

Carbene adduct zwitterionic species and their carbene isomers

Supplementary Information

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	X											
	CH ₂		SiH ₂		NH		PH		O		S	
	R'=H	R'=Me	R'=H	R'=Me	R'=H	R'=Me	R'=H	R'=Me	R'=H	R'=Me	R'=H	R'=Me
1	-0.3	-1.9	2.8	0.6	-21.0	-22.3	-16.6	-17.1	-44.7	-45.6	-36.4	-38.2
2	23.3	19.8	18.6	14.9	0.9	-3.0	2.0	1.0	-22.1	-24.7	-18.0	-21.0
3	18.4	18.4	19.1	19.8	17.7	16.0	17.4	19.3	18.9	17.6	18.9	18.5
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table S1 Relative energies of **1-4** with R'=H and R'=Me at B3LYP/6-311+G** level of theory

	X					
	CH ₂	SiH ₂	NH	PH	O	S
1	-1.1	1.6	-21.7	-17.1	-44.9	-36.2
2	22.3	17.4	0.1	1.5	-22.4	-17.9
3	18.5	19.0	17.8	17.3	18.7	18.8
4	0.0	0.0	0.0	0.0	0.0	0.0

Table S2 Relative energies of **1-4** (R'=H) at B3LYP/cc-pvTZ level of theory

	X					
	CH ₂	SiH ₂	NH	PH	O	S
1	1.2	4.2	-19.8	-15.4	-63.9	-35.5
2	26.9	20.6	3.9	4.4	-39.3	-16.0
3	19.5	20.7	18.5	19.0	0.0	20.3
4	0.0	0.0	0.0	0.0	0.0	0.0

Table S3 Relative energies of **1-4** (R'=H) at ω -B97XD/6-311+G** level of theory

	X					
	CH ₂	SiH ₂	NH	PH	O	S
1	1.7	4.2	-18.8	-15.2	-41.5	-35.0
2	27.6	20.5	5.1	4.5	-16.8	-15.6
3	19.5	20.6	18.5	19.0	19.6	20.4
4	0.0	0.0	0.0	0.0	0.0	0.0

Table S4 Relative energies of **1-4** (R'=H) at M06-2X/6-311+G** level of theory

	X					
	SiH ₂	CH ₂	NH	PH	O	S
1	0.12	-0.89	-0.49	-0.32	-0.44	-0.63
2	0.11	-0.98	-0.47	-0.37	-0.45	-0.74
3	0.64	-0.69	-0.52	0.02	-0.32	-0.20
4	0.64	-0.77	-0.45	-0.03	-0.31	-0.26

Table S5 B3LYP/6-311+G** Mulliken charges at the X heteroatom in **1-4** (R'=H)

	X					
	SiH ₂	CH ₂	NH	PH	O	S
1	-0.25	-0.68	-0.31	-0.41	-0.44	-0.63
2	-0.29	-0.79	-0.31	-0.49	-0.45	-0.74
3	0.31	-0.21	-0.01	0.03	-0.04	-0.12
4	0.28	-0.32	0.03	0.08	-0.04	-0.20

Table S6 B3LYP/6-311+G** Mulliken charges with the hydrogens summed up to the X heteroatom in **1-4** (R'=H)

	X					
	SiH ₂	CH ₂	NH	PH	O	S
1	0.19	-0.64	-0.80	-0.04	-0.66	-0.27
2	0.17	-0.68	-0.82	-0.08	-0.69	-0.32
3	0.81	-0.62	-0.86	0.30	-0.61	0.02
4	0.85	-0.61	-0.83	0.30	-0.67	0.02

Table S7 B3LYP/6-311+G** NPA charges at the X heteroatom in **1-4** (R'=H)

	X					
	CH ₂	SiH ₂	NH	PH	O	S
1'	-8.1	4.1	-22.7	-18.4	-45.4	-37.2
2'	16.3	20.5	0.6	1.3	-23.6	-17.9
3'	16.2	16.7	14.5	17.6	16.1	16.6
4'	0.0	0.0	0.0	0.0	0.0	0.0

Table S8 B3LYP/6-311+G** relative energies of the thiazol analogues **1' – 4'** R: H showing similar relative energies as for the imidazol compounds **1-4** in **Table S1**.

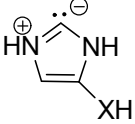
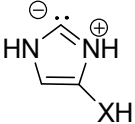
	O	S	NH	PH	CH ₂	SiH ₂
 4a	37.0	34.8	32.5	33.2	35.9	32.8
 4b	31.3	32.7	35.7	35.3	34.5	35.1

Table S9 The two leading resonance structures of **4** at the B3LYP/6-311+G** level of theory

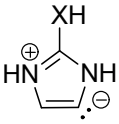
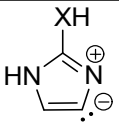
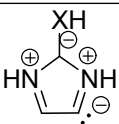
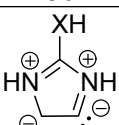
	O	S	NH	PH	CH ₂	SiH ₂
 3a	33.4	17.5	32.0	17.9	33.0	17.6
	32.4	19.1	30.6	19.0	32.8	19.1
 3c	<6	11.5	<6	10.0	<6	9.7
 3d	<6	9.7	<6	11.6	<6	11.7

Table S10 The four leading resonance structures of **3** at the B3LYP/6-311+G** level of theory

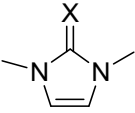
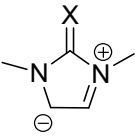
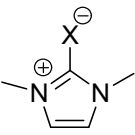
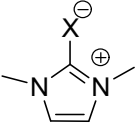
	O	S	N	P	C	Si
	50.4	34.0	55.1	39.8	60.6	15.1
	7.3	4.4	12.5	6.4	11.8	3.1
	12.5	18.5	16.1	21.6	8.4	27.4
	10.3	15.4	4.3	15.1	8.4	27.4

Table S11 The four leading resonance structures of **1** at the B3LYP/6-311+G** level of theory

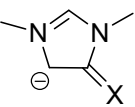
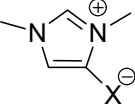
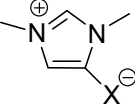
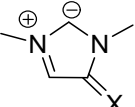
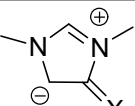
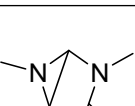
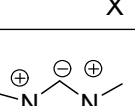
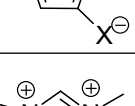
	O	S	N	P	C	Si
	28	21	26	15.3	18.2	
	15	14	9.1	11.7	6.5	30.6
	13	16	8.4	8.7	6.0	30.6
	8		9.7	9.4	15.0	
	8	7	5.4			
		5.6	7.4	4.1	7.1	
	6			7.5		
				6.2	8.7	

Table S12 The leading resonance structures of **2** at the B3LYP/6-311+G** level of theory

X	1					2				
	bond length (Å)	NBO	Mayer	Wiberg	Gordy	bond length (Å)	NBO	Mayer	Wiberg	Gordy
CH ₂	1.352	1.83	1.44	1.67	1.9	1.366	1.49	1.50	1.58	1.8
SiH ₂	1.927	1.20	0.73	0.93	0.5	1.954	1.06	0.83	0.82	0.3
NH	1.285	1.85	1.82	1.67	1.9	1.298	1.60	1.86	1.61	1.8
PH	1.785	1.52	1.04	1.39	1.4	1.776	1.34	0.86	1.28	1.4
O	1.218	1.86	1.78	1.62	1.9	1.228	1.61	1.71	1.56	1.9
S	1.672	1.47	1.11	1.50	1.7	1.689	1.37	0.98	1.40	1.6

Table S13 The bond length between the heteroatom and the imidazole unit and the different bond orders (NBO, Mayer, Wiberg, Gordy) of **1** and **2**

