:

Zero-point correction= 0.171918 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.133867

Sum of electronic and zero-point Energies= -468.941239

Sum of electronic and thermal Energies= -468.930029

Sum of electronic and thermal Enthalpies= -468.929085

Sum of electronic and thermal Free Energies= -468.979291

PBE0-D3/def2-TZVP Electronic Energy = -469.113158 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -469.117387010 a.u.

***E*.1a.H$^+$**

N	0.10913100	-0.79488300	-0.12713700
N	-0.65068500	0.15313500	0.17516700
C	1.46833300	-0.65193100	-0.09339000
C	2.27982100	0.63900800	0.00367600
C	3.60184000	0.44938800	0.21076600
C	2.14893600	-1.82352900	-0.10739500
H	1.67129200	-2.78941500	-0.19804500
C	-2.86300200	1.01221100	0.40557900
C	-2.02946000	-0.00252300	0.12117500
C	-2.61194000	-1.33085100	-0.27662700
C	-3.94820400	-1.40010200	-0.32600900
H	-2.57765400	2.01357000	0.69565600
H	-1.94654200	-2.15572000	-0.50164200
H	-4.50186700	-2.28735900	-0.59326100
H	4.32077000	1.25382100	0.28321400
Si	3.90952600	-1.33051800	0.17886600
Si	-4.51976300	0.25508200	0.13939500
H	-5.84015500	0.87386500	0.27702200
H	5.09646100	-2.18072900	0.29530700
H	-0.29576300	1.07402200	0.48145500
Si	1.68296500	2.42428400	-0.29344300
H	1.22866000	2.49694200	-1.69899500
H	0.52258800	2.65590800	0.61279800
H	2.81697100	3.30342700	0.03617900

PBE0-D3/def2-TZVP:

Zero-point correction= 0.166382 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.125112

Sum of electronic and zero-point Energies= -1287.808522

Sum of electronic and thermal Energies= -1287.794536

Sum of electronic and thermal Enthalpies= -1287.793592

Sum of electronic and thermal Free Energies= -1287.849792

PBE0-D3/def2-TZVP Electronic Energy = -1287.974904 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1287.97878720 a.u.

***Z*.1a.H$^+$**

C	-1.68242500	-0.16748200	0.89045800
C	-1.80298400	-0.51229800	-0.39255400
C	-3.14049500	-0.36404800	-1.07027800
H	-3.24641900	-0.64472100	-2.11322900
C	-4.13384300	0.13516100	-0.32666600
C	0.82687800	1.40748600	-0.91478900
C	1.07573600	0.12700200	-0.58340700
C	2.32637200	-0.21413500	0.22128500
C	3.03653900	0.85796000	0.61367200
H	-0.80979100	-0.26323600	1.52039900
H	-5.13635600	0.31134900	-0.68557800
H	0.02346700	1.76013500	-1.54580600
H	3.92810400	0.80972300	1.22291900
Si	-3.39257100	0.41247200	1.30153500
Si	2.22912600	2.29677300	-0.13904000
H	-3.89339000	0.90791000	2.58552600
H	2.54034600	3.72854400	-0.18678100
N	0.44323900	-0.94884500	-1.17155800
N	-0.77364900	-1.14117100	-1.15710100
H	-1.07802100	-1.91025700	-1.76598600
Si	2.76469300	-2.02323100	0.59753400
H	3.43124700	-2.56812400	-0.60605900
H	3.63841100	-2.02250900	1.78686400
H	1.46313800	-2.70076800	0.82160300

PBE0-D3/def2-TZVP:

Zero-point correction= 0.166140 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.124615

Sum of electronic and zero-point Energies= -1287.794901

Sum of electronic and thermal Energies= -1287.780709

Sum of electronic and thermal Enthalpies= -1287.779765

Sum of electronic and thermal Free Energies= -1287.836426

PBE0-D3/def2-TZVP Electronic Energy = -1287.961041 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1287.96464470 a.u.

***E*.2a.H$^+$**

N	0.25064500	-0.53088200	0.02142200
N	-0.57599900	0.40690600	-0.07068400
C	1.59981600	-0.33096400	0.02239700
C	2.41196500	0.97117100	0.04214200

C	3.75573900	0.80635600	-0.02632000
C	2.31431200	-1.48346300	-0.00107100
H	1.85213500	-2.46125100	-0.00078400
C	-2.83936500	1.14771000	-0.13134900
C	-1.93959400	0.15243600	-0.04817800
C	-2.43074900	-1.26258800	0.08367600
C	-3.75909800	-1.42609200	0.11294700
H	-2.61774500	2.20204500	-0.22172500
H	-1.71164600	-2.07043800	0.14786400
H	-4.25252700	-2.38182200	0.20342000
H	4.44339000	1.63948300	-0.00915300
Si	4.09229100	-0.94302000	-0.05896900
Si	-4.43868900	0.24882400	-0.03076800
H	-5.79957900	0.78969100	-0.06138100
H	5.29966900	-1.76941300	-0.09336200
H	-0.29360600	1.38674300	-0.16201700
C	1.77856600	2.30395300	0.15588800
H	1.20623600	2.54221900	-0.75022300
H	1.11603300	2.36031100	1.02570800
H	2.53513300	3.07789600	0.26200600

PBE0-D3/def2-TZVP:

Zero-point correction= 0.179796 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.139966

Sum of electronic and zero-point Energies= -1036.509348

Sum of electronic and thermal Energies= -1036.496341

Sum of electronic and thermal Enthalpies= -1036.495397

Sum of electronic and thermal Free Energies= -1036.549179

PBE0-D3/def2-TZVP Electronic Energy = -1036.689145 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1036.69345278 a.u.

***Z*.2a.H$^+$**

C	1.56669300	0.07417400	0.96814700
C	1.64537900	0.60102400	-0.25406800
C	2.88703100	0.37328600	-1.07692700
H	2.95166900	0.79522100	-2.07457400
C	3.84374100	-0.37305600	-0.51427200
C	-1.13114600	-0.88077400	-0.98394200
C	-1.27624400	0.32212200	-0.40191300
C	-2.51331000	0.56868900	0.46246200
C	-3.31533700	-0.50521700	0.62143300
H	0.76933600	0.19904700	1.68628600
H	4.77573900	-0.63421300	-0.99198300
H	-0.35773700	-1.16117300	-1.68419600

H	-4.20068600	-0.49655300	1.23957700
Si	3.19048900	-0.79647700	1.12160800
Si	-2.62953400	-1.79228300	-0.41219700
H	3.70990900	-1.55654300	2.26081400
H	-3.05939700	-3.14312400	-0.78063300
N	-0.56165400	1.44144000	-0.77264800
N	0.67030400	1.49574400	-0.79674400
H	1.04107300	2.34549500	-1.23901100
C	-2.70966400	1.90982900	1.03450900
H	-1.80836400	2.21908800	1.57790400
H	-2.84807400	2.63919300	0.22936600
H	-3.57023600	1.93545200	1.69787100

PBE0-D3/def2-TZVP:

Zero-point correction= 0.179118 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.138240

Sum of electronic and zero-point Energies= -1036.496477

Sum of electronic and thermal Energies= -1036.483184

Sum of electronic and thermal Enthalpies= -1036.482239

Sum of electronic and thermal Free Energies= -1036.537355

PBE0-D3/def2-TZVP Electronic Energy = -1036.675595 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1036.67968822 a.u.

***E*.3a.H$^+$**

N	0.24884300	-0.57281700	0.00016500
N	-0.56460700	0.38470800	0.00006600
C	1.59164800	-0.36529700	0.00008900
C	2.34905400	0.95365700	0.00009000
C	3.71627000	0.90133500	0.00024700
C	2.38129800	-1.46397900	0.00000300
H	1.98535600	-2.47107000	0.00008600
C	-2.81376300	1.16205100	-0.00011100
C	-1.92948200	0.14909700	0.00003400
C	-2.44413600	-1.26402900	0.00016300
C	-3.77504800	-1.40786900	0.00003300
H	-2.57311200	2.21583100	-0.00031600
H	-1.73882700	-2.08642200	0.00032300
H	-4.28423300	-2.35960100	0.00012200
H	4.33947500	1.78441600	0.00020100
Si	4.13153800	-0.80766600	-0.00017000
Si	-4.42628900	0.28499000	-0.00012200
H	-5.77865200	0.84792300	-0.00016300
H	5.38352200	-1.56309400	-0.00097500
H	-0.24364600	1.36103200	0.00004600

O	1.58888300	2.00864700	-0.00002000
H	2.08085300	2.84624700	0.00002000

PBE0-D3/def2-TZVP:

Zero-point correction= 0.157111 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.117534

Sum of electronic and zero-point Energies= -1072.452024

Sum of electronic and thermal Energies= -1072.439530

Sum of electronic and thermal Enthalpies= -1072.438586

Sum of electronic and thermal Free Energies= -1072.491601

PBE0-D3/def2-TZVP Electronic Energy = -1072.609135 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1072.61361809 a.u.

***Z*.3a.H$^+$**

C	1.63449100	-0.02516500	0.99079500
C	1.67607900	0.62994900	-0.17019300
C	2.89249700	0.49884000	-1.05030700
H	2.92334900	1.02540900	-1.99912400
C	3.86775500	-0.29685000	-0.59832000
C	-1.09922600	-0.81283900	-0.89719000
C	-1.26428500	0.37885400	-0.29980200
C	-2.57900400	0.57672200	0.44044100
C	-3.42604800	-0.49629400	0.50177600
H	0.85124800	0.01830000	1.73344100
H	4.78596700	-0.50081700	-1.12776600
H	-0.26835300	-1.09208500	-1.52978700
H	-4.35891200	-0.48948200	1.04608800
Si	3.25888300	-0.90374300	0.99794300
Si	-2.66271000	-1.73675500	-0.47980900
H	3.80416500	-1.79877000	2.02125600
H	-3.04536000	-3.08104600	-0.91211800
N	-0.54638200	1.52398800	-0.54426400
N	0.68805900	1.57470200	-0.58519500
H	1.05065600	2.47141000	-0.92813600
O	-2.71687600	1.76517000	0.93084400
H	-3.55945700	1.88256700	1.39853300

PBE0-D3/def2-TZVP:

Zero-point correction= 0.156679 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.115243

Sum of electronic and zero-point Energies= -1072.428684

Sum of electronic and thermal Energies= -1072.416015

Sum of electronic and thermal Enthalpies= -1072.415071

Sum of electronic and thermal Free Energies= -1072.470120

PBE0-D3/def2-TZVP Electronic Energy = -1072.585362 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1072.58974028 a.u.

***E*.4a.H$^+$**

N	0.03639400	-0.81901500	0.00106800
N	-0.70727000	0.19441400	-0.01248500
C	1.38944300	-0.70496300	0.00048600
C	2.23496800	0.56003000	0.00096300
C	3.60024800	0.40458100	-0.00561100
C	2.10066700	-1.85709400	0.00011200
H	1.63316500	-2.83305500	0.00159300
C	-2.90026100	1.12409700	-0.02101500
C	-2.08506800	0.05461800	-0.00767900
C	-2.69381300	-1.32136100	0.01485100
C	-4.03123300	-1.37580500	0.01987000
H	-2.59035100	2.15879100	-0.03683100
H	-2.04466500	-2.18857500	0.02572600
H	-4.60385200	-2.29058800	0.03540200
H	4.29720100	1.22862500	-0.00472000
Si	3.89095800	-1.32733500	-0.00634700
Si	-4.56619300	0.35706200	-0.00428900
H	-5.87855700	1.00779000	-0.01087300
H	5.08723700	-2.16842300	-0.00986100
H	-0.31147000	1.14361500	-0.02608300
O	1.55206700	1.65646600	0.01065700
C	2.22630900	2.93828500	0.01695000
H	2.83603100	3.01227800	0.91618300
H	2.83019800	3.02475100	-0.88511800
H	1.43039200	3.67476800	0.02458900

PBE0-D3/def2-TZVP:

Zero-point correction= 0.184742 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.142836

Sum of electronic and zero-point Energies= -1111.692513

Sum of electronic and thermal Energies= -1111.678311

Sum of electronic and thermal Enthalpies= -1111.677367

Sum of electronic and thermal Free Energies= -1111.734420

PBE0-D3/def2-TZVP Electronic Energy = -1111.877255 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1111.88154081 a.u.

***Z*.4a.H$^+$**

C	-1.84510200	-0.09948700	0.94416900
C	-1.92466700	-0.59735800	-0.29184000
C	-3.24627300	-0.55404600	-1.01673300

H	-3.31494900	-0.95532600	-2.02305600
C	-4.26677400	0.01044900	-0.36269800
C	0.68346100	1.25563300	-0.84423300
C	0.98152800	-0.01482100	-0.52038100
C	2.35120400	-0.23880200	0.10532800
C	3.10372800	0.88033100	0.36597800
H	-0.98477300	-0.10192400	1.59675000
H	-5.26225500	0.12611200	-0.76321700
H	-0.20238800	1.58219100	-1.37192900
H	4.05886500	0.86151200	0.86679800
Si	-3.56919700	0.48895000	1.23988400
Si	2.18026100	2.21624600	-0.29758800
H	-4.11639700	1.12830200	2.43871300
H	2.41338200	3.65429900	-0.43240600
N	0.34536600	-1.14514500	-0.96518200
N	-0.88080300	-1.31231000	-0.94896100
H	-1.18293800	-2.14948000	-1.45801000
O	2.61718700	-1.47718000	0.31619100
C	3.88394400	-1.83940800	0.90450300
H	3.95302700	-1.40773000	1.90249400
H	3.87645600	-2.92296700	0.95111800
H	4.69135100	-1.48305400	0.26552300

PBE0-D3/def2-TZVP:

Zero-point correction= 0.185098 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.143656

Sum of electronic and zero-point Energies= -1111.667873

Sum of electronic and thermal Energies= -1111.653792

Sum of electronic and thermal Enthalpies= -1111.652848

Sum of electronic and thermal Free Energies= -1111.709315

PBE0-D3/def2-TZVP Electronic Energy = -1111.852971 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1111.85712312 a.u.

***E*.5a.H$^+$**

N	0.25560500	-0.56064900	0.21698800
N	-0.54549600	0.34268700	-0.15791700
C	1.58721800	-0.36075800	0.21401300
C	2.34545500	0.95372100	0.21690300
C	3.67738700	0.86911600	-0.20122100
C	2.36764900	-1.46513700	0.06790100
H	1.95421800	-2.46561200	0.08784900
C	-2.78543600	1.08052200	-0.51996800
C	-1.91472900	0.13403300	-0.12459100
C	-2.44799200	-1.17990600	0.38008300

C	-3.77968200	-1.30501000	0.40339700
H	-2.53334800	2.06214000	-0.89451700
H	-1.75288800	-1.95058300	0.69050100
H	-4.30365000	-2.18883800	0.73398300
H	4.32440300	1.73468100	-0.20571000
Si	4.06088700	-0.82679600	-0.34870100
Si	-4.40250800	0.27666600	-0.23587100
H	-5.74880200	0.80155900	-0.47686000
H	5.26760100	-1.59486900	-0.65138700
H	-0.22354400	1.22866100	-0.56048900
N	1.76643000	2.04051400	0.65702800
H	2.27196800	2.91782100	0.66659500
H	0.89175800	2.03949800	1.16224400

PBE0-D3/def2-TZVP:

Zero-point correction= 0.169536 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.129946

Sum of electronic and zero-point Energies= -1052.593192

Sum of electronic and thermal Energies= -1052.580508

Sum of electronic and thermal Enthalpies= -1052.579564

Sum of electronic and thermal Free Energies= -1052.632782

PBE0-D3/def2-TZVP Electronic Energy = -1052.762728 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1052.76752997 a.u.

***Z*.5a.H$^+$**

C	1.72552700	-0.56489900	0.63575000
C	1.75551200	0.55827800	-0.10196900
C	3.07912900	0.98322500	-0.69222000
H	3.12030900	1.87515200	-1.30974400
C	4.13545200	0.20789800	-0.43332500
C	-1.16988600	-0.92720400	-0.57173000
C	-1.32655900	0.34853400	-0.11103100
C	-2.74527600	0.66321900	0.31547100
C	-3.65255500	-0.41035400	0.30330400
H	0.88003800	-0.98153500	1.15984700
H	5.13296000	0.38635600	-0.80448700
H	-0.24786600	-1.32240900	-0.97692200
H	-4.66495300	-0.30426000	0.66554800
Si	3.46911700	-1.11377700	0.61544900
Si	-2.82040600	-1.75640700	-0.42740500
H	4.06872500	-2.27499500	1.27728300
H	-3.18073100	-3.11074400	-0.84362700
N	-0.53408600	1.42603400	-0.17035300
N	0.72081900	1.47830900	-0.29804400

H	1.03781900	2.42973000	-0.49009000
N	-3.01500600	1.88963500	0.63031500
H	-2.29502900	2.60188400	0.57403200
H	-3.94338100	2.17338300	0.91661700

PBE0-D3/def2-TZVP:

Zero-point correction= 0.169543 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.129494

Sum of electronic and zero-point Energies= -1052.584039

Sum of electronic and thermal Energies= -1052.571361

Sum of electronic and thermal Enthalpies= -1052.570416

Sum of electronic and thermal Free Energies= -1052.624088

PBE0-D3/def2-TZVP Electronic Energy = -1052.753582 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1052.75829016 a.u.

***E*.6a.H$^+$**

N	-0.05137300	-0.86613000	0.36584900
N	-0.75861300	0.02367500	-0.19536900
C	1.28937100	-0.79579000	0.33521600
C	2.17144600	0.37989000	-0.03938000
C	3.39060600	0.00047800	-0.63864000
C	1.92682500	-2.00530900	0.36610600
H	1.39740300	-2.91340000	0.62609500
C	-2.90568000	0.89026800	-0.77240400
C	-2.13881500	-0.04696200	-0.18197400
C	-2.80840300	-1.20145700	0.51458500
C	-4.14549900	-1.20264700	0.49804500
H	-2.54880600	1.76230800	-1.30118800
H	-2.19816900	-1.96285000	0.98500400
H	-4.76099300	-1.96440700	0.95168000
H	4.13493600	0.72506500	-0.93273000
Si	3.58859600	-1.71558100	-0.38637700
Si	-4.59311000	0.29592300	-0.42911500
H	-5.87831800	0.88550300	-0.81265200
H	4.66996300	-2.67129800	-0.62135700
H	-0.33796000	0.79419600	-0.72103100
N	1.83978500	1.61586400	0.24898000
C	2.61267900	2.73393800	-0.28020000
H	1.98441400	3.62106800	-0.24199600
H	3.49693900	2.89656700	0.34003400
H	2.90212600	2.53806400	-1.30933100
C	0.91744900	1.98828200	1.31775200
H	1.49479300	2.55086500	2.05438000
H	0.13248300	2.63663600	0.92892800

H	0.50591800	1.11888300	1.82018300

PBE0-D3/def2-TZVP:

Zero-point correction= 0.226954 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.184991

Sum of electronic and zero-point Energies= -1131.081106

Sum of electronic and thermal Energies= -1131.066035

Sum of electronic and thermal Enthalpies= -1131.065090

Sum of electronic and thermal Free Energies= -1131.123069

PBE0-D3/def2-TZVP Electronic Energy = -1131.308060 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1131.31339071 a.u.

***Z*.6a.H$^+$**

C	-2.16758800	0.42064600	0.69207100
C	-2.13596700	-0.43520400	-0.34734500
C	-3.45467300	-0.94134000	-0.88349700
H	-3.45521100	-1.62593100	-1.72682300
C	-4.56414300	-0.50035800	-0.28562100
C	0.52566900	1.50237700	-0.54972600
C	0.86510800	0.19250900	-0.32966600
C	2.31459000	-0.00896300	0.08548200
C	3.06741900	1.18554800	0.16194000
H	-1.33155800	0.87165900	1.20070400
H	-5.56685200	-0.77797000	-0.57205000
H	-0.43356000	1.80543300	-0.94939700
H	4.07068900	1.20245200	0.55858900
Si	-3.94986400	0.58564800	1.03231000
Si	2.02901200	2.51574000	-0.27731700
H	-4.61479700	1.37846600	2.06968800
H	2.18702500	3.96474200	-0.39238900
N	0.22236600	-0.86899300	-0.82819800
N	-1.02820400	-1.02213200	-0.95739700
H	-1.24816100	-1.83140500	-1.53725100
N	2.79969400	-1.19484100	0.33548000
C	1.99628300	-2.38411700	0.58853500
H	1.87391500	-2.95005800	-0.33758000
H	2.54937300	-2.99739000	1.29996700
H	1.03873700	-2.13794200	1.03271700
C	4.23676600	-1.41036700	0.45018300
H	4.44815000	-2.42122400	0.10495700
H	4.78188300	-0.69882400	-0.16201700
H	4.53451000	-1.32406600	1.49765700

PBE0-D3/def2-TZVP:

Zero-point correction= 0.225252 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.181585

Sum of electronic and zero-point Energies= -1131.069947

Sum of electronic and thermal Energies= -1131.054189

Sum of electronic and thermal Enthalpies= -1131.053245

Sum of electronic and thermal Free Energies= -1131.113613

PBE0-D3/def2-TZVP Electronic Energy = -1131.295198 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1131.30050522 a.u.