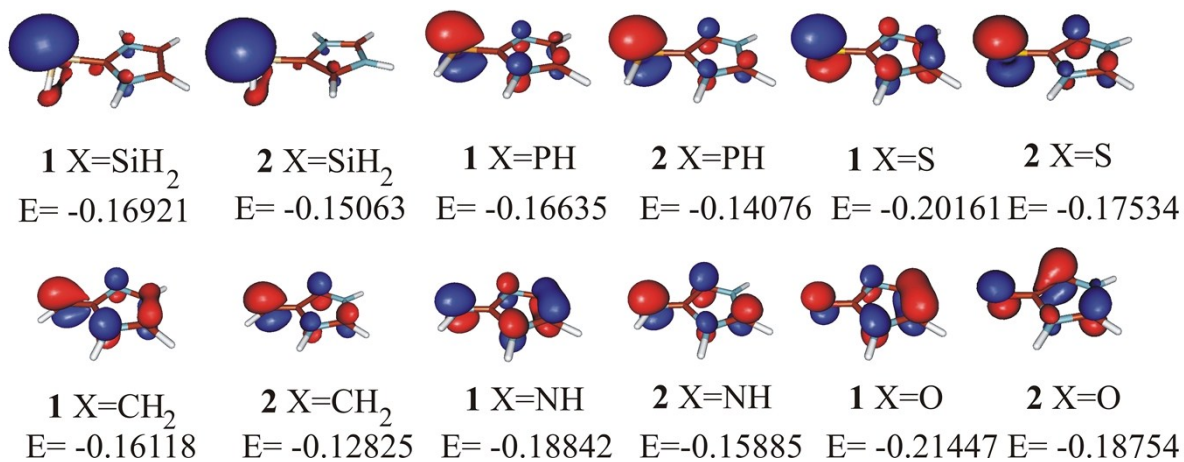


Figure S1 Kohn—Sham HOMOs of **1** and **2** and their energies in au.

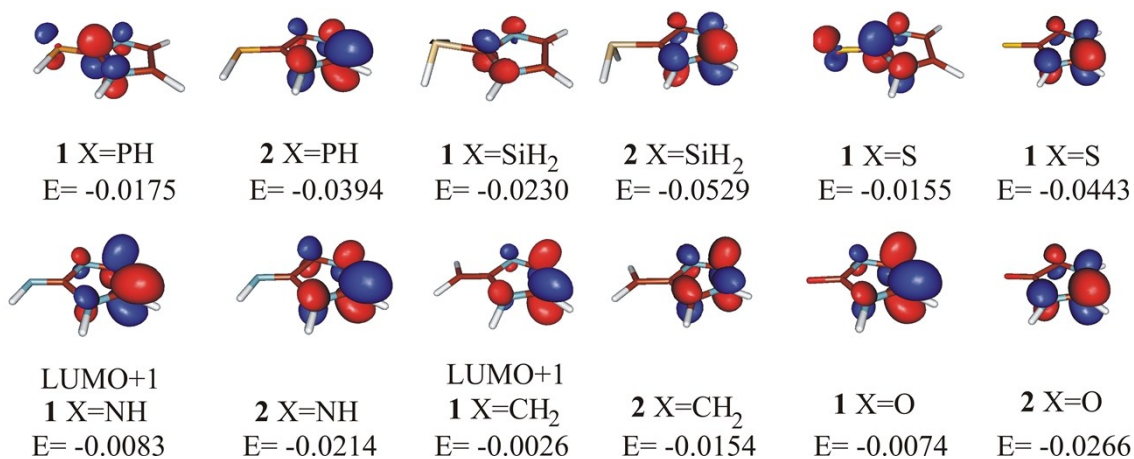


Figure S2 Kohn—Sham LUMO of **1** and **2** and their energies in au. In case of **1** X: NH and **1** X: CH₂ the LUMO+1 is shown, since the LUMO is a diffuse orbital.

XYZ coordinates and total energies of 1-4 X:CH₂ at different level of theory

1 X:CH₂

$$E(B3LYP/6-311+G^{**}) = -265.572740$$

C	0.016915	-0.006281	0.001622
C	-0.003499	0.059568	1.343712
N	1.315174	-0.091069	1.797100
C	2.197985	-0.134614	0.713889
N	1.348527	-0.198533	-0.394643
C	3.549944	-0.118164	0.733738
H	-0.834775	0.130509	2.023235
H	-0.793249	-0.002927	-0.706490
H	1.626002	0.171819	2.716203
H	1.687461	-0.026086	-1.325164
H	4.116555	-0.171966	-0.184157
H	4.088117	-0.081152	1.669403

$$E(B3LYP/cc-pVTZ) = -265.595308$$

N	-0.001282	0.017956	-0.003565
C	-0.001693	0.011081	1.391318
N	1.354873	0.018388	1.716018
C	2.129645	-0.157884	0.563600
C	1.300006	-0.158158	-0.488360
C	-1.060247	0.002113	2.226147
H	-0.826994	-0.205341	-0.526579
H	1.514289	-0.199691	-1.539802
H	1.671075	-0.204709	2.640926
H	-0.919283	0.010520	3.294642
H	-2.066462	0.010137	1.840023
H	3.202081	-0.199184	0.600286

$$E(\omega B97X-D/6-311+G^{**}) = -265.477730$$

C	-0.088787	0.199762	-0.029033
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N	-0.047169	0.262135	1.358845
C	1.270054	0.157131	1.812760
C	2.067403	0.129131	0.736934
N	1.252138	0.216594	-0.394477
C	-1.172744	0.136617	-0.830572
H	1.549668	-0.000186	-1.327422
H	3.140950	0.110600	0.665881
H	-0.858227	0.085528	1.921759
H	-2.167630	0.142922	-0.409857
H	-1.060256	0.104355	-1.904406
H	1.514466	0.168008	2.860620

$E(M06-2X/6-311+G^{**}) = -265.453654$

C	-0.090059	0.205514	-0.030095
N	-0.048487	0.273017	1.359972
C	1.270388	0.156796	1.813244
C	2.067853	0.128644	0.737141
N	1.253060	0.227089	-0.396367
C	-1.173195	0.135839	-0.830929
H	1.546876	-0.008467	-1.327756
H	3.140996	0.108582	0.669165
H	-0.859462	0.076434	1.919412
H	-2.166283	0.141163	-0.409449
H	-1.059351	0.102087	-1.903211
H	1.517530	0.165899	2.859904

2 X:CH₂

$E(B3LYP/6-311+G^{**}) = -265.535113$

N	0.038476	0.049951	0.112577
C	-0.017183	-0.013537	1.488808
C	1.320335	-0.142290	1.976166
N	2.078320	-0.149518	0.766862
C	1.286787	-0.029538	-0.335064

C	1.860292	-0.240125	3.226936
H	-0.765249	0.141599	-0.487991
H	1.602925	-0.012715	-1.360969
H	-0.947956	0.045829	2.020444
H	3.081085	-0.221150	0.739794
H	2.927511	-0.332994	3.374470
H	1.222072	-0.228129	4.097597

$E(B3LYP/cc-pVTZ) = -265.557996$

N	-0.000620	-0.004254	-0.003466
C	-0.000285	0.012595	1.420574
C	1.395984	0.009696	1.716180
N	2.079989	-0.009427	0.521952
C	1.257839	-0.018074	-0.515308
C	-1.123600	0.026947	2.188516
H	-0.836564	-0.008263	-0.557562
H	1.534060	-0.029780	-1.550564
H	1.906517	0.014775	2.658014
H	3.081016	-0.015039	0.438100
H	-1.048029	0.039106	3.263120
H	-2.106844	0.025275	1.743526

$E(\omega B97X-D/6-311+G^{**}) = -265.436750$

C	-0.132974	0.095284	0.033022
C	-0.070198	-0.023753	1.452627
N	1.256767	-0.061816	1.815883
C	2.050847	0.016783	0.764634
N	1.240495	0.127819	-0.320137
C	-1.163228	0.179101	-0.859734
H	1.567189	0.193963	-1.266873

H	3.124909	0.018242	0.767955
H	-0.855716	-0.074913	2.177639
H	1.584988	-0.134684	2.764189
H	-2.178633	0.195731	-0.512904
H	-0.967128	0.291758	-1.911335

$E(M06-2X/6-311+G^{**}) = -265.412506$

C	-0.134252	0.107503	0.037074
C	-0.072284	-0.014006	1.455739
N	1.256351	-0.060508	1.815144
C	2.050206	0.021129	0.763304
N	1.240196	0.123832	-0.318628
C	-1.158014	0.194386	-0.859731
H	1.564331	0.199641	-1.267637
H	3.123837	0.009608	0.768721
H	-0.857965	-0.071806	2.183658
H	1.590304	-0.144896	2.761811
H	-2.179735	0.175805	-0.515764
H	-0.965655	0.282826	-1.918722

3 X:CH₂

$E(B3LYP/6-311+G^{**}) = -265.542914$

C	0.114071	0.011489	0.037574
C	0.055151	-0.039121	1.415369
N	1.433291	-0.033207	1.725266
C	2.258854	0.013296	0.663679
N	1.449991	0.040692	-0.401355
C	3.747275	0.073003	0.663104
H	-0.679356	0.021041	-0.691911
H	1.775556	-0.065936	2.673774
H	1.776519	0.078965	-1.356026

H	4.171328	-0.545789	-0.131680
H	4.138007	-0.295499	1.613779
H	4.112774	1.096616	0.526686

$E(B3LYP/cc-pVTZ) = -265.595308$

N	-0.001282	0.017956	-0.003565
C	-0.001693	0.011081	1.391318
N	1.354873	0.018388	1.716018
C	2.129645	-0.157884	0.563600
C	1.300006	-0.158158	-0.488360
C	-1.060247	0.002113	2.226147
H	-0.826994	-0.205341	-0.526579
H	1.514289	-0.199691	-1.539802
H	1.671075	-0.204709	2.640926
H	-0.919283	0.010520	3.294642
H	-2.066462	0.010137	1.840023
H	3.202081	-0.199184	0.600286

$E(\omega B97X-D/6-311+G^{**}) = -265.448613$

C	0.007056	0.062969	-0.063830
N	-0.027959	0.049159	1.273840
C	1.229903	-0.007844	1.904357
C	2.052029	-0.026097	0.800269
N	1.298724	0.015546	-0.378968
C	-1.139497	0.162578	-1.005652
H	1.649238	0.012239	-1.323071
H	3.127211	-0.074252	0.734918
H	-0.891792	0.074358	1.791128
H	-2.043283	-0.236354	-0.541969
H	-1.334042	1.201240	-1.288865
H	-0.949977	-0.410117	-1.915666

$E(M06-2X/6-311+G^{**}) = -265.425284$

C	0.007402	0.063951	-0.064620
N	-0.028147	0.042659	1.272572
C	1.230760	-0.014663	1.907075
C	2.052818	-0.024916	0.801300
N	1.299759	0.021157	-0.379815
C	-1.140653	0.163111	-1.007009
H	1.649214	0.024235	-1.326221
H	3.127233	-0.069890	0.736824
H	-0.894925	0.063321	1.788181
H	-2.045618	-0.215182	-0.530579
H	-1.320497	1.198676	-1.306110
H	-0.959735	-0.429031	-1.905109

4 X:CH₂

$E(B3LYP/6-311+G^{**}) = -265.572311$

C	0.022484	0.209720	-0.026328
N	0.141800	-0.049115	1.306526
C	1.460901	-0.181006	1.741705
C	2.239230	-0.000665	0.646096
N	1.338517	0.231522	-0.396215
C	3.719497	-0.020843	0.465376
H	-0.664408	-0.133424	1.902765
H	1.731521	-0.386484	2.763693
H	1.613453	0.404004	-1.349763
H	4.027622	-0.797962	-0.241944
H	4.216004	-0.219961	1.416120
H	4.091742	0.937612	0.088265

$E(B3LYP/cc-pVTZ) = -265.593513$

N	0.010302	-0.040344	0.028074
C	-0.069037	-0.103759	1.415883

C	1.198958	0.018733	1.870608
N	1.976392	0.149750	0.721937
C	1.274487	0.118072	-0.447336
C	1.760528	0.027909	3.248650
H	-0.991973	-0.227115	1.953042
H	-0.780878	-0.103659	-0.586112
H	2.974909	0.259230	0.732191
H	2.475533	-0.785147	3.396538
H	2.279433	0.964986	3.465186
H	0.966663	-0.089882	3.983898

$$E(\omega B97X-D/6-311+G^{**}) = -265.479678$$

N	0.010980	-0.040257	0.030167
C	-0.068906	-0.104016	1.416060
C	1.197105	0.018787	1.870283
N	1.975639	0.150746	0.725671
C	1.274351	0.118932	-0.441700
C	1.762133	0.027394	3.247587
H	-0.994147	-0.228300	1.953387
H	-0.778682	-0.103635	-0.587426
H	2.975049	0.261391	0.735721
H	2.475820	-0.789551	3.389590
H	2.279502	0.967888	3.459125
H	0.966473	-0.090606	3.984095

$$E(M06-2X/6-311+G^{**}) = -265.456413$$

N	0.011249	-0.039990	0.030054
C	-0.070411	-0.104002	1.416786
C	1.197097	0.018529	1.871113
N	1.974856	0.151014	0.725990
C	1.275285	0.119171	-0.443785
C	1.763331	0.027050	3.249297

H	-0.994547	-0.228161	1.954814
H	-0.779359	-0.103388	-0.588658
H	2.975766	0.261905	0.737816
H	2.476072	-0.789662	3.388418
H	2.279668	0.967381	3.458000
H	0.966309	-0.091073	3.982714

XYZ coordinates and total energies of 1-4 X:CSi₂ at different level of theory

1 X:SiH₂

$$E(B3LYP/6-311+G^{**}) = -516.961757$$

C	-0.009705	0.117633	-0.128655
N	-0.237100	0.172042	1.240399
C	0.907889	0.001040	1.958346
N	1.854477	-0.167651	0.993344
C	1.316820	-0.097851	-0.285323
Si	1.180038	0.308011	3.840978
H	-0.795294	0.228258	-0.855182
H	1.911050	-0.211275	-1.174849
H	-1.132930	0.309289	1.680723
H	2.823664	-0.333445	1.213399
H	2.189112	-0.821895	3.967108
H	-0.075210	-0.454508	4.234389

$$E(B3LYP/cc-pVTZ) = -516.985763$$

C	0.004272	-0.003599	0.001723
C	0.004252	-0.003595	1.351283
N	1.334107	0.006185	1.739948
C	2.178000	0.014607	0.676535
N	1.334139	0.006271	-0.386902
Si	4.079883	0.325358	0.676589

H	-0.807894	-0.014514	2.053316
H	-0.807850	-0.014511	-0.700336
H	1.666618	-0.004642	2.688212
H	1.666674	-0.004486	-1.335158
H	4.317666	-0.638363	-0.474736
H	4.317612	-0.638452	1.827848

$E(\omega B97X-D/6-311+G^{**}) = -516.855734$

C	0.044150	-0.006064	-0.022193
N	0.032582	0.109872	1.323807
C	1.308974	0.208660	1.847688
C	2.153785	0.150767	0.797411
N	1.360102	0.018208	-0.329216
Si	-1.447464	-0.400401	-1.190510
H	1.694239	-0.072005	-1.274150
H	3.227383	0.200760	0.750232
H	-0.828829	0.147262	1.843112
H	-2.427295	0.185358	-0.182253
H	-1.219644	0.862319	-2.004490
H	1.501882	0.307861	2.901593