***E*.7a.H$^+$**

N	0.24841700	-0.55876500	0.00140500
N	-0.56299000	0.39647700	-0.02495200
C	1.59485700	-0.36129600	0.00371000
C	2.36439000	0.94760600	0.01780100
C	3.70689600	0.93127600	0.00556200
C	2.37991900	-1.46172700	-0.00956500
H	1.99019800	-2.47102400	-0.01906200
C	-2.81616600	1.16504300	-0.04085100
C	-1.92907800	0.15570900	-0.01632600
C	-2.43873600	-1.25750900	0.02692300
C	-3.76968800	-1.40617300	0.03712100
H	-2.58285400	2.22047500	-0.06887500
H	-1.73141500	-2.07803100	0.04622200
H	-4.27383900	-2.36022800	0.06601800
H	4.31662700	1.82291300	0.01813200
Si	4.12740800	-0.80144600	-0.01687700
Si	-4.43218000	0.27977200	-0.00794000
H	-5.78447200	0.84215400	-0.01553300
H	5.39225900	-1.53457000	-0.03850900
H	-0.26288800	1.37671300	-0.05205500
F	1.65009400	2.03816400	0.04774300

PBE0-D3/def2-TZVP:

Zero-point correction= 0.143717 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.103611

Sum of electronic and zero-point Energies= -1096.446604

Sum of electronic and thermal Energies= -1096.434067

Sum of electronic and thermal Enthalpies= -1096.433122

Sum of electronic and thermal Free Energies= -1096.486709

PBE0-D3/def2-TZVP Electronic Energy = -1096.590321 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1096.59353799 a.u.

***Z*.7a.H$^+$**

C	1.59954300	0.01335700	0.98792700

C	1.66395100	0.62406800	-0.19516400
C	2.87886800	0.43247300	-1.06446100
H	2.92559400	0.92547400	-2.03043200
C	3.83209100	-0.37161600	-0.58056100
C	-1.15892200	-0.80042700	-0.98754400
C	-1.25824300	0.37666100	-0.35141500
C	-2.50716700	0.57774200	0.49021400
C	-3.38924200	-0.42759200	0.58639500
H	0.82215500	0.11140500	1.73245600
H	4.74504900	-0.61853700	-1.10090900
H	-0.39165400	-1.08306200	-1.69430400
H	-4.27985300	-0.39842000	1.19589100
Si	3.20604000	-0.90977500	1.03183400
Si	-2.70912600	-1.68473500	-0.48375200
H	3.72012800	-1.78661800	2.08630300
H	-3.17548200	-3.01039700	-0.88972300
N	-0.53800500	1.51923100	-0.63082400
N	0.69213000	1.57059400	-0.64903000
H	1.06459800	2.45659200	-1.01413600
F	-2.60349700	1.72776900	1.07648200

PBE0-D3/def2-TZVP:

Zero-point correction= 0.143931 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.104375

Sum of electronic and zero-point Energies= -1096.426205

Sum of electronic and thermal Energies= -1096.413800

Sum of electronic and thermal Enthalpies= -1096.412856

Sum of electronic and thermal Free Energies= -1096.465761

PBE0-D3/def2-TZVP Electronic Energy = -1096.570136 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1096.57324212 a.u.

***E*.8a.H$^+$**

N	0.21192300	-0.68653400	0.00579200
N	-0.59102900	0.27162000	-0.04868100
C	1.56661700	-0.50768200	0.00637100
C	2.36950000	0.79200300	0.00948800
C	3.71049500	0.68196000	-0.01498000
C	2.29956600	-1.64485800	0.00087900
H	1.85488200	-2.63078200	0.00198300
C	-2.83596300	1.06029100	-0.08455800
C	-1.95918700	0.04276800	-0.03156400
C	-2.48380300	-1.36207600	0.05679600
C	-3.81672200	-1.49633300	0.07510000
H	-2.59399000	2.11262400	-0.14404300

H	-1.78540100	-2.18935400	0.10023100
H	-4.33003400	-2.44401000	0.13626500
H	4.38396800	1.52721100	-0.01195300
Si	4.06729600	-1.10100500	-0.02427700
Si	-4.46497300	0.19189900	-0.01972700
H	-5.80971300	0.77146500	-0.04163300
H	5.30520500	-1.87943100	-0.04403700
H	-0.28829500	1.25441700	-0.10018100
C	1.72190400	2.05501400	0.05172600
N	1.15002200	3.05474600	0.08630200

PBE0-D3/def2-TZVP:

Zero-point correction= 0.150021 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.109151

Sum of electronic and zero-point Energies= -1089.402831

Sum of electronic and thermal Energies= -1089.389376

Sum of electronic and thermal Enthalpies= -1089.388432

Sum of electronic and thermal Free Energies= -1089.443701

PBE0-D3/def2-TZVP Electronic Energy = -1089.552852 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1089.55612161 a.u.

***Z*.8a.H$^+$**

C	1.61953500	0.16680700	0.90094800
C	1.72992300	0.50388400	-0.38452600
C	3.04049700	0.28201300	-1.09293300
H	3.13307000	0.54646300	-2.14128800
C	4.02326800	-0.26653900	-0.36971200
C	-1.02077800	-1.30271700	-0.86204400
C	-1.18060100	-0.00630400	-0.54496400
C	-2.41711500	0.38685600	0.25194800
C	-3.23785700	-0.61337000	0.60433500
H	0.77311100	0.31836900	1.55540600
H	5.00385300	-0.50279900	-0.75418300
H	-0.24036000	-1.71411200	-1.48715300
H	-4.13311200	-0.48970200	1.19602300
Si	3.30996400	-0.50613000	1.27563500
Si	-2.48763000	-2.11110600	-0.12090500
H	3.80486300	-1.03829000	2.54705500
H	-2.89300200	-3.51717800	-0.12253400
N	-0.50424100	1.04428600	-1.13204300
N	0.71681200	1.18755300	-1.12384500
H	1.04444700	1.94804700	-1.73344000
C	-2.60892400	1.75253000	0.59038300
N	-2.74017700	2.86409600	0.85778500

PBE0-D3/def2-TZVP:

Zero-point correction= 0.149710 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.108339

Sum of electronic and zero-point Energies= -1089.386951

Sum of electronic and thermal Energies= -1089.373395

Sum of electronic and thermal Enthalpies= -1089.372451

Sum of electronic and thermal Free Energies= -1089.428322

PBE0-D3/def2-TZVP Electronic Energy = -1089.536661 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1089.53977383 a.u.

***E*. 9a.H$^+$**

N	0.10389500	-0.70503600	0.00003400
N	-0.68758500	0.26518800	-0.00008200
C	1.45980500	-0.56365400	0.00008400
C	2.34052000	0.68728300	-0.00004500
C	3.67895100	0.50623400	-0.00000400
C	2.14557200	-1.73164000	0.00023200
H	1.65463000	-2.69574100	0.00030600
C	-2.92115200	1.08525000	0.00015600
C	-2.05821200	0.05485700	-0.00015300
C	-2.60089200	-1.34710300	-0.00056000
C	-3.93486600	-1.46447900	-0.00056200
H	-2.66149200	2.13451100	0.00037700
H	-1.91251400	-2.18376200	-0.00081500
H	-4.46230800	-2.40626200	-0.00087100
H	4.38586300	1.32302700	-0.00005000
Si	3.94350000	-1.25831800	0.00021000
Si	-4.55512000	0.23872900	0.00040400
H	-5.89433400	0.83193500	0.00174500
H	5.13068200	-2.11283800	0.00038000
H	-0.35467600	1.23811900	-0.00010800
Cl	1.65319500	2.22727700	-0.00024200

PBE0-D3/def2-TZVP:

Zero-point correction= 0.142378 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.101465

Sum of electronic and zero-point Energies= -1456.721333

Sum of electronic and thermal Energies= -1456.708594

Sum of electronic and thermal Enthalpies= -1456.707650

Sum of electronic and thermal Free Energies= -1456.762246

PBE0-D3/def2-TZVP Electronic Energy = -1456.863711 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1456.86714459 a.u.

***Z*.9a.H$^+$**

C	-1.73575900	-0.07835500	0.91772900
C	-1.82636300	-0.53718600	-0.33128800
C	-3.13833200	-0.42417000	-1.06401100
H	-3.21677300	-0.80183600	-2.07907600
C	-4.13958400	0.16718800	-0.40328400
C	0.85433200	1.26699600	-0.89271100
C	1.08248400	-0.00193900	-0.51700900
C	2.37679200	-0.27882200	0.23537400
C	3.15934700	0.78020000	0.51663500
H	-0.88560800	-0.13865000	1.58112100
H	-5.12609200	0.33309900	-0.80856000
H	0.02633600	1.61759300	-1.49323100
H	4.07696000	0.72190300	1.08216900
Si	-3.43977400	0.58462200	1.21363600
Si	2.34010300	2.16676500	-0.26392000
H	-3.96143700	1.23433200	2.41797300
H	2.68440600	3.58190000	-0.40752200
N	0.42774900	-1.11016900	-1.01052400
N	-0.79545500	-1.26042500	-1.00340200
H	-1.11196100	-2.07106600	-1.54806400
Cl	2.68741300	-1.86858900	0.66400200

PBE0-D3/def2-TZVP:

Zero-point correction= 0.141834 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.100830

Sum of electronic and zero-point Energies= -1456.704925

Sum of electronic and thermal Energies= -1456.691997

Sum of electronic and thermal Enthalpies= -1456.691053

Sum of electronic and thermal Free Energies= -1456.745929

PBE0-D3/def2-TZVP Electronic Energy = -1456.846758 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1456.84991786 a.u.

***E*.10a.H$^+$**

N	-0.19716400	1.03318000	-0.00194100
N	-0.91180100	0.00522800	0.00523600
C	1.16698400	0.99868700	-0.00209400
C	2.15117500	-0.17154700	0.00038800
C	3.46826800	0.12731600	0.00340900
C	1.74930500	2.22235200	-0.00272300
H	1.17444200	3.13875900	-0.00445200
C	-3.07125100	-0.99162400	0.00735100
C	-2.29457800	0.10566500	0.00388800
C	-2.95039200	1.45877300	-0.00265100

C	-4.28945500	1.46615700	-0.00505900
H	-2.72644700	-2.01558300	0.01177800
H	-2.33236800	2.34855400	-0.00497500
H	-4.89360500	2.36057100	-0.00949700
H	4.25022800	-0.61807800	0.00496700
Si	3.57985400	1.90999200	0.00240700
Si	-4.76820900	-0.28221700	0.00050600
H	-6.05423000	-0.98323600	-0.00103300
H	4.68602100	2.86702900	0.00514900
H	-0.50321400	-0.94209300	0.01039500
Br	1.57767300	-1.92880800	-0.00260700

PBE0-D3/def2-TZVP:

Zero-point correction= 0.140600 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.097563

Sum of electronic and zero-point Energies= -3570.516591

Sum of electronic and thermal Energies= -3570.503337

Sum of electronic and thermal Enthalpies= -3570.502393

Sum of electronic and thermal Free Energies= -3570.559628

PBE0-D3/def2-TZVP Electronic Energy = -3570.657192 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -3570.66058697 a.u.

***Z*.10a.H$^+$**

C	2.05790700	-0.25903500	-0.87983200
C	2.14668600	-0.50086400	0.42913700
C	3.49582900	-0.44399100	1.09859300
H	3.57230200	-0.63088300	2.16504200
C	4.53498700	-0.13214800	0.31634200
C	-0.20048100	1.74391700	0.76908400
C	-0.63481400	0.48481700	0.59531300
C	-1.97988200	0.30115100	-0.08475400
C	-2.61324000	1.41217500	-0.50193200
H	1.17498800	-0.32214400	-1.49915000
H	5.55266200	-0.03335800	0.66214800
H	0.70375200	2.04312900	1.28062300
H	-3.55125700	1.41750500	-1.03621500
Si	3.81932200	0.08807800	-1.33256300
Si	-1.56682400	2.75801800	0.05333700
H	4.36467300	0.43033700	-2.64805100
H	-1.69554400	4.21562400	0.00609000
N	-0.13141200	-0.62952700	1.23365500
N	1.05763600	-0.95610300	1.23158100
H	1.27482200	-1.71762500	1.88579800
Br	-2.57876800	-1.42241800	-0.30329900

PBE0-D3/def2-TZVP:

Zero-point correction= 0.141399 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.099675

Sum of electronic and zero-point Energies= -3570.500200

Sum of electronic and thermal Energies= -3570.487146

Sum of electronic and thermal Enthalpies= -3570.486202

Sum of electronic and thermal Free Energies= -3570.541924

PBE0-D3/def2-TZVP Electronic Energy = -3570.641599 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -3570.64472129 a.u.

***E*.11a.H$^+$**

N	-0.49443100	1.27060300	-0.13473300
N	-1.12410400	0.23878400	0.19354600
C	0.86381600	1.36415400	-0.07919500
C	1.93916900	0.29207600	0.08607400
C	3.20389500	0.73222400	0.28964600
C	1.32840100	2.63756100	-0.13561600
H	0.67474400	3.48875700	-0.27214300
C	-3.19506800	-0.90365200	0.45439400
C	-2.50856500	0.20294300	0.12125100
C	-3.26541100	1.41835000	-0.33807300
C	-4.59824700	1.30137100	-0.38399100
H	-2.76922000	-1.83766400	0.79291000
H	-2.71815200	2.31471200	-0.60451500
H	-5.26818400	2.09022900	-0.69066700
H	4.05556400	0.07639300	0.39704400
Si	3.15072900	2.51409400	0.17263700
Si	-4.93703600	-0.39121800	0.17163300
H	-6.16498300	-1.16581700	0.36441100
H	4.15344200	3.57690300	0.25199100
H	-0.64872200	-0.61913000	0.51100600
I	1.55501200	-1.70718000	-0.11449900

PBE0-D3/def2-TZVP:

Zero-point correction= 0.140835 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.098613

Sum of electronic and zero-point Energies= -1294.379223

Sum of electronic and thermal Energies= -1294.366086

Sum of electronic and thermal Enthalpies= -1294.365141

Sum of electronic and thermal Free Energies= -1294.421445

PBE0-D3/def2-TZVP Electronic Energy = -1294.520058 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1294.52344515 a.u.

***Z*.11a.2H$^+$**

C	2.32647300	-0.29607900	-0.85206800
C	2.41527900	-0.51460300	0.46222400
C	3.77787600	-0.62699900	1.09662200
H	3.85853200	-0.78747100	2.16710100
C	4.82821100	-0.49362600	0.27964700
C	0.34945200	2.01371000	0.71888700
C	-0.23041300	0.80481500	0.61346600
C	-1.58785200	0.73294900	-0.05026800
C	-2.09852800	1.88445300	-0.52488900
H	1.42745400	-0.24390400	-1.44865500
H	5.85889300	-0.53160700	0.59771700
H	1.29198000	2.23318200	1.20025000
H	-3.03228000	1.97417300	-1.05916200
Si	4.10245600	-0.22748300	-1.35858600
Si	-0.90770700	3.13341300	-0.02774600
H	4.65581300	-0.02505900	-2.69963700
H	-0.88624400	4.59474500	-0.12720600
N	0.15036700	-0.33234600	1.29380300
N	1.30128800	-0.78540000	1.30671800
H	1.44030600	-1.52749500	2.00166700
I	-2.41859500	-1.12402000	-0.18658100

PBE0-D3/def2-TZVP:

Zero-point correction= 0.140604 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.098004

Sum of electronic and zero-point Energies= -1294.365969

Sum of electronic and thermal Energies= -1294.352645

Sum of electronic and thermal Enthalpies= -1294.351701

Sum of electronic and thermal Free Energies= -1294.408570

PBE0-D3/def2-TZVP Electronic Energy = -1294.506574 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1294.50969772 a.u.

***E*.1a.2H$^+$**

N	0.38716800	-0.50863100	-0.08360200
N	-0.38718200	0.50858200	-0.08345500
C	1.75161900	-0.50149000	-0.06920000
C	2.62851300	0.73250900	-0.00984400
C	3.94908400	0.45916200	-0.13685600
C	2.35919300	-1.71860200	-0.13131100
H	1.85206600	-2.67497200	-0.15919600
C	-2.35916800	1.71860500	-0.13106000
C	-1.75162700	0.50147500	-0.06904400
C	-2.62854400	-0.73251700	-0.00976400

C	-3.94911100	-0.45913400	-0.13672100
H	-1.85204300	2.67498000	-0.15876400
H	-4.71845900	-1.22008700	-0.12288400
H	4.71839700	1.22015300	-0.12305500
Si	4.17642500	-1.33470200	-0.19811100
Si	-4.17639200	1.33473200	-0.19823200
H	-5.30240300	2.26849700	-0.23833000
H	5.30248300	-2.26843800	-0.23745600
H	0.07990300	1.43745200	-0.11647900
Si	2.19301800	2.56372400	0.34532400
H	0.85364000	2.82621800	-0.25638900
H	2.11437900	2.69080900	1.81360100
H	3.23661900	3.36172200	-0.31475600
H	-0.07989700	-1.43752300	-0.11668500
Si	-2.19302600	-2.56373300	0.34531500
H	-0.85381100	-2.82625500	-0.25675800
H	-2.11405800	-2.69076400	1.81358600
H	-3.23683100	-3.36178200	-0.31438200

PBE0-D3/def2-TZVP:

Zero-point correction= 0.195290 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.152495

Sum of electronic and zero-point Energies= -1578.691237

Sum of electronic and thermal Energies= -1578.675315

Sum of electronic and thermal Enthalpies= -1578.674371

Sum of electronic and thermal Free Energies= -1578.734032

PBE0-D3/def2-TZVP Electronic Energy = -1578.886527 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1578.89190180 a.u.

***Z*.1a.2H$^+$**

C	-1.42607400	1.34795700	0.67373200
C	-1.59563200	0.09692100	0.15938500
C	-3.01739300	-0.34766000	-0.12765500
C	-3.97410800	0.53410700	0.24481100
C	1.42613800	1.34791000	-0.67395700
C	1.59560300	0.09690800	-0.15949400
C	3.01732500	-0.34771100	0.12764900
C	3.97411900	0.53396700	-0.24483000
H	-0.49863900	1.83996000	0.92985900
H	-5.03248600	0.36637300	0.09967800
H	0.49876000	1.83992300	-0.93026400
H	5.03247500	0.36614300	-0.09965200
Si	-3.16351200	1.96869300	0.97139000
Si	3.16362900	1.96866200	-0.97130300

H	-3.55298100	3.22226800	1.61941800
H	3.55317700	3.22253000	-1.61872200
N	0.64643300	-0.86156900	0.01301700
N	-0.64647200	-0.86157500	-0.01308800
H	-1.03256500	-1.81192900	-0.11444500
Si	3.47403200	-1.99295000	0.99272600
H	2.42280800	-2.96438600	0.58434500
H	4.81194900	-2.35699700	0.49748700
H	3.39417700	-1.71195700	2.44223300
H	1.03254200	-1.81190800	0.11449200
Si	-3.47412700	-1.99291600	-0.99266100
H	-2.42290600	-2.96434800	-0.58424900
H	-4.81206800	-2.35699600	-0.49751900
H	-3.39415800	-1.71191200	-2.44216600

PBE0-D3/def2-TZVP:

Zero-point correction= 0.191936 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.145741

Sum of electronic and zero-point Energies= -1578.678995

Sum of electronic and thermal Energies= -1578.661657

Sum of electronic and thermal Enthalpies= -1578.660713

Sum of electronic and thermal Free Energies= -1578.725190

PBE0-D3/def2-TZVP Electronic Energy = -1578.870931 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1578.87608177 a.u.

***E*.2a.2H$^+$**

N	0.46222900	-0.44576500	-0.04379100
N	-0.46204400	0.44517200	-0.04335400
C	1.81159300	-0.26182100	-0.02493500
C	2.54758100	1.06687600	0.04846200
C	3.89853300	0.94888000	0.00338900
C	2.56952000	-1.39314900	-0.07310000
H	2.18128700	-2.40431500	-0.11400600
C	-2.56901900	1.39306500	-0.07276400
C	-1.81143700	0.26149200	-0.02463800
C	-2.54788100	-1.06694200	0.04863900
C	-3.89880200	-0.94851700	0.00314100
H	-2.18046700	2.40411500	-0.11348200
H	-4.55146000	-1.80904900	0.04936500
H	4.55093300	1.80961300	0.04948800
Si	4.33079000	-0.78665200	-0.06976900
Si	-4.33049600	0.78713900	-0.06992400
H	-5.56107600	1.57621500	-0.10342200
H	5.56164900	-1.57530900	-0.10290400

H	-0.13477900	1.41389300	-0.05157300
C	1.86128700	2.36962500	0.18584800
H	1.25108000	2.59749400	-0.69811800
H	1.24376800	2.40368200	1.09108700
H	2.59182100	3.17047900	0.26883100
H	0.13512100	-1.41452000	-0.05231700
C	-1.86204300	-2.36989600	0.18607300
H	-1.25287600	-2.59829600	-0.69850600
H	-1.24354800	-2.40397100	1.09059100
H	-2.59286400	-3.17039100	0.26998400

PBE0-D3/def2-TZVP:

Zero-point correction= 0.221115 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.179866

Sum of electronic and zero-point Energies= -1076.094004

Sum of electronic and thermal Energies= -1076.079597

Sum of electronic and thermal Enthalpies= -1076.078653

Sum of electronic and thermal Free Energies= -1076.135253

PBE0-D3/def2-TZVP Electronic Energy = -1076.315119 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1076.32129841 a.u.

***Z*.2a.2H$^+$**

C	1.47207600	-0.94016300	0.67080500
C	1.59320600	0.28079300	0.07927900
C	2.98273500	0.66232300	-0.40768100
C	3.94990100	-0.25996800	-0.16120600
C	-1.42777900	-1.00760600	-0.51410200
C	-1.58775000	0.24615100	-0.00374600
C	-3.01082000	0.64347300	0.36414400
C	-3.96495900	-0.26641100	0.03373700
H	0.57595000	-1.37787800	1.08797000
H	4.97269300	-0.12654200	-0.48362200
H	-0.50205000	-1.50081900	-0.77695900
H	-5.01129700	-0.11595000	0.25863100
Si	3.20906000	-1.61776700	0.72942000
Si	-3.16313200	-1.64654600	-0.76394700
H	3.65580400	-2.85660400	1.36532200
H	-3.56323800	-2.88247800	-1.43553700
N	-0.65242300	1.22113200	0.11773200
N	0.63992000	1.24002600	-0.02306300
H	0.98080800	2.18964600	-0.19023900
C	-3.26263900	1.92294400	1.03669000
H	-2.56543300	2.07909900	1.86941300
H	-3.12616500	2.75840000	0.33406500

H	-4.28198600	1.97476400	1.40978400
H	-1.02154800	2.16732500	0.23989300
C	3.19142700	1.93797300	-1.10167100
H	2.47444400	2.05570200	-1.92559900
H	3.04250100	2.78315600	-0.41424700
H	4.20165500	2.00739500	-1.49567900

PBE0-D3/def2-TZVP:

Zero-point correction= 0.219277 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.177710

Sum of electronic and zero-point Energies= -1076.086219

Sum of electronic and thermal Energies= -1076.071464

Sum of electronic and thermal Enthalpies= -1076.070519

Sum of electronic and thermal Free Energies= -1076.127786

PBE0-D3/def2-TZVP Electronic Energy = -1076.305496 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1076.31146102 a.u.