$E(M06-2X/6-311+G^{**}) = -516.818309$

C	0.037488	-0.003264	-0.018856
N	0.032053	0.101242	1.328892
C	1.310916	0.199525	1.850948
C	2.151807	0.157015	0.795009
N	1.354083	0.030504	-0.329393
Si	-1.457671	-0.411895	-1.182791
H	1.684171	-0.047785	-1.278789
H	3.225045	0.205572	0.747744
H	-0.829702	0.138196	1.851390
H	-2.416606	0.223063	-0.188698

H	-1.199681	0.826485	-2.018318
H	1.507964	0.293939	2.903894

2 X:SiH₂

$E(B3LYP/6-311+G^{**}) = -516.936582$

N	0.000984	0.069397	-0.005358
C	-0.089329	0.205301	1.371718
C	1.169631	0.035992	1.918327
N	1.967361	-0.193998	0.791748
C	1.268943	-0.168510	-0.350764
Si	1.934857	0.309092	3.694897
H	-0.762049	0.149108	-0.660783
H	1.642287	-0.305419	-1.350435
H	-1.027592	0.426941	1.848846
H	2.956682	-0.385529	0.875320
H	3.270269	-0.294085	3.223776
H	1.355370	-0.980908	4.262338

$E(B3LYP/cc-pVTZ) = -516.960713$

C	0.002613	0.004935	0.002317
N	0.004450	-0.005420	1.333537
C	1.308719	-0.003708	1.795858
C	2.162858	-0.000403	0.712382
N	1.284805	0.003420	-0.371996
Si	4.086219	0.234708	0.481927
H	-0.825849	-0.004564	1.901844
H	-0.863505	0.015256	-0.632319
H	1.525043	0.009858	2.847237
H	1.621728	-0.020467	-1.322121
H	3.966046	-0.164763	-0.999250
H	4.424839	-1.156749	0.999357

$$E(\omega B97X-D/6-311+G^{**}) = -516.829544$$

C	-0.001889	-0.048871	0.045962
C	-0.000775	-0.034415	1.419759
N	1.311477	0.005720	1.861809
C	2.127852	0.022587	0.814594
N	1.354748	-0.015495	-0.268196
Si	-1.357323	-0.284248	-1.327087
H	1.694555	-0.036637	-1.218626
H	3.202967	0.058642	0.843175
H	-0.826336	-0.035871	2.109573
H	1.614678	0.028562	2.821936
H	-2.491939	0.021159	-0.358662
H	-1.170695	1.142382	-1.839270

$$E(M06-2X/6-311+G^{**}) = -516.792215$$

C	0.010784	-0.035145	0.029780
C	-0.001305	0.006392	1.402913
N	1.308581	0.024443	1.858950
C	2.136087	0.000407	0.818733
N	1.372655	-0.042461	-0.269767
Si	-1.327069	-0.236573	-1.382600
H	1.715695	-0.101215	-1.220268
H	3.211297	0.008272	0.860877
H	-0.833268	0.037942	2.083574
H	1.605647	0.057231	2.822745
H	-2.468499	-0.144100	-0.386167
H	-1.273285	1.248321	-1.713803

3 X:SiH₂

$$E(B3LYP/6-311+G^{**}) = -516.935913$$

C	-0.037173	0.035873	0.035147
C	-0.080183	-0.196733	1.402713
N	1.284534	-0.192378	1.700068
C	2.118792	0.018996	0.645613
N	1.278849	0.161686	-0.398458
Si	3.988604	0.090326	0.666056
H	-0.842340	0.123824	-0.676505
H	1.631679	-0.336622	2.636607
H	1.583154	0.333878	-1.346374
H	4.568258	-0.964224	-0.202819
H	4.386056	-0.132533	2.076545
H	4.473232	1.413456	0.199666

$E(B3LYP/cc-pVTZ) = -516.958082$

N	0.002120	0.000001	0.000962
C	0.002529	0.000002	1.387720
C	1.298789	0.000002	1.876271
N	2.013959	-0.000003	0.680323
C	1.266909	-0.000006	-0.452985
Si	1.876996	0.000027	-2.219387
H	-0.933917	-0.000003	1.917517
H	3.020103	-0.000017	0.653132
H	-0.807830	-0.000009	-0.598265
H	1.405711	-1.204217	-2.946053
H	3.356087	-0.000557	-2.139838
H	1.406693	1.204848	-2.945737

$E(\omega B97X-D/6-311+G^{**}) = -516.829337$

C	0.120777	0.065617	0.017857
N	0.092915	0.023102	1.369069
C	1.334479	-0.046562	1.998272
C	2.167054	-0.042069	0.891805
N	1.427458	0.024051	-0.277144

Si	-1.324589	0.188541	-1.158593
H	1.794731	0.032122	-1.215590
H	3.243205	-0.087375	0.836079
H	-0.770224	0.031085	1.888876
H	-2.518864	-0.273858	-0.414798
H	-1.526622	1.584544	-1.615103
H	-1.062710	-0.675771	-2.334242

$E(M06-2X/6-311+G^{**}) = -516.792037$

C	0.121870	0.065185	0.014276
N	0.091495	0.009826	1.364512
C	1.332816	-0.058208	1.999835
C	2.167705	-0.038478	0.893766
N	1.429668	0.034068	-0.277884
Si	-1.327130	0.188518	-1.161203
H	1.797874	0.053608	-1.217677
H	3.243424	-0.076566	0.840578
H	-0.775509	0.009125	1.880929
H	-2.515867	-0.241364	-0.396918
H	-1.504100	1.576702	-1.635966
H	-1.084634	-0.698987	-2.317758

4 X:SiH₂

$E(B3LYP/6-311+G^{**}) = -516.966290$

C	-0.145247	-0.358950	0.052490
N	0.003830	0.104858	1.330493
C	1.324685	0.316196	1.698097
C	2.091938	-0.019505	0.622963
N	1.154874	-0.421654	-0.346548
Si	3.945970	0.028523	0.440503
H	-0.788771	0.269616	1.929216

H	1.614240	0.679792	2.670241
H	1.397823	-0.736114	-1.271892
H	4.343902	0.937586	-0.665501
H	4.480902	-1.323920	0.136027
H	4.514215	0.516969	1.720204

$E(B3LYP/cc-pVTZ) = -516.988368$

N	0.002213	0.000032	0.001286
C	0.001984	0.000078	1.359439
N	1.343550	0.000056	1.611201
C	2.125154	-0.000024	0.470500
C	1.274920	0.000031	-0.589952
Si	1.668867	-0.000023	-2.408741
H	1.705883	0.000057	2.547556
H	3.200085	-0.000080	0.494265
H	-0.857847	0.000006	-0.517062
H	1.100753	1.200163	-3.073685
H	1.098123	-1.198828	-3.073913
H	3.142938	-0.001508	-2.557665

$E(\omega B97X-D/6-311+G^{**}) = -516.862391$

C	-0.030567	-0.196342	-0.012197
C	-0.025961	0.020277	1.327861
N	1.319010	0.268653	1.625228
C	2.156366	0.221469	0.558706
N	1.277003	-0.070560	-0.440494
Si	-1.454065	0.000434	2.517202
H	-0.848302	-0.425208	-0.676013
H	1.577546	-0.179382	-1.393356
H	1.666475	0.468806	2.547206
H	-1.250721	-1.030207	3.566297
H	-1.599948	1.318032	3.185662
H	-2.675893	-0.307652	1.737356

$$E(M06-2X/6-311+G^{**}) = -516.824945$$

C	-0.032370	-0.197870	-0.009222
C	-0.025156	0.020922	1.331728
N	1.320908	0.268809	1.624901
C	2.159144	0.220014	0.557233
N	1.275471	-0.073325	-0.439659
Si	-1.456219	0.002706	2.519044
H	-0.852311	-0.427068	-0.669623
H	1.575113	-0.183826	-1.394264
H	1.669520	0.470473	2.547784
H	-1.255697	-1.028119	3.561299
H	-1.598199	1.317206	3.183026
H	-2.669262	-0.301602	1.731209

XYZ coordinates and total energies of 1-4 X:NH at different level of theory

1 X:NH

$$E(B3LYP/6-311+G^{**}) = -281.646503$$

C	-0.043445	0.004639	0.079270
N	-0.013269	0.003068	1.474289
C	1.304535	0.008610	1.949164
C	2.114392	0.017609	0.872713
N	1.302229	0.019538	-0.260206
N	-1.005209	-0.004541	-0.772143
H	1.538574	0.006270	2.999081
H	-0.840911	-0.013756	2.043360
H	-1.914047	-0.015289	-0.318774
H	1.599420	0.011577	-1.220539
H	3.188182	0.027724	0.811303

$$E(B3LYP/cc-pVTZ) = -281.668236$$

N	0.001311	-0.000840	0.001704
C	0.000978	-0.000410	1.387325
N	1.358089	-0.000647	1.697725
C	2.138975	-0.008160	0.538923
C	1.296010	-0.009160	-0.506658
N	-1.056414	-0.000029	2.110211
H	3.212011	-0.010060	0.568014
H	1.705191	-0.007659	2.637300
H	-0.837398	0.000298	3.100131
H	-0.853617	-0.011453	-0.521251
H	1.499806	-0.011016	-1.560597

$E(\omega B97X-D/6-311+G^{**}) = -281.547639$

C	-0.038316	0.003927	0.081002
N	-0.012281	0.002161	1.468250
C	1.300685	0.008323	1.943840
C	2.108978	0.018018	0.872331
N	1.300303	0.018680	-0.258085
N	-0.999008	-0.004718	-0.766814
H	1.531846	0.007176	2.994464
H	-0.839712	-0.013554	2.034481
H	-1.902228	-0.014546	-0.306473
H	1.597095	0.012610	-1.216662
H	3.183091	0.027371	0.811182

$E(M06-2X/6-311+G^{**}) = -281.527231$

C	-0.039495	0.003719	0.079648
N	-0.012888	0.001933	1.468459
C	1.301375	0.008250	1.944809
C	2.110277	0.017883	0.872976
N	1.300935	0.018479	-0.258586
N	-0.998803	-0.004824	-0.767682

H	1.534331	0.007191	2.994401
H	-0.842741	-0.012914	2.033861
H	-1.901669	-0.014628	-0.305758
H	1.595199	0.012834	-1.219620
H	3.183932	0.027525	0.815009

2 X:NH

isomer-1

$E(B3LYP/6-311+G^{**}) = -281.606687$

C	-0.061421	-0.011838	0.012780
N	0.013765	-0.026409	1.451591
C	1.298372	-0.010653	1.894081
N	2.064365	0.014710	0.807493
C	1.314082	0.016351	-0.349184
N	-1.119379	-0.021846	-0.736191
H	3.071386	0.034057	0.834840
H	1.636111	-0.014917	2.913843
H	-0.792925	-0.050171	2.053820
H	-1.978023	-0.042375	-0.191728
H	1.761692	0.033313	-1.324640

$E(B3LYP/cc-pVTZ) = -281.628676$

C	0.001431	0.000002	0.000415
C	-0.001108	-0.000004	1.421686
N	1.406964	-0.000167	1.714056
C	2.160022	-0.001746	0.587566
N	1.309028	-0.001704	-0.428026
N	-0.988401	0.000254	2.254387
H	1.593569	-0.000784	-1.391405
H	3.230051	-0.001016	0.520833
H	1.781447	-0.002504	2.645679
H	-0.673449	0.000563	3.219834

H -0.824778 -0.001297 -0.681259

isomer-2

$E(B3LYP/6-311+G^{**}) = -281.611752$

C -0.007701 -0.059626 -0.062314

C -0.045220 -0.035905 1.361657

N 1.344372 -0.054411 1.696864

C 2.134056 -0.085645 0.602288

N 1.323234 -0.088784 -0.450688

N -0.929711 -0.005234 2.310479

H 1.644901 -0.109750 -1.405330

H 3.208084 -0.104206 0.578213

H 1.655707 -0.043730 2.655548

H -1.870055 0.004730 1.926962

H -0.806356 -0.057900 -0.780167

$E(B3LYP/cc-pVTZ) = -281.633439$

N 0.003018 0.000007 0.002705

C 0.003052 -0.000010 1.386412

C 1.357385 0.000044 1.822051

N 2.065732 0.000079 0.582594

C 1.236646 0.000066 -0.479147

N 2.018532 0.000092 2.933295

H -0.820176 -0.000048 -0.573060

H 1.512485 0.000198 -1.515346

H 3.070231 0.000353 0.550767

H 1.383475 0.000049 3.724026

H -0.908749 -0.000295 1.949424

$E(\omega B97X-D/6-311+G^{**}) = -281.509868$

C -0.005503 -0.059183 -0.059145

C -0.040206 -0.035912 1.359202

N 1.339664 -0.054882 1.691982

C 2.125671 -0.085736 0.602235

N 1.322040 -0.088577 -0.446466

N	-0.920915	-0.005448	2.308727
H	1.643321	-0.109108	-1.399130
H	3.200172	-0.103821	0.581304
H	1.649776	-0.043494	2.649365
H	-1.857878	0.004745	1.921961
H	-0.804832	-0.059044	-0.776526

$E(M06-2X/6-311+G^{**}) = -281.489178$

C	-0.006662	-0.059407	-0.059539
C	-0.042345	-0.035854	1.359479
N	1.340700	-0.054670	1.691926
C	2.126595	-0.085499	0.602018
N	1.322430	-0.088622	-0.446320
N	-0.920804	-0.005439	2.309784
H	1.645472	-0.109062	-1.400220
H	3.200730	-0.104085	0.578609
H	1.648036	-0.043680	2.651908
H	-1.857941	0.004473	1.922373
H	-0.804902	-0.058617	-0.776508

3 X:NH

$E(B3LYP/6-311+G^{**}) = -281.584923$

C	0.004089	-0.071666	-0.012996
N	-0.006866	-0.171177	1.393004
C	1.208269	-0.100573	1.975491
N	2.071477	0.049399	0.964973
C	1.363959	0.068890	-0.239491
N	1.582053	-0.160512	3.322096
H	-0.855647	-0.286453	1.926739
H	3.067479	0.130444	1.112308
H	1.381249	-1.047446	3.769454

H	1.228988	0.604562	3.885214
H	1.899020	0.182967	-1.168287

$E(B3LYP/cc-pVTZ) = -281.605308$

C	0.004187	-0.000023	0.002469
C	0.004985	-0.000068	1.384697
N	1.390634	0.000006	1.630761
C	2.161322	0.000046	0.527920
N	1.305945	0.000026	-0.495528
N	3.552353	0.000132	0.383671
H	1.782307	0.000000	2.557986
H	1.612900	0.000098	-1.454900
H	3.997818	-0.825901	0.761382
H	3.997775	0.825819	0.762181
H	-0.824176	-0.000058	-0.683977

$E(\omega B97X-D/6-311+G^{**}) = -281.486538$

C	0.007556	-0.000032	0.002478
C	0.009752	-0.000023	1.384055
N	1.393094	0.000000	1.630173
C	2.159089	0.000039	0.528729
N	1.308011	0.000037	-0.493175
N	3.547824	0.000125	0.390068
H	1.783168	-0.000033	2.559120
H	1.614433	0.000110	-1.453036
H	3.992669	-0.830644	0.756891
H	3.992627	0.830577	0.757651
H	-0.822172	-0.000077	-0.686293