***E*.3a.2H$^+$**

N	0.44345800	-0.46619500	-0.00016600
N	-0.44346700	0.46627600	-0.00006000
C	1.79010600	-0.30125800	-0.00003200
C	2.49263300	1.03580100	0.00001500
C	3.85919300	1.01237800	0.00015700
C	2.60577500	-1.38645000	-0.00003400
H	2.26831100	-2.41576500	-0.00005900
C	-2.60582200	1.38644300	-0.00006500
C	-1.79013000	0.30129000	-0.00007100
C	-2.49262500	-1.03579200	-0.00003300
C	-3.85918100	-1.01243700	-0.00007600
H	-2.26845300	2.41578800	-0.00017800
H	-4.45882300	-1.91221600	-0.00008800
H	4.45889400	1.91211700	0.00015400
Si	4.33854900	-0.68938400	0.00008200
Si	-4.33855900	0.68932500	0.00009900
H	-5.60491200	1.41846100	0.00071400
H	5.60494800	-1.41844200	-0.00005300
H	-0.06304900	1.42444800	-0.00006500
O	1.69809800	2.06166500	-0.00010400
H	2.14992600	2.92352600	-0.00012000
H	0.06299500	-1.42438500	-0.00017100
O	-1.69804000	-2.06161600	0.00006100
H	-2.14979000	-2.92351600	0.00008500

PBE0-D3/def2-TZVP:

Zero-point correction= 0.174852 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.134783

Sum of electronic and zero-point Energies= -1147.981278

Sum of electronic and thermal Energies= -1147.967866

Sum of electronic and thermal Enthalpies= -1147.966922

Sum of electronic and thermal Free Energies= -1148.021347

PBE0-D3/def2-TZVP Electronic Energy = -1148.156130 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1148.16253155 a.u.

***Z*.3a.2H$^+$**

C	1.49205100	-0.99600000	0.52471600
C	1.57725900	0.27578800	0.05087400
C	2.97881300	0.71526200	-0.32008300
C	3.98621800	-0.20393300	-0.16875800
C	-1.49225700	-0.99533900	-0.52612700
C	-1.57740800	0.27606900	-0.05141100
C	-2.97871700	0.71524600	0.32070000
C	-3.98601300	-0.20418500	0.17005800
H	0.59900300	-1.50004800	0.86509800
H	5.01183000	0.00030400	-0.44158200
H	-0.59949500	-1.49868800	-0.86828600
H	-5.01147900	-0.00031700	0.44369700
Si	3.24271700	-1.64046200	0.54006100
Si	-3.24276800	-1.64035400	-0.53978900
H	3.70964500	-2.93652300	1.02691400
H	-3.70989400	-2.93645400	-1.02635800
N	-0.64682900	1.25054700	0.05026300
N	0.64681900	1.25028700	-0.05133400
H	1.03170700	2.19014100	-0.20047900
O	-3.02682300	1.93268100	0.73363300
H	-3.91422200	2.24819800	0.98068700
H	-1.03138100	2.19050600	0.19950700
O	3.02694900	1.93265800	-0.73307600
H	3.91439400	2.24832200	-0.97978200

PBE0-D3/def2-TZVP:

Zero-point correction= 0.174561 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.134327

Sum of electronic and zero-point Energies= -1147.964000

Sum of electronic and thermal Energies= -1147.950641

Sum of electronic and thermal Enthalpies= -1147.949697

Sum of electronic and thermal Free Energies= -1148.004234

PBE0-D3/def2-TZVP Electronic Energy = -1148.138561 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1148.14498041 a.u.

***E*.4a.2H$^+$**

N	-0.35921500	0.53390300	-0.02104700
N	0.35924400	-0.53436000	-0.02113500
C	-1.71325600	0.58859000	-0.01999600
C	-2.61419200	-0.62517700	0.00155900
C	-3.96492000	-0.38115100	-0.01163000
C	-2.34911100	1.78879300	-0.03858700
H	-1.85317800	2.75256700	-0.05397400
C	2.34940200	-1.78888200	-0.03871800
C	1.71334700	-0.58880500	-0.02000800
C	2.61412100	0.62515600	0.00177800
C	3.96486700	0.38136800	-0.01145900
H	1.85365800	-2.75275200	-0.05419000
H	4.70822900	1.16432000	0.00155900
H	-4.70840900	-1.16397100	0.00134200
Si	-4.16635500	1.37227700	-0.03649300
Si	4.16656900	-1.37203400	-0.03651500
H	5.30394900	-2.28908500	-0.04923900
H	-5.30361700	2.28946900	-0.04914400
H	-0.18442200	-1.41069600	-0.01780300
O	-1.99484300	-1.75583600	0.04223300
C	-2.73701700	-3.00719100	0.09068200
H	-3.36125600	-3.00495400	0.98231400
H	-3.32662200	-3.09773500	-0.82000200
H	-1.97710200	-3.77857500	0.14531400
H	0.18465900	1.41016300	-0.01740000
O	1.99465200	1.75577000	0.04258800
C	2.73658600	3.00729600	0.09034600
H	3.36191500	3.00499300	0.98121000
H	3.32505700	3.09813500	-0.82104100
H	1.97651000	3.77846300	0.14606700

PBE0-D3/def2-TZVP:

Zero-point correction= 0.230307 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.185819

Sum of electronic and zero-point Energies= -1226.464561

Sum of electronic and thermal Energies= -1226.447847

Sum of electronic and thermal Enthalpies= -1226.446903

Sum of electronic and thermal Free Energies= -1226.509049

PBE0-D3/def2-TZVP Electronic Energy = -1226.694868 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1226.70093073 a.u.

***Z*.4a.2H$^+$**

C	-1.44171300	1.35480200	0.53140100
C	-1.56667900	0.07223900	0.09552400
C	-2.99783500	-0.39084100	-0.09573500
C	-3.99381100	0.51084800	0.20590600
C	1.49045100	1.31326400	-0.68045800
C	1.57604000	0.04131300	-0.20761200
C	2.98141300	-0.41842900	0.12105500
C	3.99647800	0.49449500	-0.06278800
H	-0.52358900	1.88933400	0.72396800
H	-5.04564900	0.29364500	0.09123100
H	0.59577000	1.81397600	-1.02072000
H	5.03104900	0.28615900	0.16670600
Si	-3.18106400	1.96070800	0.79696000
Si	3.24109900	1.94178100	-0.73283400
H	-3.60143600	3.24968800	1.34182400
H	3.70827400	3.23831000	-1.21839500
N	0.64120300	-0.92339400	-0.07959200
N	-0.65613700	-0.90176500	-0.10926300
H	-1.06987100	-1.83171000	-0.24607000
O	3.02686500	-1.62862000	0.52806600
C	4.28750100	-2.24760900	0.90077400
H	4.72393900	-1.67961300	1.72075500
H	4.02232200	-3.25122300	1.21229800
H	4.93593100	-2.26164600	0.02646500
H	1.02502200	-1.86793700	0.03982900
O	-3.07781000	-1.59462700	-0.51661300
C	-4.36492400	-2.20966700	-0.79516900
H	-4.86403100	-1.62957900	-1.56977800
H	-4.12608400	-3.20872200	-1.14061800
H	-4.94156500	-2.23593000	0.12771300

PBE0-D3/def2-TZVP:

Zero-point correction= 0.231267 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.186991

Sum of electronic and zero-point Energies= -1226.446785

Sum of electronic and thermal Energies= -1226.430159

Sum of electronic and thermal Enthalpies= -1226.429215

Sum of electronic and thermal Free Energies= -1226.491062

PBE0-D3/def2-TZVP Electronic Energy = -1226.678053 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1226.68406344 a.u.

***E*.5a.2H$^+$**

N	-0.43111500	-0.49770900	-0.25021900
N	0.43110000	0.49771000	-0.25014900

C	-1.77299700	-0.35917900	-0.13745900
C	-2.44152200	0.83269400	0.49996400
C	-3.79862600	0.96592500	0.18686700
C	-2.62155100	-1.29316200	-0.65005100
H	-2.29316100	-2.22361900	-1.09763100
C	2.62151600	1.29318800	-0.64997100
C	1.77298200	0.35918100	-0.13738700
C	2.44154000	-0.83271200	0.49997500
C	3.79862200	-0.96594300	0.18678600
H	2.29310700	2.22365800	-1.09750800
H	4.39089900	-1.78037100	0.58039800
H	-4.39088400	1.78033400	0.58054600
H	0.06216200	1.41686700	-0.49534300
N	-1.79134000	1.59715600	1.33363100
H	-2.26048200	2.39019100	1.75641500
H	-0.89502100	1.36035300	1.73888700
H	-0.06217900	-1.41683900	-0.49551500
N	1.79143700	-1.59717200	1.33370800
H	0.89517600	-1.36035900	1.73908200
H	2.26062600	-2.39020200	1.75644800
Si	4.29661500	0.52911200	-0.60027300
Si	-4.29665400	-0.52910300	-0.60022300
H	5.57051300	1.07743900	-1.06003300
H	-5.57057300	-1.07741500	-1.05994100

PBE0-D3/def2-TZVP:

Zero-point correction= 0.200679 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.160335

Sum of electronic and zero-point Energies= -1108.264567

Sum of electronic and thermal Energies= -1108.250696

Sum of electronic and thermal Enthalpies= -1108.249752

Sum of electronic and thermal Free Energies= -1108.304911

PBE0-D3/def2-TZVP Electronic Energy = -1108.465246 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1108.47205055 a.u.

***Z*.5a.2H$^+$**

C	1.36429700	-0.85424200	0.62016800
C	1.55032900	0.35145700	0.00717500
C	2.97730000	0.60254800	-0.43395800
C	3.91365700	-0.32936300	0.04854800
C	-1.41844700	-0.75522500	-0.78579700
C	-1.55969000	0.40204000	-0.07888100
C	-2.94366400	0.61316700	0.49897900
C	-3.89868800	-0.33560200	0.08960300

H	0.40966900	-1.25225800	0.93857800
H	4.96130200	-0.25504700	-0.20748000
H	-0.49762100	-1.08519700	-1.24938600
H	-4.91509900	-0.30108200	0.45582500
Si	3.02987400	-1.57661700	0.91020400
Si	-3.08370900	-1.52379100	-0.91121400
H	3.37547600	-2.79859600	1.63197900
H	-3.47462100	-2.73053200	-1.63562500
N	-0.64041400	1.38497500	0.05890800
N	0.65960300	1.35447700	-0.14533700
H	1.02595100	2.29216300	-0.28835700
N	-3.19310600	1.57058800	1.33967500
H	-2.50399900	2.20786500	1.71554700
H	-4.12529100	1.67567400	1.72521000
H	-0.96658600	2.33858400	0.20191400
N	3.27610700	1.58093800	-1.23333700
H	2.60335000	2.19458200	-1.67344500
H	4.23526400	1.71401000	-1.53500400

PBE0-D3/def2-TZVP:

Zero-point correction= 0.200826 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.159565

Sum of electronic and zero-point Energies= -1108.260045

Sum of electronic and thermal Energies= -1108.246067

Sum of electronic and thermal Enthalpies= -1108.245123

Sum of electronic and thermal Free Energies= -1108.301306

PBE0-D3/def2-TZVP Electronic Energy = -1108.460871 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1108.46778517 a.u.

***E*.6a.2H$^+$**

N	0.32750600	0.56694100	-0.29146200
N	-0.32761100	-0.56713000	-0.29152100
C	1.67223700	0.72067600	-0.27817800
C	2.68258700	-0.37323900	-0.00321000
C	3.91464600	-0.14318000	-0.64559600
C	2.19710300	1.89177800	-0.75168300
H	1.58738200	2.75199300	-1.00139500
C	-2.19745000	-1.89160300	-0.75192900
C	-1.67237500	-0.72073200	-0.27812500
C	-2.68255500	0.37322300	-0.00266000
C	-3.91472200	0.14353200	-0.64496400
H	-1.58786900	-2.75180000	-1.00204200
H	-4.73973200	0.83559500	-0.56772100
H	4.73974700	-0.83517700	-0.56873300

H	0.22902900	-1.40200600	-0.46819200
N	2.46115300	-1.37851400	0.81274500
H	-0.22922700	1.40183000	-0.46774300
N	-2.46088100	1.37823700	0.81355200
C	3.38935900	-2.50442200	0.86680400
H	2.85413800	-3.35074600	1.29177700
H	3.73562100	-2.75793200	-0.13135500
H	4.23152300	-2.25439000	1.51568100
C	1.51863800	-1.35026100	1.92536700
H	0.99957600	-0.40011700	1.98566800
H	0.83187600	-2.19476500	1.86842800
H	2.10902600	-1.45216200	2.83867600
C	-1.51819500	1.34956900	1.92600600
H	-0.99928300	0.39932500	1.98601200
H	-0.83130900	2.19398000	1.86914700
H	-2.10841200	1.45135400	2.83943800
C	-3.38892800	2.50425100	0.86806900
H	-3.73526500	2.75810100	-0.12997700
H	-4.23105400	2.25411900	1.51696000
H	-2.85355600	3.35037800	1.29324800
Si	3.94798700	1.54450100	-1.14298400
Si	-3.94833900	-1.54398000	-1.14288800
H	4.97854500	2.43395000	-1.67410500
H	-4.97908200	-2.43311800	-1.67416700

PBE0-D3/def2-TZVP:

Zero-point correction= 0.313827 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.268058

Sum of electronic and zero-point Energies= -1265.239776

Sum of electronic and thermal Energies= -1265.220663

Sum of electronic and thermal Enthalpies= -1265.219719

Sum of electronic and thermal Free Energies= -1265.285545

PBE0-D3/def2-TZVP Electronic Energy = -1265.553603 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1265.56170050 a.u.

***Z*.6a.2H$^+$**

C	1.20902500	-1.23464400	0.97653500
C	1.53287000	-0.05640800	0.35831700
C	3.00624100	0.08886400	0.00253600
C	3.73409600	-1.10470400	0.18228600
C	-1.20898300	-1.23458500	-0.97653100
C	-1.53289600	-0.05641600	-0.35823500
C	-3.00625500	0.08878900	-0.00246900
C	-3.73407000	-1.10476500	-0.18222900

H	0.19894300	-1.50273200	1.25117600
H	4.78562100	-1.18015600	-0.04929800
H	-0.19889600	-1.50262600	-1.25118500
H	-4.78559300	-1.18024700	0.04933700
Si	2.71182100	-2.23171500	1.08357300
Si	-2.71178000	-2.23165900	-1.08365000
H	2.95990100	-3.51355500	1.73943100
H	-2.95996000	-3.51333500	-1.73979300
N	-0.66576800	0.90156500	0.02352600
N	0.66573000	0.90155000	-0.02341900
H	1.03216300	1.79849700	-0.32325900
N	-3.57083900	1.20325000	0.39936400
C	-3.08105300	2.54849400	0.12029900
H	-3.94787600	3.15056600	-0.15191000
H	-2.64592800	2.99299700	1.01943500
H	-2.40841100	2.56327800	-0.73361100
C	-4.88981300	1.18883100	1.02324600
H	-4.94430200	2.05265200	1.68348400
H	-5.65808600	1.28460500	0.25204400
H	-5.03119000	0.28083800	1.60149900
H	-1.03218200	1.79852000	0.32336600
N	3.57081800	1.20329900	-0.39935200
C	3.08101700	2.54857900	-0.12040900
H	3.94785500	3.15070500	0.15161700
H	2.64577200	2.99296800	-1.01954600
H	2.40845500	2.56344800	0.73356200
C	4.88982100	1.18882400	-1.02321300
H	4.94433500	2.05263300	-1.68346000
H	5.65807200	1.28456800	-0.25199100
H	5.03114300	0.28081000	-1.60144900

PBE0-D3/def2-TZVP:

Zero-point correction= 0.312808 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.265830

Sum of electronic and zero-point Energies= -1265.231420

Sum of electronic and thermal Energies= -1265.211951

Sum of electronic and thermal Enthalpies= -1265.211007

Sum of electronic and thermal Free Energies= -1265.278398

PBE0-D3/def2-TZVP Electronic Energy = -1265.544228 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1265.55252823 a.u.

***E*.7a.2H$^+$**

N	0.44467300	-0.46373600	0.04569000
N	-0.44469000	0.46378100	0.04549600

C	1.79314400	-0.29923500	0.02497100
C	2.50403800	1.02672100	-0.03092800
C	3.84698500	1.04133800	-0.03484500
C	2.60874500	-1.38511200	0.05072900
H	2.28236100	-2.41801400	0.08681200
C	-2.60878200	1.38511600	0.05066600
C	-1.79316900	0.29925700	0.02489100
C	-2.50402100	-1.02672500	-0.03092900
C	-3.84697200	-1.04137100	-0.03481700
H	-2.28239900	2.41802000	0.08671500
H	-4.42885300	-1.95186900	-0.07616100
H	4.42887100	1.95183900	-0.07608500
Si	4.34675400	-0.67742400	0.01689900
Si	-4.34675700	0.67738600	0.01694300
H	-5.62347700	1.38840900	0.03111300
H	5.62347700	-1.38844800	0.03094500
H	-0.09070800	1.42668000	0.05426800
F	1.75303000	2.08636300	-0.07900600
H	0.09068600	-1.42663900	0.05471900
F	-1.75298600	-2.08633000	-0.07908800

PBE0-D3/def2-TZVP:

Zero-point correction= 0.148329 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.107208

Sum of electronic and zero-point Energies= -1195.959330

Sum of electronic and thermal Energies= -1195.945825

Sum of electronic and thermal Enthalpies= -1195.944880

Sum of electronic and thermal Free Energies= -1196.000451

PBE0-D3/def2-TZVP Electronic Energy = -1196.107659 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1196.11157702 a.u.

***Z*.7a.2H$^+$**

C	-1.48660600	0.97738800	0.53777500
C	-1.57807200	-0.28679300	0.04538600
C	-2.98147900	-0.69590400	-0.33897000
C	-3.99351500	0.17752100	-0.17506300
C	1.48686500	0.97667100	-0.53917800
C	1.57825200	-0.28718700	-0.04606600
C	2.98140000	-0.69596100	0.33944600
C	3.99337800	0.17760500	0.17590000
H	-0.59788700	1.48268300	0.88965200
H	-5.01561900	-0.03965200	-0.45344600
H	0.59829800	1.48086900	-0.89290000
H	5.01535000	-0.03922200	0.45503000

Si	-3.25447000	1.62195000	0.56558100
Si	3.25450800	1.62188900	-0.56524300
H	-3.72434700	2.90807900	1.07616200
H	3.72448400	2.90846700	-1.07459700
N	0.64470800	-1.26675900	0.04628000
N	-0.64466900	-1.26647100	-0.04735200
H	-1.02036300	-2.21390900	-0.17362400
F	3.09291500	-1.88961200	0.81226200
H	1.02008700	-2.21433100	0.17244200
F	-3.09315400	-1.88974000	-0.81129900

PBE0-D3/def2-TZVP:

Zero-point correction= 0.148329 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.107117

Sum of electronic and zero-point Energies= -1195.941523

Sum of electronic and thermal Energies= -1195.928172

Sum of electronic and thermal Enthalpies= -1195.927228

Sum of electronic and thermal Free Energies= -1195.982735

PBE0-D3/def2-TZVP Electronic Energy = -1196.089852 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1196.09368681 a.u.

***E*.8a.2H$^+$**

N	0.43900400	-0.46567500	0.04872200
N	-0.43906800	0.46591200	0.04828200
C	1.79665800	-0.32988700	0.03300400
C	2.56174100	0.97271600	-0.01119400
C	3.90658600	0.87876200	-0.00178500
C	2.54535500	-1.46485100	0.05517900
H	2.15583100	-2.47550800	0.08235800
C	-2.54560300	1.46485900	0.05447400
C	-1.79672000	0.33002000	0.03264200
C	-2.56167100	-0.97272800	-0.01114300
C	-3.90651900	-0.87893900	-0.00146100
H	-2.15641200	2.47564900	0.08122700
H	-4.56256300	-1.73868600	-0.03239100
H	4.56274800	1.73840700	-0.03296900
Si	4.32343700	-0.89444200	0.03513900
Si	-4.32361200	0.89420500	0.03527500
H	-5.55910700	1.67557900	0.04142800

H	5.55875500	-1.67610000	0.04068200
H	-0.07743900	1.43433600	0.04933100
C	1.87866900	2.21292600	-0.07893100
N	1.25134400	3.17826000	-0.13511100
H	0.07736400	-1.43407700	0.05012900
C	-1.87840600	-2.21282200	-0.07905400
N	-1.25088900	-3.17801300	-0.13560500

PBE0-D3/def2-TZVP:

Zero-point correction= 0.161403 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.118875

Sum of electronic and zero-point Energies= -1181.867961

Sum of electronic and thermal Energies= -1181.852805

Sum of electronic and thermal Enthalpies= -1181.851860

Sum of electronic and thermal Free Energies= -1181.910489

PBE0-D3/def2-TZVP Electronic Energy = -1182.029364 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1182.03344558 a.u.