$E(M06-2X/6-311+G^{**}) = -281.467793$

C	0.006144	-0.000017	0.002906
C	0.006433	-0.000072	1.385973

N	1.392970	-0.000008	1.629285
C	2.158308	0.000038	0.528080
N	1.307800	0.000029	-0.494153
N	3.549253	0.000117	0.386001
H	1.786170	-0.000032	2.558585
H	1.618774	0.000106	-1.454594
H	3.991683	-0.830545	0.759328
H	3.991643	0.830501	0.759988
H	-0.823127	-0.000038	-0.684737

4 X:NH

$E(B3LYP/6-311+G^{**}) = -281.613115$

C	0.037076	-0.119135	-0.003909
N	0.000725	0.011947	1.388810
C	1.226061	0.102917	1.973041
N	2.037525	0.039416	0.871759
C	1.354129	-0.095424	-0.333832
N	2.042974	-0.110876	-1.555810
H	3.038797	0.132695	0.933091
H	-0.840226	-0.224893	-0.618736
H	1.439031	0.064725	-2.347509
H	2.569991	-0.963166	-1.713182
H	-0.846192	0.043632	1.931095

$E(B3LYP/cc-pVTZ) = -281.633645$

C	-0.002745	0.006012	0.003294
C	-0.000441	0.013174	1.357885
N	1.348084	0.001244	1.724777
C	2.211462	-0.030143	0.679538
N	1.334248	-0.019117	-0.370163
N	-1.020185	0.093938	-0.955314

H	1.641022	0.014282	-1.326268
H	-0.812290	0.019283	2.061496
H	-1.922395	0.268503	-0.537516
H	-1.083285	-0.729596	-1.541448
H	1.670743	0.014911	2.674763

$$E(\omega B97X-D/6-3II+G^{**}) = -281.516052$$

C	0.044505	-0.126930	-0.002996
N	0.005054	0.009166	1.382573
C	1.225332	0.112213	1.965820
N	2.035209	0.050027	0.870446
C	1.356575	-0.094795	-0.329678
N	2.050784	-0.119581	-1.546107
H	3.034555	0.147378	0.929938
H	-0.831033	-0.240825	-0.619116
H	1.460290	0.108902	-2.332112
H	2.519610	-1.000051	-1.717172
H	-0.840990	0.036334	1.923222

$$E(M06-2X/6-3II+G^{**}) = -281.497268$$

C	0.045842	-0.133642	-0.002542
N	0.005267	0.008119	1.382394
C	1.225344	0.121239	1.968964
N	2.034793	0.058977	0.872875
C	1.359394	-0.095555	-0.328045
N	2.060969	-0.125837	-1.543943
H	3.035821	0.159164	0.928563
H	-0.826958	-0.251998	-0.620683
H	1.477925	0.136468	-2.326691
H	2.484099	-1.027915	-1.729093
H	-0.842607	0.032818	1.923019

XYZ coordinates and total energies of 1-4 X:PH at different level of theory

1 X:PH

$$E(B3LYP/6-311+G^{**}) = -568.240153$$

C	0.052256	0.004349	0.066709
N	0.047492	0.001126	1.443769
C	1.340937	0.008578	1.961995
C	2.183582	0.017452	0.908193
N	1.395961	0.016937	-0.239478
P	-1.266060	-0.004240	-1.097028
H	1.539747	0.008196	3.019114
H	-0.801987	-0.009588	1.981514
H	-2.258698	-0.017367	-0.071680
H	1.738736	0.014435	-1.185385
H	3.258487	0.025572	0.869795

$$E(B3LYP/cc-pVTZ) = -568.265266$$

N	0.002292	-0.001793	0.001637
C	0.002466	-0.000967	1.376017
N	1.339618	-0.000526	1.686011
C	2.130866	-0.003096	0.543276
C	1.293184	-0.003611	-0.509933
P	-1.422327	-0.000483	2.402852
H	3.203576	-0.002928	0.583979
H	1.671992	-0.000922	2.632041
H	-0.645323	-0.000391	3.597903
H	-0.842104	-0.006344	-0.540271
H	1.495123	-0.004189	-1.564164

$$E(\omega B97X-D/6-311+G^{**}) = -568.136641$$

N	0.001959	-0.001818	0.004641
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C	0.004333	-0.000989	1.373925
N	1.336233	-0.000542	1.686335
C	2.128339	-0.003145	0.545168
C	1.291852	-0.003526	-0.507360
P	-1.416224	-0.000340	2.397373
H	3.203115	-0.003042	0.589374
H	1.667975	-0.000776	2.633904
H	-0.635935	-0.000519	3.587054
H	-0.844151	-0.006484	-0.536794
H	1.491867	-0.004069	-1.564272

$E(M06-2X/6-311+G^{**}) = -568.103853$

N	0.001640	-0.001866	0.004709
C	0.002410	-0.000895	1.375415
N	1.335782	-0.000492	1.687224
C	2.129173	-0.003161	0.545790
C	1.292223	-0.003629	-0.507864
P	-1.420546	0.000065	2.400058
H	3.203531	-0.003032	0.588006
H	1.666150	-0.000411	2.637033
H	-0.628804	-0.001200	3.578561
H	-0.847099	-0.006357	-0.535848
H	1.494903	-0.004272	-1.563735

2 X:PH

Isomer-1

$E(B3LYP/6-311+G^{**}) = -568.209947$

C	0.045431	-0.002885	-0.001062
N	0.071810	-0.040117	1.410218
C	1.330570	-0.025238	1.901202
N	2.138799	0.020223	0.843410

C	1.410391	0.035126	-0.328379
P	-1.392514	-0.004809	-1.044791
H	3.145229	0.039350	0.901720
H	1.626491	-0.048329	2.934014
H	-0.764910	-0.071580	1.971028
H	-2.292795	-0.053595	0.068693
H	1.889524	0.072077	-1.289350

Isomer-2

$E(B3LYP/6-311+G^{**}) = -568.210512$

C	0.003285	0.000181	-0.046474
C	-0.030824	0.000112	1.356354
N	1.341568	-0.000095	1.694597
C	2.137785	-0.000048	0.605619
N	1.325533	0.000059	-0.449283
P	-1.293812	0.000302	2.605292
H	1.642922	-0.000024	-1.406546
H	3.212233	-0.000399	0.587841
H	1.675508	0.000032	2.646312
H	-2.347805	0.000609	1.645644
H	-0.802162	0.000517	-0.757068

$E(MP2/6-311+G^{**}) = -567.0347847$

C	0.111971	-0.314442	0.089143
N	-0.035698	-0.058322	1.437835
C	1.115820	0.337222	2.072328
N	1.986793	0.307659	1.020159
C	1.435661	-0.078510	-0.200841
P	2.451529	-0.172784	-1.708254
H	2.960480	0.551951	1.135931
H	-0.695986	-0.633971	-0.551835
H	1.592658	0.539301	-2.569093
H	2.042756	-1.449812	-2.141556

H -0.906093 -0.146455 1.941002

$E(B3LYP/cc-pVTZ) = -568.235565$

N -0.007734 -0.000341 -0.021133

C -0.042177 0.000336 1.358387

C 1.275323 0.000164 1.832277

N 2.026407 -0.000358 0.638231

C 1.245468 -0.000489 -0.457067

P 2.066285 0.000714 3.418182

H -0.812951 -0.000564 -0.623503

H 1.566348 -0.001030 -1.480508

H 3.032148 -0.000347 0.622782

H 0.829463 0.001501 4.123213

H -0.968617 0.000923 1.897532

$E(\omega B97X-D/6-311+G^{**}) = -568.105152$

C 0.005116 0.000202 -0.045143

C -0.026992 0.000131 1.349559

N 1.334911 -0.000078 1.687385

C 2.127982 -0.000072 0.606594

N 1.325873 0.000039 -0.446595

P -1.279971 0.000310 2.603173

H 1.644399 -0.000060 -1.401282

H 3.202999 -0.000337 0.594857

H 1.664405 -0.000015 2.639372

H -2.333381 0.000594 1.649645

H -0.801111 0.000537 -0.755275

$E(M06-2X/6-311+G^{**}) = -568.072389$

C 0.003340 0.000219 -0.044200

C -0.029158 0.000157 1.351298

N 1.335392 -0.000084 1.687864

C	2.128382	-0.000110	0.606455
N	1.324909	0.000044	-0.446310
P	-1.284266	0.000318	2.606575
H	1.644943	-0.000018	-1.402454
H	3.203150	-0.000318	0.591376
H	1.664323	-0.000039	2.641924
H	-2.324012	0.000620	1.643302
H	-0.802773	0.000460	-0.753542

3 X:PH

$E(B3LYP/6-311+G^{**}) = -568.185869$

C	0.149218	-0.073700	0.052448
N	0.105457	-0.265971	1.393360
C	1.335610	-0.171269	2.052207
C	2.173960	0.104226	0.978051
N	1.449877	0.158525	-0.205109
P	-1.141988	-0.090373	-1.238275
H	-0.756765	-0.463630	1.878869
H	-2.086881	0.736682	-0.568944
H	1.806413	0.341486	-1.133122
H	3.239357	0.267627	0.960126
H	-1.778262	-1.302886	-0.851390

$E(B3LYP/cc-pVTZ) = -568.210443$

C	0.150706	-0.074267	0.056216
N	0.108596	-0.265055	1.394215
C	1.335967	-0.169564	2.050335
C	2.170188	0.104988	0.975671
N	1.447535	0.157902	-0.202886
P	-1.134817	-0.091344	-1.233822
H	-0.752646	-0.462055	1.876374

H	-2.084916	0.732248	-0.571644
H	1.798860	0.339361	-1.130316
H	3.233292	0.268691	0.955952
H	-1.776770	-1.300189	-0.851874

$E(\omega B97X-D/6-311+G^{**}) = -568.081800$

C	0.153004	-0.071762	0.049987
N	0.104348	-0.266040	1.382420
C	1.328445	-0.173891	2.044333
C	2.164983	0.102586	0.973861
N	1.445896	0.159316	-0.206194
P	-1.141543	-0.089872	-1.226427
H	-0.758100	-0.464013	1.864092
H	-2.074366	0.736557	-0.551367
H	1.805841	0.344313	-1.129824
H	3.230779	0.266071	0.955030
H	-1.763291	-1.302548	-0.837692

$E(M06-2X/6-311+G^{**}) = -568.049410$

C	0.152223	-0.072243	0.049921
N	0.103803	-0.266913	1.381558
C	1.329233	-0.175090	2.046848
C	2.165092	0.102271	0.974388
N	1.445044	0.159336	-0.206816
P	-1.142773	-0.088251	-1.230892
H	-0.761158	-0.465393	1.861799
H	-2.067983	0.735294	-0.546933
H	1.801645	0.344055	-1.133703
H	3.229946	0.265936	0.956008
H	-1.759077	-1.298285	-0.833957

4 X:PH

$E(B3LYP/6-311+G^{**}) = -568.213675$

C	0.115021	-0.286824	0.084891
N	-0.035871	-0.058673	1.444599
C	1.119912	0.311460	2.078074
N	1.992007	0.299767	1.033942
C	1.426061	-0.059727	-0.198889
P	2.434928	-0.116423	-1.724466
H	2.964450	0.538113	1.150907
H	-0.694722	-0.584855	-0.559834
H	1.480401	0.443730	-2.615256
H	2.163886	-1.457715	-2.112643
H	-0.906181	-0.147015	1.943493

$E(B3LYP/cc-pVTZ) = -568.237953$

C	0.005349	-0.028056	-0.003248
C	0.003263	-0.055563	1.353740
N	1.327532	-0.001973	1.747090
C	2.214514	0.060657	0.709385
N	1.361130	0.043745	-0.345615
P	-1.295405	-0.042200	-1.283623
H	1.688384	0.084628	-1.295336
H	-0.818646	-0.108230	2.044602
H	-2.238381	0.789583	-0.626953
H	-1.955303	-1.245354	-0.916913
H	1.634405	-0.004002	2.703390

$E(MP2/6-311+G^{**}) = -567.02617$

N	-0.003927	0.000049	0.008358
C	-0.003619	-0.000029	1.380871
C	1.340945	0.000032	1.828259
N	2.053239	-0.000082	0.619781
C	1.249945	-0.000013	-0.471757
P	2.160109	0.000148	3.389174

H	-0.829259	-0.000018	-0.575811
H	1.546499	-0.000182	-1.506671
H	3.064165	0.000121	0.579517
H	0.934016	0.000294	4.092968
H	-0.919257	0.000095	1.949182

$E(\omega B97X-D/6-311+G^{**}) = -568.112134$

C	0.126378	-0.309305	0.090429
N	-0.026997	-0.063304	1.440811
C	1.119491	0.330810	2.065788
N	1.988964	0.314260	1.025611
C	1.429191	-0.069122	-0.195159
P	2.434322	-0.150884	-1.712719
H	2.957390	0.563576	1.139323
H	-0.679240	-0.628357	-0.549761
H	1.533905	0.505101	-2.588413
H	2.070394	-1.453342	-2.131865
H	-0.893906	-0.157596	1.940774

$E(M06-2X/6-311+G^{**}) = -568.079621$

C	0.110310	-0.247665	0.074974
N	-0.029062	-0.058061	1.437440
C	1.132170	0.268784	2.075871
N	1.995854	0.272077	1.028396
C	1.420811	-0.038861	-0.205058
P	2.405908	-0.056225	-1.739962
H	2.972381	0.492101	1.146161
H	-0.706337	-0.509123	-0.576461
H	1.367050	0.335041	-2.613552
H	2.289660	-1.434591	-2.040306
H	-0.898854	-0.141638	1.937316

XYZ coordinates and total energies of 1-4 X:O at different level of theory

1 X:O

$$E(B3LYP/6-311+G^{**}) = -301.553334$$

C	-0.011725	-0.002480	-0.005132
N	-0.034801	-0.004056	1.384782
C	1.256187	0.008929	1.913448
C	2.114006	0.019224	0.872142
N	1.348048	0.012367	-0.293876
O	-0.952069	-0.011852	-0.779817
H	1.448248	0.010983	2.971907
H	-0.898352	-0.014356	1.900442
H	1.688985	0.016547	-1.240169
H	3.189620	0.030916	0.858183

$$E(B3LYP/cc-pVTZ) = -301.576216$$

N	0.002065	0.000039	0.001316
C	0.001499	-0.000090	1.388936
N	1.353979	0.000127	1.699194
C	2.136932	-0.000076	0.548480
C	1.298918	-0.000100	-0.503986
O	-0.949938	-0.000218	2.146508
H	3.210036	0.000264	0.579577
H	1.678881	-0.000398	2.648126
H	-0.849966	-0.000373	-0.527903
H	1.508989	-0.000096	-1.556787

$$E(\omega B97X-D/6-311+G^{**}) = -301.450124$$

N	-0.000473	-0.000225	0.023163
C	0.101117	0.000716	1.409691
C	1.410774	-0.000420	1.712156
N	2.110502	-0.001259	0.509971

C	1.248646	-0.001302	-0.571311
O	1.521243	-0.002166	-1.754243
H	3.107421	-0.001814	0.391956
H	1.904447	-0.000428	2.668329
H	-0.844487	-0.000320	-0.520558
H	-0.761373	0.001881	2.052932