***Z*. 8a.2H$^+$**

C	1.39570100	-1.26356200	0.50028700
C	1.57653700	-0.00107600	0.02554100
C	3.02419900	0.40524500	-0.18844200
C	3.97407500	-0.48790200	0.15167000
C	-1.50090600	-1.18229900	-0.73565300
C	-1.59245700	0.06115300	-0.19532000
C	-2.97909200	0.48002500	0.25385000
C	-3.97615600	-0.41008600	0.07745600
H	0.46267600	-1.77538000	0.68812600
H	5.03394300	-0.30668900	0.03696500
H	-0.62281300	-1.64466300	-1.16617400
H	-4.99734900	-0.23412600	0.38626400
Si	3.11577400	-1.93404300	0.82540500
Si	-3.24795400	-1.85902700	-0.73488300
H	3.50069800	-3.20508400	1.43714900
H	-3.73344000	-3.13007900	-1.27034400
N	-0.62934600	1.02122500	-0.12959500
N	0.65974200	0.98102700	-0.18021300
H	1.06138900	1.91804600	-0.32502300
C	-3.14189200	1.76163300	0.83143800
N	-3.19198000	2.82570000	1.27152200
H	-0.97915600	1.98521200	-0.04897000
C	3.28813200	1.69267000	-0.71114200
N	3.40668800	2.76646600	-1.11363000

PBE0-D3/def2-TZVP:

Zero-point correction= 0.160990 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.116858

Sum of electronic and zero-point Energies= -1181.849517

Sum of electronic and thermal Energies= -1181.834128

Sum of electronic and thermal Enthalpies= -1181.833184

Sum of electronic and thermal Free Energies= -1181.893649

PBE0-D3/def2-TZVP Electronic Energy = -1182.010507 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1182.01437622 a.u.

***E*. 9a.2H$^+$**

N	0.41895100	-0.48379100	-0.00403700
N	-0.41900800	0.48391900	-0.00397600
C	1.77783500	-0.41844500	-0.00641000
C	2.64325600	0.82612400	0.00484900
C	3.98065800	0.62580200	-0.00007900
C	2.45116000	-1.59978100	-0.02198900
H	1.97754500	-2.57441000	-0.03893900
C	-2.45128800	1.59981400	-0.02212000
C	-1.77791300	0.41851400	-0.00645100
C	-2.64323100	-0.82611200	0.00487300
C	-3.98063000	-0.62590500	-0.00009500
H	-1.97774700	2.57447300	-0.03927200
H	-4.69271800	-1.43942000	0.00957700
H	4.69271100	1.43934800	0.00970300
Si	4.25854900	-1.14425800	-0.01666100
Si	-4.25863400	1.14416900	-0.01664100
H	-5.43016500	2.01849100	-0.02237500
H	5.42992500	-2.01878300	-0.02286300
H	0.00444400	1.42493700	0.00149600
Cl	1.96363300	2.36285500	0.02671600
H	-0.00458700	-1.42478900	0.00129000
Cl	-1.96345200	-2.36282900	0.02670900

PBE0-D3/def2-TZVP:

Zero-point correction= 0.144850 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.102577

Sum of electronic and zero-point Energies= -1916.514657

Sum of electronic and thermal Energies= -1916.500721

Sum of electronic and thermal Enthalpies= -1916.499777

Sum of electronic and thermal Free Energies= -1916.556929

PBE0-D3/def2-TZVP Electronic Energy = -1916.659507 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1916.66397448 a.u.

***Z*.9a.2H$^+$**

C	-1.42150000	1.33385400	0.48811300
C	-1.57508900	0.05609600	0.04544300
C	-3.02156700	-0.37505100	-0.14995500
C	-3.98543100	0.52505500	0.15676500
C	1.49989600	1.26468100	-0.70345500
C	1.59110300	0.00763500	-0.19291400
C	2.99346200	-0.41827100	0.20920500
C	3.98464100	0.49240300	0.05572800
H	-0.49517600	1.85930000	0.66864400
H	-5.04063800	0.32201700	0.04054200
H	0.61309300	1.74080200	-1.09762400
H	5.00910100	0.30461800	0.34489500
Si	-3.14823700	1.97560800	0.78070700
Si	3.24307800	1.92840400	-0.71040700
H	-3.54896200	3.25865300	1.35520400
H	3.71841300	3.20690700	-1.23614100
N	0.63683000	-0.94767500	-0.09930200
N	-0.65603800	-0.91527600	-0.15078700
H	-1.06556400	-1.84921800	-0.29449800
Cl	3.20395800	-1.95940700	0.80123200
H	1.00195700	-1.90304100	0.01257200
Cl	-3.30858300	-1.91553100	-0.71186400

PBE0-D3/def2-TZVP:

Zero-point correction= 0.145740 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.104349

Sum of electronic and zero-point Energies= -1916.502800

Sum of electronic and thermal Energies= -1916.489135

Sum of electronic and thermal Enthalpies= -1916.488191

Sum of electronic and thermal Free Energies= -1916.544191

PBE0-D3/def2-TZVP Electronic Energy = -1916.648540 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1916.65280660 a.u.

***E*.10a.2H$^+$**

N	-0.29370100	-0.56896700	0.00671600
N	0.29371200	0.56882900	0.00662600
C	-1.62971300	-0.82768700	0.04214400
C	-2.77037700	0.16965200	0.03076900
C	-4.01511600	-0.34633700	0.15011700
C	-1.99680400	-2.13610900	0.11802500
H	-1.30282600	-2.96854400	0.12710600
C	1.99672200	2.13608900	0.11793700
C	1.62970900	0.82761300	0.04216300

C	2.77040200	-0.16965100	0.03100600
C	4.01510800	0.34635900	0.15064500
H	1.30260700	2.96841000	0.12706500
H	4.90714200	-0.26397600	0.15335200
H	-4.90713200	0.26402700	0.15254700
Si	-3.85317700	-2.12996700	0.23650400
Si	3.85309900	2.13000600	0.23643400
H	4.77592100	3.25828700	0.34830600
H	-4.77593000	-3.25818400	0.34954100
H	-0.34581300	1.38485300	-0.00653000
Br	-2.49663100	1.97902400	-0.17218200
H	0.34577900	-1.38504500	-0.00629500
Br	2.49667900	-1.97899600	-0.17228800

PBE0-D3/def2-TZVP:

Zero-point correction= 0.144070 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.100526

Sum of electronic and zero-point Energies= -6144.104730

Sum of electronic and thermal Energies= -6144.090471

Sum of electronic and thermal Enthalpies= -6144.089527

Sum of electronic and thermal Free Energies= -6144.148274

PBE0-D3/def2-TZVP Electronic Energy = -6144.248800 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -6144.25316032 a.u.

***Z*.10a.2H$^+$**

C	-1.39935400	1.74944000	0.74821800
C	-1.57015600	0.49362200	0.25134100
C	-3.01826200	0.08080200	0.04523500
C	-3.96977300	0.98408700	0.37800500
C	1.39937600	1.74945900	-0.74820800
C	1.57016000	0.49363000	-0.25136200
C	3.01826500	0.08080200	-0.04522000
C	3.96979100	0.98406200	-0.37801100
H	-0.46068400	2.24103200	0.96251000
H	-5.02900700	0.80839900	0.25511600
H	0.46074400	2.24111400	-0.96252600
H	5.02902300	0.80837900	-0.25511400
Si	-3.11039200	2.39881500	1.06425800
Si	3.11042800	2.39881500	-1.06423700
H	-3.50387700	3.65312000	1.70418200
H	3.50390000	3.65313000	-1.70415100
N	0.64828700	-0.46651200	-0.01497500
N	-0.64828700	-0.46650800	0.01489600
H	-1.04728600	-1.40855400	-0.10996400

Br	3.37244300	-1.58457100	0.61394100
H	1.04727900	-1.40856700	0.10986000
Br	-3.37246800	-1.58454700	-0.61393100

PBE0-D3/def2-TZVP:

Zero-point correction= 0.144053 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.100125

Sum of electronic and zero-point Energies= -6144.096155

Sum of electronic and thermal Energies= -6144.081816

Sum of electronic and thermal Enthalpies= -6144.080872

Sum of electronic and thermal Free Energies= -6144.140083

PBE0-D3/def2-TZVP Electronic Energy = -6144.240209 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -6144.24434500 a.u.

***E*.11a.2H$^+$**

N	0.14545400	0.62547300	0.06018600
N	-0.14518800	-0.62558300	0.06093800
C	1.36655200	1.22540700	0.05409600
C	2.73971900	0.58023700	0.02319200
C	3.78671000	1.44474900	0.03706800
C	1.35812800	2.58963800	0.07719800
H	0.46093100	3.19652700	0.09850500
C	-1.35802000	-2.58959700	0.07770100
C	-1.36635000	-1.22538200	0.05433500
C	-2.73959200	-0.58020100	0.02275000
C	-3.78654500	-1.44475600	0.03627800
H	-0.46086400	-3.19654000	0.09908200
H	-4.81928000	-1.12502600	0.01533400
H	4.81946400	1.12506600	0.01626200
Si	3.13001000	3.11311500	0.07189000
Si	-3.12985200	-3.11308400	0.07183800
H	-3.69862200	-4.46037900	0.08838000
H	3.69856100	4.46051400	0.08739900
H	0.67503700	-1.26055900	0.05867000
I	3.07680000	-1.42941900	-0.05361200
H	-0.67469800	1.26038200	0.05557500
I	-3.07695500	1.42941400	-0.05346300

PBE0-D3/def2-TZVP:

Zero-point correction= 0.142885 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.098424

Sum of electronic and zero-point Energies= -1591.834647

Sum of electronic and thermal Energies= -1591.820070

Sum of electronic and thermal Enthalpies= -1591.819126

Sum of electronic and thermal Free Energies= -1591.879108

PBE0-D3/def2-TZVP Electronic Energy = -1591.977532 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1591.98190337 a.u.

***Z*.11a.2H$^+$**

C	-1.21784700	1.95704800	0.99262400
C	-1.50793000	0.74694200	0.43711300
C	-2.98674100	0.42324900	0.32079500
C	-3.84461500	1.34534600	0.82078300
C	1.21804600	1.95701800	-0.99287900
C	1.50801400	0.74689000	-0.43734900
C	2.98680100	0.42318100	-0.32079200
C	3.84477800	1.34532500	-0.82051800
H	-0.23057000	2.37840900	1.12467100
H	-4.92071400	1.25334500	0.77930800
H	0.23082500	2.37842600	-1.12518700
H	4.92086600	1.25331400	-0.77880900
Si	-2.83258800	2.65179400	1.53194000
Si	2.83290000	2.65184600	-1.53174800
H	-3.10108800	3.85820800	2.31370800
H	3.10145600	3.85836800	-2.31333000
N	0.64905200	-0.22633500	-0.06413900
N	-0.64903600	-0.22630200	0.06376600
H	-1.06600100	-1.15702100	-0.06990700
I	3.58145000	-1.29647600	0.56962800
H	1.06600700	-1.15707600	0.06958300
I	-3.58160600	-1.29632600	-0.56960400

PBE0-D3/def2-TZVP:

Zero-point correction= 0.143025 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.097722

Sum of electronic and zero-point Energies= -1591.832143

Sum of electronic and thermal Energies= -1591.817501

Sum of electronic and thermal Enthalpies= -1591.816557

Sum of electronic and thermal Free Energies= -1591.877446

PBE0-D3/def2-TZVP Electronic Energy = -1591.975168 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1591.97921683 a.u.

***E*.17e.H$^+$**

N	0.21571700	-0.72727300	-0.04037700
N	-0.08438900	0.45431000	-0.37842000
C	1.51159200	-1.17261200	-0.05846900
C	2.72043700	-0.27641600	-0.12110700
C	3.87437300	-0.89917900	-0.47077500

C	1.77098100	-2.50283400	-0.07463000
C	-1.41081800	2.28891300	-0.65952500
C	-1.32473900	0.94548300	-0.36336000
C	-2.67258200	0.33996100	-0.04409600
C	-3.72537700	1.20556800	0.03574800
Si	3.57278900	-2.68638800	-0.45219900
Si	-3.18523700	2.85834300	-0.41432100
H	-3.80308500	4.17476600	-0.57945300
H	4.40077200	-3.88077800	-0.62611800
F	-0.40066500	3.00699800	-0.97671200
F	-4.94303300	0.80560600	0.30249400
F	5.03351100	-0.29012600	-0.52819700
F	0.84151900	-3.41491800	-0.04818700
I	2.72713400	1.65151700	0.52214500
I	-3.02307100	-1.64994400	0.19182000
H	-0.50324800	-1.41536900	0.22094500

PBE0-D3/def2-TZVP:

Zero-point correction= 0.098893 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.048331

Sum of electronic and zero-point Energies= -1988.240334

Sum of electronic and thermal Energies= -1988.221941

Sum of electronic and thermal Enthalpies= -1988.220996

Sum of electronic and thermal Free Energies= -1988.290897

PBE0-D3/def2-TZVP Electronic Energy = -1988.339228 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1988.34066895 a.u.

***Z*.17e.H$^+$**

C	-1.21549600	1.61744600	1.01610600
C	-1.47636100	0.40487200	0.40943800
C	-2.95316900	0.15947900	0.23036900
C	-3.80215300	1.15359000	0.62055300
C	1.13954900	1.60863000	-1.00808500
C	1.45274900	0.43327600	-0.39610100
C	2.93500500	0.19310300	-0.23777400
C	3.75108400	1.18741200	-0.66076800
Si	-2.83633300	2.48282600	1.35003100
Si	2.72615900	2.50525800	-1.35814600
H	-3.10150300	3.76764900	1.99803400
H	2.96204000	3.79865200	-2.00089300
N	0.59632200	-0.55718900	-0.01295900
N	-0.67187100	-0.61397900	0.14703200
F	-0.07032700	1.95871200	-1.33656100
F	-0.03270500	1.98403400	1.38200600

F	5.05530600	1.13643400	-0.56514000
F	-5.09905200	1.07896000	0.47161800
I	3.65766600	-1.52068900	0.57964600
I	-3.59138900	-1.56782700	-0.58555600
H	1.03182400	-1.48011300	0.08143400

PBE0-D3/def2-TZVP:

Zero-point correction= 0.098711 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.050294

Sum of electronic and zero-point Energies= -1988.236120

Sum of electronic and thermal Energies= -1988.218691

Sum of electronic and thermal Enthalpies= -1988.217747

Sum of electronic and thermal Free Energies= -1988.284537

PBE0-D3/def2-TZVP Electronic Energy = -1988.334831 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1988.33620308 a.u.

***E*.17e.2H$^+$**

N	0.20456000	0.61720300	0.06542800
N	-0.20434200	-0.61504200	0.06529600
C	1.46673900	1.08065500	0.07074400
C	2.75791700	0.32552900	0.03136200
C	3.88298000	1.10216000	0.10094500
C	1.62932500	2.45183400	0.13887500
C	-1.62735900	-2.45072400	0.13817300
C	-1.46616400	-1.07939500	0.07054700
C	-2.75799800	-0.32550400	0.03149000
C	-3.88236800	-1.10318600	0.10153400
Si	3.44891800	2.85910400	0.17789600
Si	-3.44653900	-2.85970300	0.17844100
H	-4.14040000	-4.14557000	0.25733900
H	4.14452900	4.14412300	0.25512300
F	-0.63171700	-3.26018600	0.19158100
F	-5.07484600	-0.58953100	0.08073900
F	5.07502700	0.58743300	0.07968200
F	0.63468200	3.26236300	0.19342300
I	2.97214800	-1.68409300	-0.14628000
I	-2.97377400	1.68378100	-0.14661600
H	-0.55012300	1.32311700	0.04807700
H	0.55054200	-1.32078700	0.04828200

PBE0-D3/def2-TZVP:

Zero-point correction= 0.111235 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.060505

Sum of electronic and zero-point Energies= -1988.570584

Sum of electronic and thermal Energies= -1988.552125

Sum of electronic and thermal Enthalpies= -1988.551181

Sum of electronic and thermal Free Energies= -1988.621314

PBE0-D3/def2-TZVP Electronic Energy = -1988.681819 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1988.68454126 a.u.

***Z*.17e.2H$^+$**

C	-1.16929600	1.58962600	0.99210800
C	-1.49667300	0.37527500	0.40042800
C	-2.96332500	0.17107600	0.20584700
C	-3.74273600	1.24175400	0.54504200
C	1.16929300	1.58969200	-0.99197400
C	1.49669100	0.37528700	-0.40038700
C	2.96336200	0.17107400	-0.20585500
C	3.74274200	1.24174400	-0.54513400
Si	-2.70745100	2.58529300	1.22338400
Si	2.70744500	2.58529600	-1.22340700
H	-2.92707800	3.91891100	1.78376000
H	2.92740800	3.91879800	-1.78392000
N	0.66535800	-0.59317700	-0.03059500
N	-0.66534900	-0.59317600	0.03051600
F	-0.04416300	1.87016400	-1.33479700
F	0.04414100	1.87012700	1.33496700
F	5.03027600	1.23172600	-0.42036200
F	-5.03025600	1.23174100	0.42023700
I	3.72907500	-1.55935600	0.48806300
I	-3.72908700	-1.55935000	-0.48805700
H	1.08456700	-1.49853700	0.21118500
H	-1.08456100	-1.49850600	-0.21132200

PBE0-D3/def2-TZVP:

Zero-point correction= 0.111568 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.062535

Sum of electronic and zero-point Energies= -1988.576123

Sum of electronic and thermal Energies= -1988.557843

Sum of electronic and thermal Enthalpies= -1988.556899

Sum of electronic and thermal Free Energies= -1988.625156

PBE0-D3/def2-TZVP Electronic Energy = -1988.687691 a.u.

PBE0-D3/def2-TZVPP Electronic Energy = -1988.68997846 a.u.

Electronic transitions

The six lowest transitions computed in the TD single-point calculations (30 states in total) are reported. For each excited state, the energy (in eV), the associated wavelength (in nm), the oscillator strength of the transition as well as the numbers of the orbitals involved in the transition (with general formula occupied → unoccupied) are provided below.

***E*.AB.H$^+$**

Excited State	1:	3.0583 eV	405.40 nm	f=0.8723
47 -> 49		-0.15956		
48 -> 49		0.68711		
Excited State	2:	3.2589 eV	380.45 nm	f=0.1057
47 -> 49		0.68362		
48 -> 49		0.15437		
Excited State	3:	3.3410 eV	371.10 nm	f=0.0458
46 -> 49		0.69673		
Excited State	4:	3.9597 eV	313.12 nm	f=0.0042
44 -> 49		0.67255		
45 -> 49		0.16657		
Excited State	5:	4.5063 eV	275.13 nm	f=0.0356
44 -> 49		-0.16305		
45 -> 49		0.67023		
48 -> 52		-0.11507		

***Z*.AB.H$^+$**

Excited State	1:	2.8676 eV	432.36 nm	f=0.1882
44 -> 49		0.10037		
47 -> 49		-0.18169		
48 -> 49		0.67365		
Excited State	2:	3.1894 eV	388.74 nm	f=0.1632
47 -> 49		0.67562		
48 -> 49		0.16749		
Excited State	3:	3.3962 eV	365.07 nm	f=0.0061
46 -> 49		0.69970		
Excited State	4:	3.6566 eV	339.07 nm	f=0.0425
44 -> 49		-0.36514		
45 -> 49		0.58588		
Excited State	5:	4.4942 eV	275.88 nm	f=0.1695
44 -> 49		0.56046		
45 -> 49		0.37041		

***E*.1.H$^+$**

Excited State	1:	3.1182 eV	397.61 nm	f=0.6097
41 -> 43		-0.19006		
42 -> 43		0.67911		
Excited State	2:	3.4606 eV	358.28 nm	f=0.2278

41 -> 43 0.67617

42 -> 43 0.19327

Excited State 3: 3.6602 eV 338.73 nm f=0.0922

40 -> 43 0.70015

Excited State 4: 4.5306 eV 273.66 nm f=0.0015

38 -> 43 0.70472

Excited State 5: 5.3822 eV 230.36 nm f=0.0314

39 -> 43 0.68645

***Z*.1.H$^+$**

Excited State 1: 2.8734 eV 431.49 nm f=0.1372

42 -> 43 0.69558

Excited State 2: 3.3579 eV 369.24 nm f=0.0354

40 -> 43 0.12797

41 -> 43 0.68732

Excited State 3: 3.6880 eV 336.18 nm f=0.2897

40 -> 43 0.68359

41 -> 43 -0.11534

42 -> 43 -0.10886

Excited State 4: 4.1730 eV 297.11 nm f=0.0094

38 -> 43 0.52794

39 -> 43 0.46141

Excited State 5: 5.1678 eV 239.92 nm f=0.1377

38 -> 43 -0.45148

39 -> 43 0.51777

***E*.2.H$^+$**

Excited State 1: 3.1239 eV 396.89 nm f=0.9176

49 -> 51 -0.13058

50 -> 51 0.69499

Excited State 2: 3.2375 eV 382.97 nm f=0.1112

49 -> 51 0.69123

50 -> 51 0.12901

Excited State 3: 3.4102 eV 363.56 nm f=0.0066

48 -> 51 0.69971

Excited State 4: 4.2788 eV 289.76 nm f=0.0010

46 -> 51 0.69575

Excited State 5: 4.7345 eV 261.87 nm f=0.0369

47 -> 51 0.68188

48 -> 52 -0.10288

***Z*.2.H$^+$**

Excited State 1: 2.7348 eV 453.36 nm f=0.1062

49 -> 51 0.14933

50 -> 51		0.68832		
Excited State	2:	3.1929 eV	388.31 nm	f=0.0853
48 -> 51		0.25231		
49 -> 51		0.64387		
50 -> 51		-0.12239		
Excited State	3:	3.2632 eV	379.95 nm	f=0.1593
48 -> 51		0.65628		
49 -> 51		-0.23877		
Excited State	4:	3.7799 eV	328.01 nm	f=0.0146
46 -> 51		0.56334		
47 -> 51		0.41000		
Excited State	5:	4.4459 eV	278.88 nm	f=0.1999
46 -> 51		-0.40502		
47 -> 51		0.55580		

***E*.3.H$^+$**

Excited State	1:	3.1489 eV	393.74 nm	f=0.4404
40 -> 43		-0.13486		
41 -> 43		0.15933		
42 -> 43		0.67698		
Excited State	2:	3.5480 eV	349.45 nm	f=0.0932
40 -> 43		0.10906		
41 -> 43		0.67655		
42 -> 43		-0.14094		
Excited State	3:	4.0234 eV	308.16 nm	f=0.3628
40 -> 43		0.68382		
42 -> 43		0.15743		
Excited State	4:	4.4137 eV	280.91 nm	f=0.0014
39 -> 43		0.70390		
Excited State	5:	5.6787 eV	218.33 nm	f=0.0268
38 -> 43		0.67639		
42 -> 44		0.10167		

***Z*.3.H$^+$**

Excited State	1:	2.7216 eV	455.55 nm	f=0.0614
42 -> 43		0.69944		
Excited State	2:	3.2696 eV	379.20 nm	f=0.0266
41 -> 43		0.68952		
Excited State	3:	3.9420 eV	314.52 nm	f=0.0076
38 -> 43		0.36480		
39 -> 43		0.57380		
40 -> 43		-0.18185		
Excited State	4:	4.0344 eV	307.32 nm	f=0.1975
38 -> 43		0.18588		

40 -> 43 0.66775

Excited State 5: 5.0432 eV 245.84 nm f=0.1676

38 -> 43 0.56089

39 -> 43 -0.38521

***E*.4.H$^+$**

Excited State 1: 2.9769 eV 416.48 nm f=0.9279

66 -> 69 0.11166

67 -> 69 0.21693

68 -> 69 0.66525

Excited State 2: 3.1561 eV 392.84 nm f=0.1134

67 -> 69 0.66894

68 -> 69 -0.20612

Excited State 3: 3.3289 eV 372.45 nm f=0.0396

66 -> 69 0.68997

68 -> 69 -0.13100

Excited State 4: 4.2563 eV 291.30 nm f=0.0009

63 -> 69 0.19523

64 -> 69 0.67133

Excited State 5: 4.4258 eV 280.14 nm f=0.0414

65 -> 69 0.68107

***Z*.4.H$^+$**

Excited State 1: 2.6519 eV 467.53 nm f=0.1694

67 -> 69 -0.23672

68 -> 69 0.66288

Excited State 2: 2.9647 eV 418.20 nm f=0.1688

67 -> 69 0.66409

68 -> 69 0.23309

Excited State 3: 3.1353 eV 395.45 nm f=0.0294

66 -> 69 0.70166

Excited State 4: 3.6717 eV 337.67 nm f=0.0294

64 -> 69 0.50877

65 -> 69 0.46866

Excited State 5: 4.1818 eV 296.48 nm f=0.1695

64 -> 69 -0.46305

65 -> 69 0.50722

***E*.5.H$^+$**

Excited State 1: 3.0077 eV 412.22 nm f=0.3050

40 -> 43 -0.13825

42 -> 43 0.69038

Excited State 2: 3.2815 eV 377.83 nm f=0.0176

41 -> 43 0.69551

Excited State	3:	3.9377 eV	314.87 nm	f=0.0013
39 -> 43		0.69359		
40 -> 43		0.11535		
Excited State	4:	4.7536 eV	260.82 nm	f=0.6681
39 -> 43		-0.11136		
40 -> 43		0.67408		
42 -> 43		0.14566		
Excited State	5:	5.4737 eV	226.51 nm	f=0.0132
38 -> 43		0.18583		
42 -> 44		0.67752		

***Z*.5.H$^+$**

Excited State	1:	2.5372 eV	488.66 nm	f=0.0559
42 -> 43		0.70448		
Excited State	2:	3.0584 eV	405.39 nm	f=0.0125
41 -> 43		0.70158		
Excited State	3:	3.7449 eV	331.07 nm	f=0.0109
38 -> 43		0.14374		
39 -> 43		-0.16713		
40 -> 43		0.66446		
Excited State	4:	4.9504 eV	250.45 nm	f=0.1340
39 -> 43		0.65192		
40 -> 43		0.18918		
42 -> 44		0.11415		
Excited State	5:	5.0970 eV	243.25 nm	f=0.0035
38 -> 43		0.16762		
42 -> 44		0.67240		

***E*.6.H$^+$**

Excited State	1:	2.8016 eV	442.55 nm	f=0.4152
40 -> 43		-0.14224		
42 -> 43		0.69273		
Excited State	2:	3.1645 eV	391.80 nm	f=0.0188
41 -> 43		0.69576		
Excited State	3:	4.1050 eV	302.03 nm	f=0.0009
39 -> 43		0.70065		
Excited State	4:	4.2865 eV	289.24 nm	f=0.6221
40 -> 43		0.68646		
42 -> 43		0.14972		
Excited State	5:	5.1299 eV	241.69 nm	f=0.0390
42 -> 44		0.66935		
42 -> 45		-0.18436		

***Z*.6.H$^+$**

Excited State	1:	2.2569 eV	549.34 nm	f=0.0843
42 -> 43		0.70727		
Excited State	2:	2.6685 eV	464.62 nm	f=0.0118
41 -> 43		0.70298		
Excited State	3:	3.3910 eV	365.63 nm	f=0.0348
38 -> 43		0.13262		
39 -> 43		0.32491		
40 -> 43		0.60982		
Excited State	4:	4.2037 eV	294.94 nm	f=0.2363
38 -> 43		0.12119		
39 -> 43		0.59412		
40 -> 43		-0.34845		
Excited State	5:	5.0730 eV	244.40 nm	f=0.0105
38 -> 43		0.38790		
42 -> 44		0.57292		

***E*.7.H$^+$**

Excited State	1:	2.6670 eV	464.87 nm	f=0.5577
40 -> 43		-0.12518		
42 -> 43		0.69460		
42 <- 43		-0.10188		
Excited State	2:	3.0789 eV	402.69 nm	f=0.0189
41 -> 43		0.69356		
Excited State	3:	3.6066 eV	343.77 nm	f=0.5045
40 -> 43		0.68818		
42 -> 43		0.13731		
Excited State	4:	3.8849 eV	319.14 nm	f=0.0001
34 -> 43		0.20249		
35 -> 43		-0.18107		
36 -> 43		0.14476		
37 -> 43		-0.31597		
39 -> 43		0.54923		
Excited State	5:	4.2445 eV	292.10 nm	f=0.0002
35 -> 43		0.21667		
36 -> 43		-0.34211		
37 -> 43		0.42639		
39 -> 43		0.37534		

***Z*.7.H$^+$**

Excited State	1:	2.1942 eV	565.06 nm	f=0.1371
42 -> 43		0.70006		
Excited State	2:	2.6023 eV	476.45 nm	f=0.0046
41 -> 43		0.70211		
Excited State	3:	3.1051 eV	399.29 nm	f=0.0368

36 -> 43	0.14799			
39 -> 43	-0.38097			
40 -> 43	0.56290			
Excited State	4:	3.5484 eV	349.40 nm	f=0.2494
36 -> 43	-0.16350			
39 -> 43	0.51726			
40 -> 43	0.42111			
42 -> 43	0.11308			
Excited State	5:	3.9201 eV	316.28 nm	f=0.0060
36 -> 43	0.10959			
37 -> 43	0.58949			
38 -> 43	-0.35882			

***E*.8.H$^+$**

Excited State	1:	2.7686 eV	447.82 nm	f=0.3150
47 -> 51	-0.10096			
50 -> 51	0.69735			
Excited State	2:	3.0529 eV	406.13 nm	f=0.0055
49 -> 51	0.70143			
Excited State	3:	3.6310 eV	341.46 nm	f=0.0007
47 -> 51	0.44457			
48 -> 51	0.53514			
Excited State	4:	4.4746 eV	277.09 nm	f=0.0327
47 -> 51	0.10114			
50 -> 52	0.67678			
Excited State	5:	4.6056 eV	269.20 nm	f=0.7304
47 -> 51	0.51918			
48 -> 51	-0.43504			
50 -> 51	0.12972			
50 -> 52	-0.13199			

***Z*.8.H$^+$**

Excited State	1:	2.4924 eV	497.44 nm	f=0.0567
50 -> 51	0.70056			
Excited State	2:	3.0254 eV	409.80 nm	f=0.0086
49 -> 51	0.69847			
Excited State	3:	3.7136 eV	333.87 nm	f=0.0077
44 -> 51	0.13371			
47 -> 51	-0.12044			
48 -> 51	0.66228			
Excited State	4:	4.1375 eV	299.66 nm	f=0.0010
50 -> 52	0.69624			
Excited State	5:	4.5060 eV	275.15 nm	f=0.1175
49 -> 52	0.41186			

50 -> 53 0.55766

***E*.9.H$^+$**

Excited State 1: 2.7085 eV 457.77 nm f=0.4101
48 -> 51 -0.11202
50 -> 51 0.69790
Excited State 2: 3.0748 eV 403.23 nm f=0.0104
49 -> 51 0.70040
Excited State 3: 3.6387 eV 340.73 nm f=0.0003
42 -> 51 0.15791
43 -> 51 -0.19307
46 -> 51 0.14466
47 -> 51 0.63794
Excited State 4: 4.2487 eV 291.82 nm f=0.6550
48 -> 51 0.69258
50 -> 51 0.11829
Excited State 5: 4.3661 eV 283.97 nm f=0.0002
42 -> 51 -0.12512
44 -> 51 -0.11461
46 -> 51 0.66713
47 -> 51 -0.12575

***Z*.9.H$^+$**

Excited State 1: 2.1010 eV 590.11 nm f=0.0642
50 -> 51 0.70359
Excited State 2: 2.7878 eV 444.74 nm f=0.0090
49 -> 51 0.69986
Excited State 3: 3.3788 eV 366.95 nm f=0.0047
42 -> 51 0.10121
44 -> 51 -0.13045
45 -> 51 0.15946
48 -> 51 0.64791
Excited State 4: 4.2062 eV 294.76 nm f=0.0239
44 -> 51 -0.13360
47 -> 51 0.56330
50 -> 52 0.38039
Excited State 5: 4.2421 eV 292.27 nm f=0.0046
44 -> 51 -0.13618
47 -> 51 -0.41472
50 -> 52 0.53751

***E*.10.H$^+$**

Excited State 1: 2.8637 eV 432.95 nm f=0.3486
65 -> 69 -0.12058

68 -> 69 0.69683

Excited State 2: 3.1706 eV 391.04 nm f=0.0097

67 -> 69 0.70069

Excited State 3: 3.7071 eV 334.45 nm f=0.0006

63 -> 69 -0.11556

66 -> 69 0.68866

Excited State 4: 4.6090 eV 269.01 nm f=0.2606

65 -> 69 -0.39029

68 -> 70 0.56701

Excited State 5: 4.6627 eV 265.91 nm f=0.5554

65 -> 69 0.56919

68 -> 69 0.10647

68 -> 70 0.39227

***Z*.10.H$^+$**

Excited State 1: 2.5153 eV 492.92 nm f=0.0586

68 -> 69 0.69967

Excited State 2: 3.0663 eV 404.35 nm f=0.0094

67 -> 69 0.69679

Excited State 3: 3.7086 eV 334.32 nm f=0.0048

62 -> 69 -0.11715

65 -> 69 -0.11891

66 -> 69 0.66394

Excited State 4: 4.2818 eV 289.56 nm f=0.0009

68 -> 70 0.69700

Excited State 5: 4.6342 eV 267.54 nm f=0.1331

65 -> 69 -0.11387

67 -> 70 0.31680

68 -> 71 0.61070

***E*.11.H$^+$**

Excited State 1: 2.7825 eV 445.58 nm f=0.4392

65 -> 69 0.10997

68 -> 69 0.69739

Excited State 2: 3.1595 eV 392.42 nm f=0.0121

67 -> 69 0.70005

Excited State 3: 3.6331 eV 341.26 nm f=0.0002

60 -> 69 -0.21514

61 -> 69 -0.11420

64 -> 69 -0.16811

66 -> 69 0.63308

Excited State 4: 4.2023 eV 295.04 nm f=0.0000

60 -> 69 -0.10137

64 -> 69 0.66628

66 -> 69 0.14971

Excited State 5: 4.2766 eV 289.91 nm f=0.6620

65 -> 69 0.69305

68 -> 69 -0.11564

***Z*.11.H$^+$**

Excited State 1: 2.1433 eV 578.47 nm f=0.0639

68 -> 69 0.70319

Excited State 2: 2.8350 eV 437.34 nm f=0.0092

67 -> 69 0.69816

Excited State 3: 3.3516 eV 369.93 nm f=0.0024

60 -> 69 -0.10673

63 -> 69 0.16252

66 -> 69 0.65518

Excited State 4: 4.0584 eV 305.50 nm f=0.0258

64 -> 69 -0.13256

65 -> 69 0.67941

Excited State 5: 4.1626 eV 297.86 nm f=0.0107

61 -> 69 -0.11046

64 -> 69 0.67301

65 -> 69 0.14368

***E*.12.H$^+$**

Excited State 1: 2.7224 eV 455.42 nm f=0.5368

68 -> 69 0.69689

Excited State 2: 2.9478 eV 420.60 nm f=0.0000

61 -> 69 -0.11789

63 -> 69 -0.15141

65 -> 69 -0.32326

66 -> 69 0.59065

Excited State 3: 3.1153 eV 397.98 nm f=0.0103

67 -> 69 0.69600

Excited State 4: 3.1997 eV 387.48 nm f=0.0000

61 -> 69 0.14054

65 -> 69 0.59802

66 -> 69 0.33863

Excited State 5: 3.3942 eV 365.28 nm f=0.0003

59 -> 69 -0.10852

61 -> 69 0.18267

63 -> 69 0.64801

66 -> 69 0.15453

***Z*.12.H$^+$**

Excited State 1: 2.0144 eV 615.49 nm f=0.0551

63 -> 69 -0.11465
66 -> 69 -0.18302
67 -> 69 0.15209
68 -> 69 0.64505
Excited State 2: 2.5509 eV 486.04 nm f=0.0368
66 -> 69 -0.19714
67 -> 69 0.61764
68 -> 69 -0.23750
Excited State 3: 2.7542 eV 450.16 nm f=0.0201
63 -> 69 0.11224
64 -> 69 -0.19280
65 -> 69 0.12822
66 -> 69 0.54803
67 -> 69 0.29705
68 -> 69 0.15301
Excited State 4: 2.9741 eV 416.87 nm f=0.0007
61 -> 69 0.14211
63 -> 69 -0.25159
64 -> 69 0.44177
65 -> 69 0.43698
66 -> 69 0.12940
Excited State 5: 2.9939 eV 414.13 nm f=0.0063
63 -> 69 0.22284
64 -> 69 -0.28790
65 -> 69 0.49850
66 -> 69 -0.30999

***E*.13.H$^+$**

Excited State 1: 2.6775 eV 463.05 nm f=0.5068
50 -> 51 0.69879
Excited State 2: 3.0122 eV 411.61 nm f=0.0000
41 -> 51 0.10004
43 -> 51 -0.11494
44 -> 51 0.17342
46 -> 51 -0.30929
48 -> 51 0.58959
Excited State 3: 3.0837 eV 402.06 nm f=0.0093
49 -> 51 0.69725
Excited State 4: 3.2589 eV 380.45 nm f=0.0001
43 -> 51 0.16887
46 -> 51 0.57765
48 -> 51 0.35571
Excited State 5: 3.3486 eV 370.26 nm f=0.0007
43 -> 51 -0.16040

44 -> 51	0.63809			
46 -> 51	0.20513			
48 -> 51	-0.10158			

***Z*.13.H$^+$**

Excited State	1:	1.9762 eV	627.39 nm	f=0.0633
44 -> 51	0.12227			
45 -> 51	0.12971			
48 -> 51	-0.13163			
49 -> 51	0.13152			
50 -> 51	0.65811			
Excited State	2:	2.5236 eV	491.30 nm	f=0.0235
44 -> 51	0.11416			
48 -> 51	-0.14396			
49 -> 51	0.63513			
50 -> 51	-0.20598			
Excited State	3:	2.7574 eV	449.65 nm	f=0.0188
44 -> 51	-0.22029			
45 -> 51	-0.26730			
46 -> 51	-0.13795			
47 -> 51	-0.11784			
48 -> 51	0.48528			
49 -> 51	0.26866			
50 -> 51	0.15413			
Excited State	4:	2.9424 eV	421.37 nm	f=0.0013
45 -> 51	-0.12784			
46 -> 51	-0.11455			
47 -> 51	0.67988			
Excited State	5:	3.0219 eV	410.29 nm	f=0.0008
43 -> 51	-0.10147			
44 -> 51	0.12108			
45 -> 51	0.39506			
46 -> 51	0.35743			
47 -> 51	0.12907			
48 -> 51	0.41204			

***E*.14.H$^+$**

Excited State	1:	2.5180 eV	492.38 nm	f=0.3419
42 -> 49	-0.10481			
48 -> 49	0.70040			
Excited State	2:	2.9594 eV	418.95 nm	f=0.0029
47 -> 49	0.69984			
Excited State	3:	3.0569 eV	405.59 nm	f=0.0000
41 -> 49	-0.12490			

45 -> 49	-0.26444			
46 -> 49	0.62598			
Excited State	4:	3.3929 eV	365.42 nm	f=0.0002
43 -> 49	0.11989			
45 -> 49	0.62676			
46 -> 49	0.27227			
46 -> 50	0.11810			
Excited State	5:	3.6112 eV	343.33 nm	f=0.0001
41 -> 49	0.19936			
43 -> 49	-0.17019			
44 -> 49	0.64401			

***Z*.14.H$^+$**

Excited State	1:	2.0125 eV	616.07 nm	f=0.0528
48 -> 49	0.69947			
Excited State	2:	2.7035 eV	458.60 nm	f=0.0081
44 -> 49	-0.10502			
46 -> 49	-0.10148			
47 -> 49	0.68256			
Excited State	3:	3.1170 eV	397.76 nm	f=0.0073
42 -> 49	-0.11599			
44 -> 49	0.45402			
46 -> 49	0.47826			
47 -> 49	0.16156			
Excited State	4:	3.4353 eV	360.91 nm	f=0.0008
43 -> 49	-0.12936			
44 -> 49	0.29625			
45 -> 49	0.32104			
46 -> 49	-0.32919			
48 -> 50	0.40622			
Excited State	5:	3.4659 eV	357.73 nm	f=0.0005
44 -> 49	-0.27458			
45 -> 49	-0.17009			
46 -> 49	0.27445			
48 -> 50	0.54841			

***E*.15.H$^+$**

Excited State	1:	2.5133 eV	493.31 nm	f=0.3496
66 -> 67	0.69971			
Excited State	2:	2.9477 eV	420.62 nm	f=0.0000
63 -> 67	-0.28530			
64 -> 67	0.62783			
Excited State	3:	2.9841 eV	415.48 nm	f=0.0022
65 -> 67	0.69754			

Excited State	4:	3.2586 eV	380.48 nm	f=0.0003
63 -> 67		0.62400		
64 -> 67		0.28621		
64 -> 68		0.13079		
Excited State	5:	3.5900 eV	345.36 nm	f=0.0055
65 -> 69		-0.10152		
66 -> 68		0.68211		
66 -> 69		-0.11267		

***Z*.15.H$^+$**

Excited State	1:	1.9909 eV	622.77 nm	f=0.0551
66 -> 67		0.69889		
Excited State	2:	2.6896 eV	460.98 nm	f=0.0081
64 -> 67		0.18981		
65 -> 67		0.66231		
Excited State	3:	2.9883 eV	414.90 nm	f=0.0105
62 -> 67		-0.20862		
64 -> 67		0.61706		
65 -> 67		-0.22407		
Excited State	4:	3.2883 eV	377.04 nm	f=0.0019
61 -> 67		0.11771		
63 -> 67		0.64408		
64 -> 68		-0.10288		
66 -> 68		-0.21025		
Excited State	5:	3.3679 eV	368.14 nm	f=0.0003
63 -> 67		0.21300		
65 -> 69		-0.12401		
66 -> 68		0.65292		

***E*.16.H$^+$**

Excited State	1:	2.0867 eV	594.17 nm	f=0.1780
65 -> 68		-0.14393		
66 -> 67		0.68427		
Excited State	2:	2.5133 eV	493.30 nm	f=0.0001
65 -> 67		0.57839		
66 -> 68		-0.39931		
Excited State	3:	2.8537 eV	434.47 nm	f=0.0043
65 -> 67		0.39800		
66 -> 68		0.56779		
Excited State	4:	3.1866 eV	389.08 nm	f=0.0002
63 -> 67		0.11530		
64 -> 67		0.67443		
Excited State	5:	3.6668 eV	338.13 nm	f=0.4024
62 -> 67		0.14236		

65 -> 68 -0.46594
66 -> 67 -0.14682
66 -> 69 0.48080

***Z*.16.H$^+$**

Excited State 1: 1.9203 eV 645.66 nm f=0.0419
66 -> 67 0.69863
Excited State 2: 2.4312 eV 509.97 nm f=0.0008
65 -> 67 0.52329
66 -> 68 -0.46464
Excited State 3: 2.6704 eV 464.29 nm f=0.0018
65 -> 67 0.44807
66 -> 68 0.50636
66 -> 69 -0.13002
Excited State 4: 3.1108 eV 398.56 nm f=0.0531
64 -> 67 -0.13842
65 -> 67 0.14361
65 -> 68 0.46541
66 -> 68 0.10376
66 -> 69 0.47353
Excited State 5: 3.4181 eV 362.73 nm f=0.0105
64 -> 67 0.55858
64 -> 69 0.12790
65 -> 68 0.33207
66 -> 69 -0.12881

***E*.17.H$^+$**

Excited State 1: 2.0135 eV 615.76 nm f=0.1736
47 -> 50 -0.14368
48 -> 49 0.68611
Excited State 2: 2.4436 eV 507.38 nm f=0.0001
47 -> 49 0.61175
48 -> 50 -0.34683
Excited State 3: 2.8097 eV 441.27 nm f=0.0033
47 -> 49 0.34418
48 -> 50 0.60247
Excited State 4: 3.1200 eV 397.39 nm f=0.0003
46 -> 49 0.68296
Excited State 5: 3.6707 eV 337.76 nm f=0.3991
44 -> 49 -0.14611
47 -> 50 0.47786
48 -> 49 0.14523
48 -> 51 -0.46837

***Z*.17.H$^+$**

Excited State	1:	1.8857 eV	657.48 nm	f=0.0422
48 -> 49		0.69868		
Excited State	2:	2.3887 eV	519.04 nm	f=0.0010
47 -> 49		0.56344		
48 -> 50		-0.41572		
Excited State	3:	2.6228 eV	472.72 nm	f=0.0015
47 -> 49		0.39750		
48 -> 50		0.54645		
48 -> 51		0.13244		
Excited State	4:	3.1207 eV	397.30 nm	f=0.0569
46 -> 49		-0.12153		
47 -> 49		-0.14293		
47 -> 50		0.49693		
48 -> 50		-0.11192		
48 -> 51		0.44373		
Excited State	5:	3.4409 eV	360.32 nm	f=0.0088
46 -> 49		0.44687		
46 -> 51		0.13368		
47 -> 50		0.39941		
48 -> 51		-0.29889		

***E*.18.H$^+$**

Excited State	1:	1.9060 eV	650.48 nm	f=0.2247
39 -> 42		-0.12181		
40 -> 41		0.69747		
40 <- 41		-0.13920		
Excited State	2:	2.4696 eV	502.05 nm	f=0.0002
39 -> 41		0.64219		
40 -> 42		-0.28646		
Excited State	3:	2.7901 eV	444.37 nm	f=0.0024
39 -> 41		0.28677		
40 -> 42		0.63688		
Excited State	4:	3.2442 eV	382.17 nm	f=0.000
37 -> 41		0.16648		
38 -> 41		0.67013		
Excited State	5:	3.6147 eV	343.00 nm	f=0.2326
35 -> 41		0.14369		
39 -> 42		-0.11212		
40 -> 43		0.67190		

***Z*.18.H$^+$**

Excited State	1:	1.8426 eV	672.87 nm	f=0.0995
39 -> 42		-0.12145		

40 -> 41 0.69297

40 <- 41 -0.11361

Excited State 2: 2.0615 eV 601.43 nm f=0.0028

39 -> 41 0.69472

Excited State 3: 2.8200 eV 439.65 nm f=0.0011

38 -> 41 -0.11716

39 -> 43 0.11062

40 -> 42 0.68428

Excited State 4: 3.1369 eV 395.24 nm f=0.0089

38 -> 41 0.63780

39 -> 42 -0.22315

40 -> 42 0.11361

40 -> 43 -0.10322

Excited State 5: 3.3391 eV 371.31 nm f=0.1700

38 -> 41 0.23654

39 -> 42 0.62291

40 -> 41 0.13419

40 -> 43 0.15177

***E*.AB.2H$^+$**

Excited State 1: 2.3109 eV 536.52 nm f=0.0861

47 -> 49 0.66628

48 -> 49 0.23929

Excited State 2: 2.3376 eV 530.40 nm f=0.0001

46 -> 49 0.70634

Excited State 3: 2.4928 eV 497.37 nm f=1.0172

47 -> 49 -0.23438

48 -> 49 0.68062

48 <- 49 -0.14764

Excited State 4: 4.1207 eV 300.88 nm f=0.0005

45 -> 49 0.68968

48 -> 50 0.11876

Excited State 5: 4.3842 eV 282.79 nm f=0.0004

44 -> 49 0.70438

***Z*.AB.2H$^+$**

Excited State 1: 2.0649 eV 600.43 nm f=0.0430

47 -> 49 0.62011

48 -> 49 -0.34272

Excited State 2: 2.3398 eV 529.89 nm f=0.0036

46 -> 49 0.70621

Excited State 3: 2.4262 eV 511.02 nm f=0.6093

47 -> 49 0.33922

48 -> 49 0.63062

48 <- 49	-0.13059			
Excited State	4:	3.9372 eV	314.90 nm	f=0.0822
44 -> 49	0.20100			
45 -> 49	0.66447			
48 -> 50	0.10671			
Excited State	5:	4.3727 eV	283.54 nm	f=0.0012
43 -> 49	0.69972			

***E*.1.2H$^+$**

Excited State	1:	2.4610 eV	503.79 nm	f=0.4322
40 -> 43	-0.35310			
42 -> 43	0.62468			
42 <- 43	-0.13229			
Excited State	2:	2.6087 eV	475.27 nm	f=0.0000
41 -> 43	0.70333			
Excited State	3:	2.9446 eV	421.06 nm	f=0.5396
40 -> 43	0.61295			
42 -> 43	0.36770			
42 <- 43	-0.11074			
Excited State	4:	5.3319 eV	232.53 nm	f=0.0001
39 -> 43	0.68841			
Excited State	5:	6.2353 eV	198.84 nm	f=0.1349
42 -> 44	0.69347			

***Z*.1.2H$^+$**

Excited State	1:	2.2014 eV	563.21 nm	f=0.1260
40 -> 43	-0.29792			
42 -> 43	0.64993			
42 <- 43	-0.11189			
Excited State	2:	2.4538 eV	505.28 nm	f=0.0125
41 -> 43	0.70507			
Excited State	3:	3.0185 eV	410.75 nm	f=0.4327
40 -> 43	0.64197			
42 -> 43	0.30977			
Excited State	4:	5.2088 eV	238.03 nm	f=0.0897
39 -> 43	0.68175			
Excited State	5:	6.2894 eV	197.13 nm	f=0.0002
38 -> 43	0.67013			
42 -> 44	0.17744			

***E*.2.2H$^+$**

Excited State	1:	2.4112 eV	514.20 nm	f=0.1258
48 -> 51	0.61005			
50 -> 51	-0.35882			

Excited State	2:	2.4329 eV	509.62 nm	f=0.0003
49 -> 51		0.70415		
Excited State	3:	2.5943 eV	477.91 nm	f=0.9714
48 -> 51		0.35358		
50 -> 51		0.62780		
50 <- 51		-0.14963		
Excited State	4:	4.5099 eV	274.92 nm	f=0.0000
47 -> 51		0.68454		
48 -> 53		-0.10489		
49 -> 52		0.10710		
Excited State	5:	4.8479 eV	255.75 nm	f=0.0000
46 -> 51		0.70555		

***Z*.2.2H$^+$**

Excited State	1:	2.0456 eV	606.10 nm	f=0.0875
48 -> 51		0.44062		
50 -> 51		0.56051		
Excited State	2:	2.2735 eV	545.34 nm	f=0.0025
49 -> 51		0.70655		
Excited State	3:	2.5649 eV	483.38 nm	f=0.4874
48 -> 51		0.55366		
50 -> 51		-0.45293		
50 <- 51		0.11605		
Excited State	4:	4.3352 eV	285.99 nm	f=0.0866
45 -> 51		-0.13034		
47 -> 51		0.67631		
Excited State	5:	4.6697 eV	265.51 nm	f=0.0074
46 -> 51		0.70512		

***E*.3.2H$^+$**

Excited State	1:	2.4306 eV	510.11 nm	f=0.4038
40 -> 43		-0.27944		
42 -> 43		0.66314		
42 <- 43		-0.14088		
Excited State	2:	2.6494 eV	467.97 nm	f=0.0000
41 -> 43		0.70159		
Excited State	3:	3.3409 eV	371.11 nm	f=0.5322
40 -> 43		0.64995		
42 -> 43		0.29511		
42 <- 43		-0.10766		
Excited State	4:	5.5515 eV	223.33 nm	f=0.0000
39 -> 43		0.68329		
Excited State	5:	5.6742 eV	218.50 nm	f=0.0000
38 -> 43		0.70183		

***Z*.3.2H$^+$**

Excited State	1:	2.0991 eV	590.67 nm	f=0.1111
40 -> 43		-0.22120		
42 -> 43		0.68301		
42 <- 43		-0.12491		
Excited State	2:	2.3483 eV	527.98 nm	f=0.0144
41 -> 43		0.70398		
Excited State	3:	3.2661 eV	379.61 nm	f=0.3615
40 -> 43		0.67267		
42 -> 43		0.23570		
Excited State	4:	5.1725 eV	239.70 nm	f=0.0439
37 -> 43		0.30484		
39 -> 43		0.61956		
Excited State	5:	5.4716 eV	226.60 nm	f=0.0008
38 -> 43		0.70064		

***E*.4.2H$^+$**

Excited State	1:	2.3245 eV	533.39 nm	f=0.2204
67 -> 69		0.63637		
68 -> 69		0.31190		
Excited State	2:	2.3609 eV	525.15 nm	f=0.0000
66 -> 69		0.70571		
Excited State	3:	2.4629 eV	503.41 nm	f=0.9206
67 -> 69		-0.30501		
68 -> 69		0.65284		
68 <- 69		-0.15347		
Excited State	4:	4.1480 eV	298.90 nm	f=0.0000
65 -> 69		0.68386		
66 -> 70		0.10075		
Excited State	5:	4.5327 eV	273.53 nm	f=0.0000
64 -> 69		0.70557		

***Z*.4.2H$^+$**

Excited State	1:	1.9896 eV	623.16 nm	f=0.0999
67 -> 69		0.52644		
68 -> 69		-0.48127		
68 <- 69		0.10033		
Excited State	2:	2.2127 eV	560.33 nm	f=0.0001
66 -> 69		0.70601		
Excited State	3:	2.3161 eV	535.33 nm	f=0.4678
67 -> 69		0.47196		
68 -> 69		0.53960		
68 <- 69		-0.13057		

Excited State	4:	3.9540 eV	313.57 nm	f=0.0878
63 -> 69		-0.10260		
65 -> 69		0.68045		
68 -> 70		0.10588		
Excited State	5:	4.3252 eV	286.65 nm	f=0.0097
64 -> 69		0.70487		

***E*.5.2H$^+$**

Excited State	1:	2.0985 eV	590.84 nm	f=0.3032
40 -> 43		-0.20087		
42 -> 43		0.69442		
42 <- 43		-0.14934		
Excited State	2:	2.3494 eV	527.73 nm	f=0.0000
41 -> 43		0.70306		
Excited State	3:	3.9847 eV	311.15 nm	f=0.6780
40 -> 43		0.67459		
42 -> 43		0.22012		
42 <- 43		-0.11227		
Excited State	4:	5.2521 eV	236.07 nm	f=0.0002
39 -> 43		-0.29900		
42 -> 44		0.63701		
Excited State	5:	5.4567 eV	227.21 nm	f=0.1185
42 -> 45		0.69954		

***Z*.5.2H$^+$**

Excited State	1:	1.5434 eV	803.30 nm	f=0.0792
40 -> 43		-0.12928		
42 -> 43		0.71317		
42 <- 43		-0.15081		
Excited State	2:	1.7847 eV	694.70 nm	f=0.0077
41 -> 43		0.70608		
Excited State	3:	3.5987 eV	344.53 nm	f=0.2598
40 -> 43		0.69652		
42 -> 43		0.15118		
42 <- 43		-0.10277		
Excited State	4:	4.8492 eV	255.68 nm	f=0.0330
38 -> 43		-0.18362		
39 -> 43		0.59603		
42 -> 44		0.30431		
Excited State	5:	5.2805 eV	234.80 nm	f=0.0025
38 -> 43		0.48716		
42 -> 44		0.49394		

***E*.6.2H$^+$**

Excited State	1:	2.0734 eV	597.96 nm	f=0.3991
40 -> 43		-0.20456		
42 -> 43		0.69774		
42 <- 43		-0.17267		
Excited State	2:	2.4040 eV	515.75 nm	f=0.0000
41 -> 43		0.70285		
Excited State	3:	3.5604 eV	348.23 nm	f=0.6034
40 -> 43		0.67585		
42 -> 43		0.22375		
42 <- 43		-0.10829		
Excited State	4:	5.0120 eV	247.38 nm	f=0.0003
39 -> 43		-0.14664		
42 -> 44		0.68634		
Excited State	5:	5.0273 eV	246.62 nm	f=0.0070
38 -> 43		0.67223		
42 -> 45		-0.19658		

***Z*.6.2H$^+$**

Excited State	1:	1.6314 eV	760.01 nm	f=0.1273
40 -> 43		-0.14979		
42 -> 43		0.71267		
42 <- 43		-0.17280		
Excited State	2:	1.8962 eV	653.84 nm	f=0.0041
41 -> 43		0.70564		
Excited State	3:	3.2494 eV	381.56 nm	f=0.2338
40 -> 43		0.69132		
42 -> 43		0.16948		
42 <- 43		-0.10213		
Excited State	4:	4.6705 eV	265.46 nm	f=0.0213
36 -> 43		-0.11792		
38 -> 43		0.64919		
39 -> 43		-0.23616		
Excited State	5:	4.7945 eV	258.60 nm	f=0.0032
35 -> 43		0.10259		
37 -> 43		0.67628		
39 -> 43		0.10938		
42 -> 44		-0.12601		

***E*.7.2H$^+$**

Excited State	1:	2.0525 eV	604.07 nm	f=0.4949
40 -> 43		0.21826		
42 -> 43		0.69148		
42 <- 43		-0.17857		

Excited State	2:	2.3567 eV	526.10 nm	f=0.0000
41 -> 43		0.70405		
Excited State	3:	2.7975 eV	443.20 nm	f=0.5245
40 -> 43		0.67198		
42 -> 43		-0.23308		
Excited State	4:	3.3733 eV	367.55 nm	f=0.0000
36 -> 43		0.11946		
39 -> 43		0.69619		
Excited State	5:	3.4147 eV	363.09 nm	f=0.0012
35 -> 43		0.10496		
38 -> 43		0.69856		

***E*.8.2H$^+$**

Excited State	1:	2.0022 eV	619.22 nm	f=0.3471
48 -> 51		-0.17272		
50 -> 51		0.70171		
50 <- 51		-0.15445		
Excited State	2:	2.3194 eV	534.54 nm	f=0.0000
49 -> 51		0.70363		
Excited State	3:	3.8796 eV	319.58 nm	f=0.7267
48 -> 51		0.68308		
50 -> 51		0.19061		
50 <- 51		-0.10076		
Excited State	4:	4.3531 eV	284.82 nm	f=0.0000
50 -> 52		0.69667		
Excited State	5:	4.4329 eV	279.69 nm	f=0.0000
47 -> 51		0.70321		

***Z*.8.2H$^+$**

Excited State	1:	1.4435 eV	858.94 nm	f=0.1039
50 -> 51		0.71911		
50 <- 51		-0.16085		
Excited State	2:	1.7796 eV	696.70 nm	f=0.0037
49 -> 51		0.70671		
Excited State	3:	3.4505 eV	359.32 nm	f=0.2033
48 -> 51		0.69627		
50 -> 51		-0.11295		
Excited State	4:	4.0870 eV	303.36 nm	f=0.0073
47 -> 51		0.69715		
Excited State	5:	4.1046 eV	302.06 nm	f=0.0008
46 -> 51		0.69756		

***E*.9.2H$^+$**

Excited State	1:	2.0052 eV	618.30 nm	f=0.4259

48 -> 51 0.15483

50 -> 51 0.70496

50 <- 51 -0.16828

Excited State 2: 2.3965 eV 517.36 nm f=0.0000

49 -> 51 0.70351

Excited State 3: 3.3273 eV 372.63 nm f=0.0000

44 -> 51 -0.13467

47 -> 51 0.69294

Excited State 4: 3.3906 eV 365.67 nm f=0.5261

48 -> 51 0.68937

50 -> 51 -0.16586

Excited State 5: 3.4123 eV 363.34 nm f=0.0002

46 -> 51 0.70031

***Z*.9.2H$^+$**

Excited State 1: 1.4521 eV 853.83 nm f=0.134

50 -> 51 0.72129

50 <- 51 -0.18547

Excited State 2: 1.8347 eV 675.77 nm f=0.0009

49 -> 51 0.70651

Excited State 3: 2.9189 eV 424.77 nm f=0.0402

44 -> 51 -0.29442

47 -> 51 0.43506

48 -> 51 0.47136

Excited State 4: 3.0008 eV 413.17 nm f=0.0861

47 -> 51 0.52740

48 -> 51 -0.46430

Excited State 5: 3.0214 eV 410.35 nm f=0.0001

46 -> 51 0.70371

***E*.10.2H$^+$**

Excited State 1: 2.0568 eV 602.80 nm f=0.3754

66 -> 69 -0.16935

68 -> 69 0.70092

68 <- 69 -0.14658

Excited State 2: 2.3892 eV 518.93 nm f=0.0000

67 -> 69 0.70366

Excited State 3: 3.9007 eV 317.85 nm f=0.7468

66 -> 69 0.68315

68 -> 69 0.18441

Excited State 4: 4.1261 eV 300.48 nm f=0.0000

65 -> 69 0.70148

Excited State 5: 4.2442 eV 292.12 nm f=0.0001

64 -> 69 0.70309

***Z*.10.2H$^+$**

Excited State	1:	1.4327 eV	865.38 nm	f=0.1058
68 -> 69		0.71965		
68 <- 69		-0.15674		
Excited State	2:	1.8297 eV	677.63 nm	f=0.0041
67 -> 69		0.70655		
Excited State	3:	3.4210 eV	362.42 nm	f=0.1902
62 -> 69		-0.10337		
66 -> 69		0.68863		
Excited State	4:	3.7620 eV	329.57 nm	f=0.0193
65 -> 69		0.69261		
66 -> 69		0.10953		
Excited State	5:	3.8096 eV	325.45 nm	f=0.0000
64 -> 69		0.70317		

***E*.11.2H$^+$**

Excited State	1:	2.0441 eV	606.54 nm	f=0.4430
66 -> 69		0.15608		
68 -> 69		0.70264		
68 <- 69		-0.16004		
Excited State	2:	2.4322 eV	509.77 nm	f=0.0000
67 -> 69		0.70347		
Excited State	3:	3.1068 eV	399.08 nm	f=0.0000
62 -> 69		0.15199		
65 -> 69		0.68923		
Excited State	4:	3.2058 eV	386.75 nm	f=0.0000
61 -> 69		0.10743		
64 -> 69		0.69782		
Excited State	5:	3.3895 eV	365.79 nm	f=0.5360
66 -> 69		0.68919		
68 -> 69		-0.16650		

***Z*.11.2H$^+$**

Excited State	1:	1.4664 eV	845.52 nm	f=0.1301
68 -> 69		0.71749		
68 <- 69		-0.17496		
Excited State	2:	1.8530 eV	669.09 nm	f=0.0011
67 -> 69		0.70627		
Excited State	3:	2.7004 eV	459.13 nm	f=0.0019
63 -> 69		-0.24356		
65 -> 69		0.60601		
66 -> 69		-0.26316		

Excited State	4:	2.8343 eV	437.43 nm	f=0.0000
64 -> 69		0.70046		

Excited State	5:	2.9539 eV	419.73 nm	f=0.1196
63 -> 69		-0.24863		
65 -> 69		0.17899		
66 -> 69		0.63350		

***E*.12.2H$^+$**

Excited State	1:	2.0329 eV	609.88 nm	f=0.4411
60 -> 69		-0.11341		
66 -> 69		0.21145		
68 -> 69		0.68272		
68 <- 69		-0.16049		
Excited State	2:	2.1374 eV	580.08 nm	f=0.0000
63 -> 69		-0.22173		
65 -> 69		0.67056		
Excited State	3:	2.2301 eV	555.96 nm	f=0.0000
61 -> 69		-0.14499		
64 -> 69		0.69145		
Excited State	4:	2.2404 eV	553.40 nm	f=0.0000
67 -> 69		0.70598		
Excited State	5:	2.4235 eV	511.58 nm	f=0.3989
66 -> 69		0.67406		
68 -> 69		-0.22107		

***E*.13.2H$^+$**

Excited State	1:	2.0112 eV	616.46 nm	f=0.4586
42 -> 51		-0.12133		
48 -> 51		0.17148		
50 -> 51		0.69463		
50 <- 51		-0.16917		
Excited State	2:	2.2261 eV	556.95 nm	f=0.0000
49 -> 51		0.70585		
Excited State	3:	2.2275 eV	556.61 nm	f=0.0000
44 -> 51		0.19560		
47 -> 51		0.67887		
Excited State	4:	2.2958 eV	540.04 nm	f=0.0004
43 -> 51		0.12126		
46 -> 51		0.69608		
Excited State	5:	2.3529 eV	526.93 nm	f=0.2978
48 -> 51		0.68528		
50 -> 51		-0.17961		

***E*.14.2H$^+$**

Excited State	1:	1.9620 eV	631.93 nm	f=0.4272
42 -> 49		-0.13593		
48 -> 49		0.71504		
48 <- 49		-0.18116		
Excited State	2:	2.4599 eV	504.01 nm	f=0.0000
44 -> 49		-0.20482		
46 -> 49		0.67488		
Excited State	3:	2.5290 eV	490.24 nm	f=0.0000
47 -> 49		0.70244		
Excited State	4:	2.5632 eV	483.72 nm	f=0.0003
43 -> 49		-0.15176		
45 -> 49		0.68887		
Excited State	5:	2.9086 eV	426.26 nm	f=0.0000
44 -> 49		0.66920		
46 -> 49		0.20555		

***Z*.14.2H$^+$**

Excited State	1:	1.4017 eV	884.51 nm	f=0.1417
44 -> 49		-0.12920		
48 -> 49		0.71713		
48 <- 49		-0.20544		
Excited State	2:	1.9654 eV	630.85 nm	f=0.0018
47 -> 49		0.70584		
Excited State	3:	2.1028 eV	589.61 nm	f=0.0154
44 -> 49		-0.23145		
46 -> 49		0.65518		
48 -> 49		-0.11798		
Excited State	4:	2.1924 eV	565.52 nm	f=0.0000
43 -> 49		0.11934		
45 -> 49		0.69521		
Excited State	5:	2.4593 eV	504.14 nm	f=0.0270
44 -> 49		0.64282		
46 -> 49		0.25204		

***E*.15.2H$^+$**

Excited State	1:	1.9922 eV	622.35 nm	f=0.4520
60 -> 67		-0.13230		
66 -> 67		0.71458		
66 <- 67		-0.17793		
Excited State	2:	2.3206 eV	534.27 nm	f=0.0000
62 -> 67		0.13971		
64 -> 67		0.69082		
Excited State	3:	2.4627 eV	503.44 nm	f=0.0004

61 -> 67 0.12802
63 -> 67 0.69299
Excited State 4: 2.5835 eV 479.91 nm f=0.0000
65 -> 67 0.70218
Excited State 5: 3.0287 eV 409.37 nm f=0.0000
62 -> 67 0.68800
64 -> 67 -0.14181

***Z*.15.2H$^+$**

Excited State 1: 1.4188 eV 873.87 nm f=0.1288
62 -> 67 0.10900
64 -> 67 -0.19439
66 -> 67 0.69441
66 <- 67 -0.19045
Excited State 2: 1.9637 eV 631.39 nm f=0.0517
62 -> 67 -0.13537
64 -> 67 0.65667
66 -> 67 0.22026
Excited State 3: 2.0241 eV 612.53 nm f=0.0023
65 -> 67 0.70386
Excited State 4: 2.1737 eV 570.40 nm f=0.0001
61 -> 67 0.15315
63 -> 67 0.68622
Excited State 5: 2.6099 eV 475.05 nm f=0.0150
62 -> 67 0.67791
64 -> 67 0.16735

***E*.16.2H$^+$**

Excited State 1: 1.8478 eV 670.99 nm f=0.3193
62 -> 67 -0.10864
66 -> 67 0.70721
66 <- 67 -0.17629
Excited State 2: 2.4139 eV 513.62 nm f=0.0000
65 -> 67 0.67654
66 -> 68 -0.19010
Excited State 3: 2.7761 eV 446.61 nm f=0.0000
65 -> 67 0.19612
66 -> 68 0.67377
Excited State 4: 3.2328 eV 383.53 nm f=0.1981
62 -> 67 0.12073
65 -> 68 -0.11947
66 -> 69 0.67906
Excited State 5: 3.2475 eV 381.79 nm f=0.0004
64 -> 67 0.69262

***Z*.16.2H$^+$**

Excited State	1:	1.4243 eV	870.47 nm	f=0.1497
66 -> 67		0.72778		
66 <- 67		-0.20747		
Excited State	2:	1.9530 eV	634.84 nm	f=0.0005
65 -> 67		0.70443		
Excited State	3:	2.7793 eV	446.09 nm	f=0.0007
66 -> 68		0.69598		
Excited State	4:	2.8935 eV	428.49 nm	f=0.0055
61 -> 67		0.13105		
62 -> 67		-0.10505		
64 -> 67		0.67744		
Excited State	5:	3.0902 eV	401.22 nm	f=0.0001
63 -> 67		0.69391		

***E*.17.2H$^+$**

Excited State	1:	1.7663 eV	701.93 nm	f=0.2949
44 -> 49		-0.10438		
47 -> 50		-0.10686		
48 -> 49		0.71027		
48 <- 49		-0.19192		
Excited State	2:	2.3457 eV	528.55 nm	f=0.0001
47 -> 49		0.66844		
48 -> 50		-0.21717		
Excited State	3:	2.6967 eV	459.76 nm	f=0.0001
47 -> 49		0.22246		
48 -> 50		0.66689		
Excited State	4:	3.2228 eV	384.71 nm	f=0.2029
44 -> 49		-0.12135		
47 -> 50		0.10236		
48 -> 49		0.10466		
48 -> 51		0.68157		
Excited State	5:	3.4526 eV	359.10 nm	f=0.0009
45 -> 50		0.10067		
46 -> 49		0.69140		

***Z*.17.2H$^+$**

Excited State	1:	1.3608 eV	911.09 nm	f=0.1442
48 -> 49		0.73348		
48 <- 49		-0.22714		
Excited State	2:	1.9091 eV	649.43 nm	f=0.0003
47 -> 49		0.70343		
Excited State	3:	2.6987 eV	459.42 nm	f=0.0005

48 -> 50	0.69726			
Excited State	4:	3.1432 eV	394.45 nm	f=0.0007
43 -> 49	0.15443			
44 -> 49	0.11932			
46 -> 49	0.66925			
Excited State	5:	3.2299 eV	383.86 nm	f=0.0000
45 -> 49	0.69796			

***E*.18.2H$^+$**

Excited State	1:	1.6801 eV	737.94 nm	f=0.3084
40 -> 41	0.72979			
40 -> 43	0.10193			
40 <- 41	-0.24844			
Excited State	2:	2.4576 eV	504.49 nm	f=0.0001
39 -> 41	0.60948			
40 -> 42	0.34881			
Excited State	3:	2.6860 eV	461.60 nm	f=0.0001
39 -> 41	-0.35169			
40 -> 42	0.61190			
Excited State	4:	3.1644 eV	391.80 nm	f=0.1819
40 -> 41	-0.11106			
40 -> 43	0.69491			
Excited State	5:	3.3582 eV	369.20 nm	f=0.0008
36 -> 41	-0.16877			
37 -> 42	-0.10124			
38 -> 41	0.67674			

***E*.1a.H$^+$**

Excited State	1:	1.9673 eV	630.22 nm	f=0.1341
55 -> 57	-0.10682			
55 -> 58	-0.14163			
56 -> 57	0.68094			
Excited State	2:	2.3854 eV	519.76 nm	f=0.0106
55 -> 57	0.62005			
56 -> 58	-0.31353			
Excited State	3:	2.7721 eV	447.25 nm	f=0.0025
54 -> 57	-0.23309			
55 -> 57	0.26955			
56 -> 58	0.58673			
Excited State	4:	2.8334 eV	437.58 nm	f=0.0020
53 -> 57	0.23970			
54 -> 57	0.58238			
55 -> 57	0.17157			
56 -> 58	0.20013			

Excited State	5:	3.1052 eV	399.28 nm	f=0.0075
49 -> 57		0.10682		
51 -> 57		-0.11577		
53 -> 57		0.61713		
54 -> 57		-0.26148		
54 -> 58		-0.10038		

***Z*.1a.H$^+$**

Excited State	1:	1.7966 eV	690.09 nm	f=0.0417
56 -> 57		0.69799		
Excited State	2:	2.3397 eV	529.93 nm	f=0.0004
55 -> 57		0.59623		
56 -> 58		0.36119		
Excited State	3:	2.5646 eV	483.45 nm	f=0.0024
55 -> 57		-0.34373		
56 -> 58		0.58424		
56 -> 59		-0.13483		
Excited State	4:	2.9897 eV	414.70 nm	f=0.0144
51 -> 57		-0.12959		
54 -> 57		0.64345		
54 -> 58		-0.16790		
Excited State	5:	3.1222 eV	397.10 nm	f=0.0587
53 -> 57		-0.11321		
54 -> 57		0.11606		
55 -> 57		-0.13244		
55 -> 58		0.47810		
56 -> 59		0.43795		

***E*.2a.H$^+$**

Excited State	1:	1.9376 eV	639.88 nm	f=0.1386
51 -> 53		-0.10141		
51 -> 54		-0.14228		
52 -> 53		0.68283		
Excited State	2:	2.3775 eV	521.49 nm	f=0.0146
51 -> 53		0.61126		
52 -> 54		-0.33499		
Excited State	3:	2.7622 eV	448.86 nm	f=0.0003
51 -> 53		0.33754		
52 -> 54		0.60805		
Excited State	4:	3.0143 eV	411.32 nm	f=0.0008
50 -> 53		0.68692		
Excited State	5:	3.5927 eV	345.10 nm	f=0.3895
48 -> 53		-0.11070		
51 -> 54		0.58275		

52 -> 53 0.15157
52 -> 55 -0.32597

***Z*.2a.H$^+$**

Excited State 1: 1.7962 eV 690.26 nm f=0.0456
52 -> 53 0.69722
Excited State 2: 2.3443 eV 528.88 nm f=0.0014
51 -> 53 0.56864
51 -> 54 0.10401
52 -> 54 0.40053
Excited State 3: 2.5756 eV 481.38 nm f=0.0032
51 -> 53 -0.39504
52 -> 54 0.55896
52 -> 55 0.12071
Excited State 4: 3.1020 eV 399.69 nm f=0.0629
50 -> 53 0.17216
51 -> 53 -0.12476
51 -> 54 0.47275
52 -> 55 -0.46151
Excited State 5: 3.3236 eV 373.04 nm f=0.0197
47 -> 53 -0.10828
50 -> 53 0.57084
50 -> 55 0.12693
51 -> 54 -0.31824

***E*.3a.H$^+$**

Excited State 1: 1.9402 eV 639.03 nm f=0.1574
51 -> 54 0.13956
52 -> 53 0.68834
Excited State 2: 2.3846 eV 519.93 nm f=0.0141
51 -> 53 0.62156
52 -> 54 0.31676
Excited State 3: 2.7851 eV 445.18 nm f=0.0000
51 -> 53 -0.32505
52 -> 54 0.61631
Excited State 4: 3.1646 eV 391.78 nm f=0.0003
48 -> 53 0.11516
50 -> 53 0.68406
Excited State 5: 3.5695 eV 347.34 nm f=0.3740
49 -> 53 0.15849
51 -> 54 0.58594
52 -> 53 -0.14726
52 -> 55 0.31394

***Z*.3a.H$^+$**

Excited State	1:	1.7573 eV	705.52 nm	f=0.0630
52 -> 53		0.69720		
Excited State	2:	2.3187 eV	534.72 nm	f=0.0039
51 -> 53		0.62072		
51 -> 54		-0.12939		
52 -> 54		0.30377		
Excited State	3:	2.5793 eV	480.70 nm	f=0.0029
51 -> 53		-0.31103		
52 -> 54		0.61584		
Excited State	4:	3.1383 eV	395.07 nm	f=0.0673
50 -> 53		-0.21280		
51 -> 53		0.10183		
51 -> 54		0.55347		
52 -> 55		-0.33907		
Excited State	5:	3.2609 eV	380.21 nm	f=0.0155
49 -> 53		-0.13104		
50 -> 53		0.60599		
50 -> 55		0.11346		
51 -> 54		0.24917		

***E*.4a.H$^+$**

Excited State	1:	1.9124 eV	648.31 nm	f=0.1588
55 -> 58		-0.13318		
56 -> 57		0.68963		
Excited State	2:	2.3764 eV	521.74 nm	f=0.0204
55 -> 57		0.62552		
55 -> 58		-0.10504		
56 -> 58		-0.30014		
Excited State	3:	2.7787 eV	446.19 nm	f=0.0000
55 -> 57		0.31338		
56 -> 58		0.62158		
Excited State	4:	3.0949 eV	400.61 nm	f=0.0003
54 -> 57		0.68626		
Excited State	5:	3.5398 eV	350.26 nm	f=0.2984
53 -> 57		-0.21253		
55 -> 58		0.57922		
56 -> 57		0.13644		
56 -> 58		-0.10072		
56 -> 59		-0.29376		

***Z*.4a.H$^+$**

Excited State	1:	1.6796 eV	738.17 nm	f=0.0765
56 -> 57		0.69788		

Excited State	2:	2.2810 eV	543.56 nm	f=0.0057
55 -> 57		0.65524		
55 -> 58		0.12025		
56 -> 58		-0.22104		
Excited State	3:	2.5731 eV	481.84 nm	f=0.0039
55 -> 57		0.22629		
56 -> 58		0.64969		
56 -> 59		-0.10054		
Excited State	4:	3.1189 eV	397.52 nm	f=0.0295
52 -> 57		0.17652		
53 -> 57		-0.18779		
54 -> 57		0.56636		
54 -> 59		-0.11303		
55 -> 58		0.21309		
56 -> 59		-0.17676		
Excited State	5:	3.2239 eV	384.58 nm	f=0.0557
54 -> 57		-0.27702		
55 -> 58		0.52924		
56 -> 59		-0.34017		

***E*.5a.H$^+$**

Excited State	1:	1.8554 eV	668.22 nm	f=0.1981
51 -> 54		0.11355		
52 -> 53		0.69754		
52 <- 53		-0.10398		
Excited State	2:	2.3855 eV	519.75 nm	f=0.0222
51 -> 53		0.61439		
51 -> 54		0.15801		
52 -> 54		0.29424		
Excited State	3:	2.6945 eV	460.14 nm	f=0.0046
51 -> 53		-0.31757		
52 -> 54		0.61987		
Excited State	4:	3.2503 eV	381.45 nm	f=0.0126
48 -> 53		-0.10438		
49 -> 53		-0.20368		
50 -> 53		0.60358		
51 -> 54		-0.15849		
52 -> 55		0.19582		
Excited State	5:	3.4680 eV	357.51 nm	f=0.3548
49 -> 53		-0.23704		
50 -> 53		0.13374		
51 -> 53		-0.10488		
51 -> 54		0.50593		
52 -> 53		-0.11860		

52 -> 55 -0.33507

***Z*.5a.H$^+$**

Excited State 1: 1.5695 eV 789.96 nm f=0.1607
51 -> 53 0.12967
52 -> 53 0.69708
52 <- 53 -0.13815
Excited State 2: 2.1426 eV 578.65 nm f=0.0222
51 -> 53 0.67802
52 -> 53 -0.12884
52 -> 54 0.10541
Excited State 3: 2.5770 eV 481.12 nm f=0.0170
51 -> 53 -0.12206
51 -> 54 0.16387
52 -> 54 0.66793
Excited State 4: 2.8461 eV 435.63 nm f=0.0139
49 -> 53 0.29844
50 -> 53 0.62211
Excited State 5: 3.3093 eV 374.65 nm f=0.1078
49 -> 53 0.13758
51 -> 54 0.62174
52 -> 54 -0.14288
52 -> 55 -0.22297

***E*.6a.H$^+$**

Excited State 1: 1.7396 eV 712.73 nm f=0.1874
60 -> 61 0.70311
60 <- 61 -0.10626
Excited State 2: 2.3387 eV 530.15 nm f=0.0396
58 -> 61 0.10163
59 -> 61 0.63165
59 -> 62 -0.20345
60 -> 62 -0.20770
Excited State 3: 2.5763 eV 481.25 nm f=0.0079
59 -> 61 0.24949
59 -> 62 0.10351
60 -> 62 0.64232
Excited State 4: 3.1370 eV 395.23 nm f=0.0047
57 -> 61 0.18496
58 -> 61 0.58770
59 -> 62 0.17627
60 -> 63 -0.26654
Excited State 5: 3.3960 eV 365.09 nm f=0.1684
57 -> 61 -0.17389

59 -> 61	0.14943			
59 -> 62	0.62114			
60 -> 62	-0.17579			

***Z*.6a.H$^+$**

Excited State	1:	1.4706 eV	843.07 nm	f=0.1785
59 -> 61	-0.11194			
60 -> 61	0.70355			
60 <- 61	-0.14878			
Excited State	2:	2.0750 eV	597.50 nm	f=0.0154
59 -> 61	0.68557			
60 -> 61	0.11777			
Excited State	3:	2.4598 eV	504.03 nm	f=0.0219
58 -> 61	0.22891			
59 -> 62	-0.13776			
60 -> 62	0.63999			
Excited State	4:	2.6958 eV	459.91 nm	f=0.0317
57 -> 61	-0.23784			
58 -> 61	0.60806			
60 -> 62	-0.22132			
Excited State	5:	3.1958 eV	387.96 nm	f=0.0329
57 -> 61	0.33886			
59 -> 62	0.49677			
60 -> 63	-0.30917			

***E*.7a.H$^+$**

Excited State	1:	2.0212 eV	613.43 nm	f=0.1730
51 -> 54	-0.13805			
52 -> 53	0.68699			
Excited State	2:	2.4630 eV	503.38 nm	f=0.0013
51 -> 53	0.61616			
52 -> 54	-0.34032			
Excited State	3:	2.8144 eV	440.53 nm	f=0.0035
51 -> 53	0.33810			
52 -> 54	0.60496			
Excited State	4:	3.1562 eV	392.83 nm	f=0.0004
48 -> 53	0.15011			
50 -> 53	0.67740			
50 -> 55	-0.10059			
Excited State	5:	3.6851 eV	336.45 nm	f=0.3865
49 -> 53	0.16181			
51 -> 54	-0.45756			
52 -> 53	-0.13238			
52 -> 55	0.48502			

***Z*.7a.H$^+$**

Excited State 1: 1.9129 eV 648.16 nm f=0.0480
51 -> 54 0.10198
52 -> 53 0.69894
Excited State 2: 2.3930 eV 518.10 nm f=0.0017
51 -> 53 0.60426
52 -> 54 0.35177
Excited State 3: 2.6844 eV 461.86 nm f=0.0023
51 -> 53 -0.35013
51 -> 55 -0.10085
52 -> 54 0.59660
Excited State 4: 3.1186 eV 397.57 nm f=0.0667
50 -> 53 0.13547
51 -> 54 0.53736
52 -> 55 -0.41715
Excited State 5: 3.4334 eV 361.11 nm f=0.0105
50 -> 53 0.57131
50 -> 55 0.14370
51 -> 54 -0.28785
52 -> 55 -0.15974

***E*.8a.H$^+$**

Excited State 1: 1.9313 eV 641.98 nm f=0.1436
53 -> 56 -0.12110
54 -> 55 0.68716
Excited State 2: 2.4025 eV 516.07 nm f=0.0090
53 -> 55 0.62747
54 -> 56 -0.30924
Excited State 3: 2.7011 eV 459.02 nm f=0.0034
53 -> 55 0.30731
54 -> 56 0.61669
Excited State 4: 2.9305 eV 423.09 nm f=0.0004
49 -> 55 0.11401
52 -> 55 0.68347
Excited State 5: 3.5927 eV 345.10 nm f=0.2140
51 -> 55 0.27973
53 -> 56 0.33267
54 -> 57 0.53609

***Z*.8a.H$^+$**

Excited State 1: 1.8707 eV 662.78 nm f=0.0417
54 -> 55 0.69801
Excited State 2: Singlet-A 2.3384 eV 530.20 nm f=0.0010 <S**2>=0.000

53 -> 55	0.61317			
54 -> 56	-0.33184			
Excited State	3:	2.5921 eV	478.31 nm	f=0.0030
53 -> 55	0.31759			
54 -> 56	0.60898			
Excited State	4:	3.0527 eV	406.14 nm	f=0.0574
53 -> 55	-0.12741			
53 -> 56	0.57454			
54 -> 57	-0.34679			
Excited State	5:	3.3410 eV	371.10 nm	f=0.0142
49 -> 55	-0.18372			
52 -> 55	0.61673			
52 -> 57	-0.11977			
53 -> 56	0.17589			

***E*.9a.H$^+$**

Excited State	1:	1.9061 eV	650.46 nm	f=0.1220
55 -> 57	0.13126			
55 -> 58	0.12931			
56 -> 57	0.68118			
Excited State	2:	2.3515 eV	527.26 nm	f=0.0261
55 -> 57	0.62368			
56 -> 57	-0.10749			
56 -> 58	0.29853			
Excited State	3:	2.7221 eV	455.48 nm	f=0.0004
55 -> 57	-0.30355			
56 -> 58	0.62365			
Excited State	4:	2.8246 eV	438.94 nm	f=0.0001
54 -> 57	0.68455			
Excited State	5:	3.5228 eV	351.95 nm	f=0.2875
53 -> 57	-0.24014			
55 -> 58	0.54369			
56 -> 57	-0.12917			
56 -> 59	0.34370			

***Z*.9a.H$^+$**

Excited State	1:	1.7267 eV	718.03 nm	f=0.0439
56 -> 57	0.69897			
Excited State	2:	2.2740 eV	545.23 nm	f=0.0035
55 -> 57	0.64144			
55 -> 58	0.10994			
56 -> 58	-0.26673			
Excited State	3:	2.5524 eV	485.75 nm	f=0.0051
55 -> 57	0.26345			

56 -> 58	0.63578			
56 -> 59	-0.10606			
Excited State	4:	3.0467 eV	406.95 nm	f=0.0172
52 -> 57	-0.16092			
53 -> 57	-0.14219			
54 -> 57	0.61377			
55 -> 58	-0.13178			
56 -> 59	0.15036			
Excited State	5:	3.1100 eV	398.66 nm	f=0.0679
54 -> 57	0.22061			
55 -> 57	-0.10390			
55 -> 58	0.53668			
56 -> 59	-0.36196			

***E*.10a.H$^+$**

Excited State	1:	1.8306 eV	677.30 nm	f=0.0970
64 -> 66	0.15403			
64 -> 67	0.10960			
65 -> 66	0.67987			
Excited State	2:	2.3032 eV	538.30 nm	f=0.0483
64 -> 66	0.63234			
64 -> 67	-0.11256			
65 -> 66	-0.13265			
65 -> 67	0.24345			
Excited State	3:	2.5039 eV	495.16 nm	f=0.0000
61 -> 66	0.10991			
63 -> 66	0.68914			
Excited State	4:	2.6752 eV	463.45 nm	f=0.0000
64 -> 66	-0.26440			
65 -> 67	0.63883			
Excited State	5:	3.3751 eV	367.35 nm	f=0.1513
62 -> 66	-0.36171			
64 -> 67	0.51498			
65 -> 66	-0.10918			
65 -> 68	0.28272			

***Z*.10a.H$^+$**

Excited State	1:	1.6530 eV	750.04 nm	f=0.0347
65 -> 66	0.69563			
Excited State	2:	2.2172 eV	559.19 nm	f=0.0107
64 -> 66	0.64814			
64 -> 67	0.12533			
65 -> 67	0.22724			

Excited State	3:	2.4809 eV	499.76 nm	f=0.0049
63 -> 66		-0.11695		
64 -> 66		-0.24346		
65 -> 67		0.62861		
65 -> 68		-0.11337		
Excited State	4:	2.5722 eV	482.02 nm	f=0.0302
63 -> 66		0.66519		
63 -> 67		-0.10959		
64 -> 67		0.11307		
65 -> 67		0.13234		
Excited State	5:	3.0470 eV	406.91 nm	f=0.0693
61 -> 66		0.13194		
62 -> 66		0.17206		
64 -> 66		-0.13293		
64 -> 67		0.53661		
64 -> 68		0.11680		
65 -> 68		0.32094		

***E*.11a.H$^+$**

Excited State	1:	1.6326 eV	759.41 nm	f=0.0609
59 -> 61		0.16308		
60 -> 61		0.68252		
Excited State	2:	1.8889 eV	656.37 nm	f=0.0163
58 -> 61		-0.15881		
59 -> 61		0.66398		
60 -> 61		-0.15522		
Excited State	3:	2.2456 eV	552.13 nm	f=0.0767
57 -> 61		-0.10082		
58 -> 61		0.64716		
58 -> 62		-0.16128		
59 -> 61		0.13588		
Excited State	4:	2.5476 eV	486.68 nm	f=0.0060
57 -> 61		-0.16627		
58 -> 61		-0.13437		
58 -> 62		-0.17626		
60 -> 62		0.63502		
Excited State	5:	2.9771 eV	416.46 nm	f=0.0068
56 -> 61		-0.24504		
57 -> 61		0.46863		
58 -> 62		-0.25778		
59 -> 62		0.32516		
59 -> 63		0.12646		
60 -> 63		-0.10643		

***Z*.11a.H$^+$**

Excited State	1:	1.3235 eV	936.78 nm	f=0.0072
59 -> 61		0.15464		
60 -> 61		0.67963		
60 -> 62		-0.10264		
Excited State	2:	1.8931 eV	654.92 nm	f=0.0834
58 -> 61		-0.19492		
59 -> 61		0.63459		
60 -> 61		-0.15988		
60 -> 62		-0.14956		
Excited State	3:	2.1626 eV	573.31 nm	f=0.0102
58 -> 61		0.64495		
59 -> 61		0.13287		
60 -> 62		-0.17914		
Excited State	4:	2.3221 eV	533.93 nm	f=0.0327
57 -> 61		0.10148		
58 -> 61		0.11568		
58 -> 62		0.17201		
59 -> 61		0.20453		
60 -> 62		0.62350		
Excited State	5:	2.6079 eV	475.42 nm	f=0.0019
57 -> 61		-0.25321		
59 -> 62		0.61520		
59 -> 63		-0.13247		

***E*.1a.2H$^+$**

Excited State	1:	1.6073 eV	771.36 nm	f=0.1865
60 -> 65		0.10991		
63 -> 66		-0.10275		
64 -> 65		0.69976		
64 <- 65		-0.15611		
Excited State	2:	2.0688 eV	599.30 nm	f=0.0007
63 -> 65		0.69257		
64 -> 66		-0.12880		
Excited State	3:	2.4654 eV	502.90 nm	f=0.0001
59 -> 65		-0.18344		
60 -> 65		0.12964		
62 -> 65		0.66420		
Excited State	4:	2.4905 eV	497.84 nm	f=0.0005
58 -> 65		0.11044		
61 -> 65		0.68863		
Excited State	5:	2.6051 eV	475.93 nm	f=0.0002
63 -> 65		0.12615		
64 -> 66		0.68410		

***Z*.1a.2H$^+$**

Excited State	1:	1.2287 eV	1009.06 nm	f=0.1512
64 -> 65		0.72853		
64 <- 65		-0.21095		
Excited State	2:	1.6825 eV	736.89 nm	f=0.0049
63 -> 65		0.70178		
Excited State	3:	2.0098 eV	616.89 nm	f=0.0029
59 -> 65		-0.15729		
60 -> 65		-0.14317		
62 -> 65		0.67006		
Excited State	4:	2.0266 eV	611.80 nm	f=0.0006
58 -> 65		-0.18102		
61 -> 65		0.67766		
Excited State	5:	2.4821 eV	499.51 nm	f=0.0171
59 -> 65		0.65580		
60 -> 65		0.16876		
62 -> 65		0.18950		

***E*.2a.2H$^+$**

Excited State	1:	1.5610 eV	794.27 nm	f=0.2187
55 -> 58		0.10947		
56 -> 57		0.71035		
56 <- 57		-0.18386		
Excited State	2:	2.0988 eV	590.75 nm	f=0.0001
55 -> 57		0.68458		
56 -> 58		0.17118		
Excited State	3:	2.5726 eV	481.94 nm	f=0.0000
55 -> 57		-0.17336		
56 -> 58		0.68119		
Excited State	4:	3.1837 eV	389.44 nm	f=0.1617
52 -> 57		0.12896		
54 -> 57		-0.13522		
55 -> 58		-0.12231		
56 -> 59		0.66585		
Excited State	5:	3.3424 eV	370.95 nm	f=0.0031
52 -> 57		0.38097		
54 -> 57		0.57891		

***Z*.2a.2H$^+$**

Excited State	1:	1.2636 eV	981.20 nm	f=0.1775
56 -> 57		0.73765		
56 <- 57		-0.23859		
Excited State	2:	1.8991 eV	652.87 nm	f=0.0028

55 -> 57 0.70155

Excited State 3: 2.5770 eV 481.11 nm f=0.0056

56 -> 58 0.69646

Excited State 4: 3.0545 eV 405.90 nm f=0.0076

48 -> 57 0.11935

53 -> 57 0.67174

54 -> 57 -0.12639

Excited State 5: 3.1928 eV 388.33 nm f=0.0115

52 -> 57 0.62097

54 -> 57 -0.20625

56 -> 59 0.23259

***E*.3a.2H$^+$**

Excited State 1: 1.5290 eV 810.87 nm f=0.2518

55 -> 58 0.10130

56 -> 57 0.71525

56 <- 57 -0.18864

Excited State 2: 2.0792 eV 596.31 nm f=0.0000

55 -> 57 0.69303

56 -> 58 0.14042

Excited State 3: 2.6194 eV 473.33 nm f=0.0000

55 -> 57 -0.14198

56 -> 58 0.68819

Excited State 4: 3.1926 eV 388.35 nm f=0.1641

54 -> 57 -0.20341

55 -> 58 -0.14426

56 -> 59 0.65710

Excited State 5: 3.6863 eV 336.34 nm f=0.0298

54 -> 57 0.32826

55 -> 58 0.57781

56 -> 59 0.23133

***Z*.3a.2H$^+$**

Excited State 1: 1.3173 eV 941.22 nm f=0.2343

56 -> 57 0.74127

56 <- 57 -0.24794

Excited State 2: 1.9992 eV 620.18 nm f=0.0024

55 -> 57 0.70328

Excited State 3: 2.6247 eV 472.38 nm f=0.0096

56 -> 58 0.69707

Excited State 4: 3.2235 eV 384.63 nm f=0.0908

53 -> 57 -0.12067

54 -> 57 0.45850

55 -> 58 0.15043

56 -> 59	0.49565			
Excited State	5:	3.3648 eV	368.47 nm	f=0.0292
51 -> 57	-0.11383			
53 -> 57	0.43185			
54 -> 57	-0.34614			
56 -> 59	0.41688			

***E*.4a.2H$^+$**

Excited State	1:	1.4636 eV	847.09 nm	f=0.2462
64 -> 65	0.71410			
64 <- 65	-0.18301			
Excited State	2:	2.0001 eV	619.90 nm	f=0.0000
63 -> 65	0.69918			
64 -> 66	0.11161			
Excited State	3:	2.6153 eV	474.07 nm	f=0.0000
63 -> 65	-0.11204			
64 -> 66	0.69267			
Excited State	4:	3.1367 eV	395.27 nm	f=0.0635
62 -> 65	-0.37701			
63 -> 66	-0.18837			
64 -> 67	0.56383			
Excited State	5:	3.5056 eV	353.67 nm	f=0.1014
62 -> 65	0.45004			
63 -> 66	0.33949			
64 -> 67	0.41403			

***Z*.4a.2H$^+$**

Excited State	1:	1.3198 eV	939.43 nm	f=0.2831
64 -> 65	0.73926			
64 <- 65	-0.24083			
Excited State	2:	1.9970 eV	620.86 nm	f=0.0071
63 -> 65	0.70564			
63 <- 65	-0.10143			
Excited State	3:	2.6382 eV	469.96 nm	f=0.0136
64 -> 66	0.69768			
Excited State	4:	3.0288 eV	409.35 nm	f=0.0404
60 -> 65	0.10240			
62 -> 65	0.62592			
63 -> 66	0.14135			
64 -> 67	0.25518			
Excited State	5:	3.3259 eV	372.79 nm	f=0.0239
58 -> 65	0.20646			
60 -> 65	-0.43600			
61 -> 65	-0.15699			

64 -> 67 0.46692

***E*.5a.2H$^+$**

Excited State 1: 1.4591 eV 849.76 nm f=0.3510
56 -> 57 0.74259
56 <- 57 -0.26417
Excited State 2: 2.1944 eV 565.01 nm f=0.0179
55 -> 57 0.70609
55 <- 57 -0.11668
Excited State 3: 2.4305 eV 510.11 nm f=0.0031
56 -> 58 0.69797
Excited State 4: 2.7700 eV 447.60 nm f=0.1306
54 -> 57 -0.24984
56 -> 59 0.65123
Excited State 5: 3.1859 eV 389.16 nm f=0.1041
54 -> 57 0.59866
55 -> 58 -0.25894
56 -> 59 0.25390

***Z*.5a.2H$^+$**

Excited State 1: 1.1444 eV 1083.40 nm f=0.2460
56 -> 57 0.77591
56 <- 57 -0.33629
Excited State 2: 1.9732 eV 628.34 nm f=0.0006
55 -> 57 0.71150
55 <- 57 -0.12939
Excited State 3: 2.3504 eV 527.50 nm f=0.0166
56 -> 58 0.70131
Excited State 4: 2.8665 eV 432.53 nm f=0.0928
54 -> 57 -0.44124
55 -> 58 0.12005
56 -> 59 0.53323
Excited State 5: 3.0955 eV 400.54 nm f=0.0242
54 -> 57 0.50566
55 -> 58 -0.15715
56 -> 59 0.45468

***E*.6a.2H$^+$**

Excited State 1: 1.2643 eV 980.67 nm f=0.2897
72 -> 73 0.73874
72 <- 73 -0.25323
Excited State 2: 1.8452 eV 671.92 nm f=0.0070
71 -> 73 0.71294
71 <- 73 -0.11559

Excited State 3: 2.3170 eV 535.11 nm f=0.0152
72 -> 74 0.69991
Excited State 4: 2.5408 eV 487.97 nm f=0.0075
70 -> 73 0.54616
71 -> 74 0.17594
72 -> 75 -0.40732
Excited State 5: Singlet-A 2.9287 eV 423.35 nm f=0.1412 <S**2>=0.000
70 -> 73 0.32754
71 -> 74 0.26436
72 -> 75 0.55678

***Z*.6a.2H$^+$**
Excited State 1: 0.7998 eV 1550.15 nm f=0.1621
72 -> 73 0.85065
72 <- 73 -0.48298
Excited State 2: 1.8259 eV 679.02 nm f=0.0024
71 -> 73 0.70738
71 <- 73 -0.12002
Excited State 3: 2.1057 eV 588.82 nm f=0.0942
70 -> 73 0.68778
72 -> 75 -0.13217
Excited State 4: 2.1990 eV 563.83 nm f=0.0273
71 -> 73 0.10162
72 -> 74 0.69356
Excited State 5: 2.6678 eV 464.74 nm f=0.0195
70 -> 73 0.12756
72 -> 75 0.68569

***E*.7a.2H$^+$**
Excited State 1: 1.7271 eV 717.87 nm f=0.2868
54 -> 57 0.10490
55 -> 58 0.10296
56 -> 57 0.71094
56 <- 57 -0.18322
Excited State 2: 2.2934 eV 540.62 nm f=0.0000
55 -> 57 0.68314
56 -> 58 0.17207
Excited State 3: 2.7509 eV 450.70 nm f=0.0000
55 -> 57 -0.17603
56 -> 58 0.68002
Excited State 4: 3.2909 eV 376.75 nm f=0.1971
54 -> 57 0.13980
55 -> 58 -0.12529
56 -> 59 0.67632

Excited State	5:	3.8751 eV	319.95 nm	f=0.0004
51 -> 57		0.14213		
53 -> 57		0.68170		

***Z*.7a.2H$^+$**

Excited State	1:	1.3947 eV	888.99 nm	f=0.1889
56 -> 57		0.73253		
56 <- 57		-0.22233		
Excited State	2:	2.0056 eV	618.19 nm	f=0.0001
55 -> 57		0.70230		
Excited State	3:	2.7541 eV	450.18 nm	f=0.0030
56 -> 58		0.69663		
Excited State	4:	3.3497 eV	370.13 nm	f=0.0137
51 -> 57		-0.12685		
53 -> 57		0.50254		
54 -> 57		0.46732		
Excited State	5:	3.4051 eV	364.12 nm	f=0.1114
53 -> 57		0.19886		
54 -> 57		-0.11103		
55 -> 58		0.20746		
56 -> 59		0.63189		

***E*.8a.2H$^+$**

Excited State	1:	1.6351 eV	758.25 nm	f=0.1782
58 -> 61		0.12031		
60 -> 61		0.70161		
60 <- 61		-0.15167		
Excited State	2:	2.1061 eV	588.68 nm	f=0.0001
59 -> 61		0.69777		
60 -> 62		0.11288		
Excited State	3:	2.6045 eV	476.03 nm	f=0.0000
59 -> 61		-0.11273		
60 -> 62		0.69244		
Excited State	4:	3.0384 eV	408.05 nm	f=0.0004
57 -> 61		0.68336		
58 -> 61		-0.15730		
Excited State	5:	3.0953 eV	400.56 nm	f=0.0420
57 -> 61		0.11328		
58 -> 61		0.34579		
59 -> 62		-0.11296		
60 -> 63		0.59188		

***Z*.8a.2H$^+$**

Excited State	1:	1.3150 eV	942.86 nm	f=0.1640

60 -> 61 0.72539

60 <- 61 -0.19396

Excited State 2: 1.8211 eV 680.81 nm f=0.0107

59 -> 61 0.70529

Excited State 3: 2.6199 eV 473.24 nm f=0.0112

57 -> 61 -0.14367

58 -> 61 0.56216

60 -> 62 -0.37716

Excited State 4: 2.6271 eV 471.95 nm f=0.0083

56 -> 61 0.15232

58 -> 61 0.35339

60 -> 62 0.58050

Excited State 5: 2.7396 eV 452.57 nm f=0.0044

56 -> 61 0.57756

57 -> 61 0.37988

***E*.9a.2H$^+$**

Excited State 1: 1.4820 eV 836.60 nm f=0.1835

61 -> 65 -0.10893

64 -> 65 0.70698

64 <- 65 -0.16191

Excited State 2: 1.9585 eV 633.05 nm f=0.0000

63 -> 65 0.69698

64 -> 66 0.12247

Excited State 3: 2.5117 eV 493.62 nm f=0.0000

63 -> 65 -0.12220

64 -> 66 0.69110

Excited State 4: 2.7348 eV 453.36 nm f=0.0000

62 -> 65 0.70428

Excited State 5: 3.0491 eV 406.63 nm f=0.0690

61 -> 65 -0.34502

63 -> 66 -0.16883

64 -> 67 0.58958

***Z*.9a.2H$^+$**

Excited State 1: 1.2713 eV 975.26 nm f=0.1974

64 -> 65 0.73115

64 <- 65 -0.21854

Excited State 2: 1.8528 eV 669.18 nm f=0.0106

63 -> 65 0.70173

Excited State 3: 2.4950 eV 496.92 nm f=0.0238

60 -> 65 0.11141

62 -> 65 0.69124

Excited State 4: 2.5424 eV 487.66 nm f=0.0083

64 -> 66 0.69362

Excited State 5: 2.6820 eV 462.29 nm f=0.0048

61 -> 65 0.69509

***E*.10a.2H$^+$**

Excited State 1: 1.3448 eV 921.94 nm f=0.1498

78 -> 83 0.11371

82 -> 83 0.70657

82 <- 83 -0.15219

Excited State 2: 1.7464 eV 709.93 nm f=0.0002

81 -> 83 0.70443

Excited State 3: 2.0994 eV 590.57 nm f=0.0002

80 -> 83 0.70509

Excited State 4: 2.4013 eV 516.33 nm f=0.0000

79 -> 83 0.69683

Excited State 5: 2.4143 eV 513.53 nm f=0.0002

82 -> 84 0.68831

***Z*.10a.2H$^+$**

Excited State 1: 1.1705 eV 1059.21 nm f=0.1897

80 -> 83 0.10096

82 -> 83 0.72933

82 <- 83 -0.22565

Excited State 2: 1.6884 eV 734.34 nm f=0.0125

79 -> 83 -0.24184

81 -> 83 0.66481

Excited State 3: 1.9081 eV 649.77 nm f=0.0451

80 -> 83 0.69448

82 -> 83 -0.11274

Excited State 4: 2.1100 eV 587.60 nm f=0.0139

79 -> 83 0.65765

81 -> 83 0.24518

Excited State 5: 2.4371 eV 508.73 nm f=0.0129

82 -> 84 0.69318

***E*.11a.2H$^+$**

Excited State 1: 1.0752 eV 1153.09 nm f=0.1302

72 -> 73 0.71695

72 <- 73 -0.16680

Excited State 2: 1.3416 eV 924.13 nm f=0.0004

70 -> 73 0.70537

Excited State 3: 1.4005 eV 885.26 nm f=0.0001

71 -> 73 0.70951

Excited State 4: 1.5827 eV 783.36 nm f=0.0000

69 -> 73 0.70278

Excited State 5: 2.1658 eV 572.45 nm f=0.0000

72 -> 74 0.69490

***Z*.11a.2H$^+$**

Excited State 1: 0.8942 eV 1386.54 nm f=0.0945

70 -> 73 0.35180

72 -> 73 0.65304

72 <- 73 -0.23313

Excited State 2: 1.1289 eV 1098.25 nm f=0.0011

69 -> 73 0.39910

71 -> 73 0.58342

Excited State 3: 1.2947 eV 957.60 nm f=0.1572

70 -> 73 0.60875

72 -> 73 -0.38903

72 <- 73 0.16879

Excited State 4: 1.7327 eV 715.57 nm f=0.0394

69 -> 73 0.57480

71 -> 73 -0.40860

Excited State 5: 2.1126 eV 586.88 nm f=0.0206

68 -> 73 0.66722

71 -> 74 0.15522

72 -> 75 0.16317

***E*.17e.H$^+$**

Excited State 1: 1.2137 eV 1021.57 nm f=0.0789

88 -> 89 0.69721

88 <- 89 -0.11174

Excited State 2: 1.5435 eV 803.29 nm f=0.0049

86 -> 89 -0.42953

87 -> 89 0.47163

88 -> 90 -0.27159

Excited State 3: 1.6864 eV 735.20 nm f=0.004

86 -> 89 0.11879

87 -> 89 0.41364

88 -> 90 0.54563

Excited State 4: 1.7651 eV 702.43 nm f=0.0022

86 -> 89 0.53932

87 -> 89 0.28790

88 -> 90 -0.33202

Excited State 5: 2.1078 eV 588.21 nm f=0.0023

84 -> 89 0.31075

85 -> 89 0.58730

87 -> 90 -0.19715

***Z*.17e.H$^+$**

Excited State 1: 1.2930 eV 958.92 nm f=0.1336
86 -> 89 0.10556
87 -> 89 -0.11633
87 -> 90 -0.12766
88 -> 89 0.68405
88 <- 89 -0.12799
Excited State 2: 1.5758 eV 786.80 nm f=0.0291
86 -> 89 -0.29951
87 -> 89 0.53734
88 -> 89 0.13773
88 -> 90 -0.29535
Excited State 3: 1.7186 eV 721.43 nm f=0.0115
86 -> 89 -0.21619
87 -> 89 0.21014
88 -> 90 0.62088
Excited State 4: 1.8778 eV 660.28 nm f=0.0330
83 -> 89 -0.10983
86 -> 89 0.56553
87 -> 89 0.36985
Excited State 5: 2.0984 eV 590.85 nm f=0.0059
85 -> 89 0.67352
85 -> 90 -0.13938

***E*.17e.2H$^+$**

Excited State 1: 0.9856 eV 1257.98 nm f=0.1145
88 -> 89 0.72719
88 <- 89 -0.23322
Excited State 2: 1.4722 eV 842.15 nm f=0.0001
87 -> 89 -0.16527
88 -> 90 0.68447
Excited State 3: 1.6358 eV 757.96 nm f=0.0003
87 -> 89 0.68712
88 -> 90 0.16252
Excited State 4: 1.7078 eV 725.98 nm f=0.0005
86 -> 89 0.70380
Excited State 5: 1.9202 eV 645.70 nm f=0.0000
85 -> 89 0.69790

***Z*.17e.2H$^+$**

Excited State 1: 1.1967 eV 1036.07 nm f=0.2641
88 -> 89 0.73815
88 <- 89 -0.25650

Excited State	2:	1.5369 eV	806.73 nm	f=0.0103
85 -> 89		0.12067		
88 -> 90		0.68978		
Excited State	3:	1.6546 eV	749.31 nm	f=0.0176
86 -> 89		0.69792		
Excited State	4:	1.6618 eV	746.09 nm	f=0.0014
85 -> 89		0.57549		
87 -> 89		-0.39028		
88 -> 90		-0.10775		
Excited State	5:	1.9475 eV	636.64 nm	f=0.0495
85 -> 89		0.38257		
87 -> 89		0.58678		