$E(M06-2X/6-311+G^{**}) = -301.430865$

N	-0.001123	-0.000231	0.023000
C	0.100472	0.000718	1.410747
C	1.410796	-0.000417	1.713437
N	2.111167	-0.001257	0.510174
C	1.248916	-0.001297	-0.572236
O	1.521138	-0.002165	-1.753548
H	3.109284	-0.001823	0.388935
H	1.901867	-0.000422	2.670221
H	-0.844721	-0.000324	-0.524276
H	-0.759978	0.001880	2.055632

2 X:O

$E(B3LYP/6-311+G^{**}) = -301.517375$

C	0.100430	-0.000121	-0.000866
N	0.001046	-0.000667	1.326584
C	1.249484	-0.000208	1.928145
C	2.233961	0.000676	0.912227
N	1.413873	0.000466	-0.290653
H	1.370185	0.000079	2.995129
H	-0.875949	-0.001560	1.822236
H	1.810886	0.001083	-1.217673
O	3.461421	0.001406	0.887197
H	-0.722918	-0.000446	-0.692589

$E(B3LYP/cc-pVTZ) = -301.540384$

N	0.002153	0.000119	0.001686
C	0.003284	-0.000187	1.343441
N	1.273960	0.000138	1.725590
C	2.128892	0.000224	0.638527
C	1.350849	0.000358	-0.540279
O	1.588269	0.000655	-1.741984
H	3.194352	0.000723	0.752237
H	1.566502	-0.000087	2.686424
H	-0.815255	0.000310	-0.583965
H	-0.847734	-0.000592	1.997143

$E(\omega B97X-D/6-311+G^{**}) = -301.410930$

N	-0.005785	-0.000152	0.044965
C	0.103501	0.000490	1.380296
N	1.397148	-0.000190	1.659254
C	2.159756	-0.001364	0.506215
C	1.285438	-0.001368	-0.599707
O	1.420924	-0.002163	-1.817036
H	3.233397	-0.002154	0.531378
H	1.768882	0.000084	2.593538
H	-0.867839	0.000095	-0.474838
H	-0.697604	0.001385	2.098020

$E(M06-2X/6-311+G^{**}) = -301.391400$

N	-0.006565	-0.000170	0.045551
C	0.102859	0.000538	1.380456
N	1.396713	-0.000285	1.659414
C	2.161214	-0.001358	0.505929
C	1.287451	-0.001422	-0.600818
O	1.419330	-0.002169	-1.817323

H	3.233829	-0.001996	0.530796
H	1.767527	-0.000060	2.595849
H	-0.868333	0.000048	-0.477772
H	-0.696209	0.001537	2.100003

3 X:O

$$E(B3LYP/6-311+G^{**}) = -301.451941$$

N	-0.001849	-0.092192	0.078396
C	0.060672	-0.106925	1.414238
N	1.340966	-0.018593	1.750446
C	2.097566	0.054639	0.550848
C	1.279461	0.004991	-0.551320
O	-0.928376	-0.149569	2.327988
H	3.169223	0.141377	0.617712
H	1.667744	-0.026366	2.705797
H	-0.864277	-0.121220	-0.443711
H	-1.711410	-0.574617	1.960457

$$E(B3LYP/cc-pVTZ) = -301.474794$$

C	0.002079	0.028068	0.005739
N	0.011124	-0.027542	1.436194
C	1.237394	-0.050666	1.958662
N	2.098090	-0.013637	0.954536
C	1.346272	0.034876	-0.249677
O	1.633495	-0.101618	3.243409
H	1.875067	0.069967	-1.185022
H	3.097366	-0.020543	1.077578
H	-0.831250	-0.046997	1.985440
H	0.870447	-0.122528	3.829852

$$E(\omega B97X-D/6-311+G^{**}) = -301.348266$$

N	0.067154	-0.097879	-0.060986
C	-0.023677	0.019953	1.358017
C	1.303988	0.060894	1.688918
N	2.119567	-0.032860	0.535449
C	1.319624	-0.127515	-0.510157
O	1.779463	-0.210424	-1.763026
H	3.124627	-0.042309	0.473866
H	1.779037	0.151792	2.651883
H	-0.745370	-0.137265	-0.654242
H	1.080203	-0.479252	-2.362000

$E(M06-2X/6-311+G^{**}) = -301.333367$

N	0.065775	-0.089657	-0.059865
C	-0.026126	0.014500	1.363294
C	1.303928	0.054436	1.690738
N	2.118611	-0.028812	0.534335
C	1.316627	-0.114258	-0.510562
O	1.772533	-0.179561	-1.768371
H	3.125142	-0.040019	0.465656
H	1.779525	0.138771	2.652912
H	-0.746749	-0.119312	-0.656356
H	1.095350	-0.530953	-2.354060

4 X:O

$E(B3LYP/6-311+G^{**}) = -301.482117$

N	-0.074677	-0.010537	0.057001
C	0.002408	0.123778	1.422536
N	1.344772	0.050637	1.609328
C	2.088507	-0.121574	0.430609
C	1.155154	-0.158685	-0.552546
O	1.203035	-0.301155	-1.899323

H	3.161143	-0.200286	0.398269
H	1.754672	0.117074	2.525753
H	-0.947224	-0.001855	-0.446529
H	2.116826	-0.392263	-2.187376

$E(B3LYP/cc-pVTZ) = -301.504656$

C	0.000689	0.000032	0.001334
N	0.002447	-0.000426	1.378884
C	1.259943	0.001378	1.927109
N	2.021293	0.001343	0.807651
C	1.295723	0.001175	-0.391192
O	-1.185600	-0.000991	-0.651427
H	1.741938	0.001171	-1.367991
H	3.023656	0.002202	0.852042
H	-0.835967	-0.001318	1.932464
H	-1.032734	0.000865	-1.601023

$E(\omega B97X-D/6-311+G^{**}) = -301.348262$

N	-0.012351	-0.000160	-0.014138
C	-0.027680	0.001043	1.412918
C	1.315198	-0.000332	1.675725
N	2.069343	-0.001143	0.476493
C	1.214765	-0.001288	-0.529424
O	1.609448	-0.002314	-1.806445
H	3.069657	-0.001785	0.361039
H	1.841362	-0.000356	2.616028
H	-0.855708	0.000099	-0.564114
H	0.851791	-0.002346	-2.394407

$E(M06-2X/6-311+G^{**}) = -301.364678$

C	0.052066	0.000040	-0.080552
N	0.037562	0.000003	1.294602

C	1.286941	-0.000115	1.857197
N	2.060201	-0.000733	0.746274
C	1.349860	-0.000279	-0.459220
O	-1.124670	0.000357	-0.740760
H	1.807382	-0.000384	-1.432353
H	3.064167	-0.001183	0.804650
H	-0.810811	0.000185	1.837765
H	-0.966139	0.000298	-1.687906

XYZ coordinates and total energies of 1-4 X:S at different level of theory

1 X:S

$E(B3LYP/6-311+G^{**}) = -624.514519$

C	0.033025	-0.001167	0.033732
N	0.008808	-0.003129	1.406497
C	1.290913	0.008700	1.942265
C	2.149326	0.018899	0.897359
N	1.374934	0.013463	-0.256452
S	-1.259037	-0.013364	-1.027610
H	1.477213	0.009739	3.001754
H	-0.859243	-0.013367	1.916767
H	1.707338	0.015801	-1.206975
H	3.224870	0.030647	0.874574

$E(B3LYP/cc-pVTZ) = -624.540646$

N	0.002419	-0.000343	0.001686
C	0.002488	-0.000290	1.371009
N	1.335540	-0.000046	1.684099
C	2.128287	-0.000965	0.546925
C	1.290702	-0.001301	-0.510119
S	-1.305654	0.000045	2.407597

H	3.201029	-0.000810	0.588224
H	1.648879	-0.000100	2.638169
H	-0.854731	-0.001721	-0.521498
H	1.495725	-0.001409	-1.563897

$E(\omega B97X-D/6-311+G^{**}) = -624.414872$

N	0.000914	-0.000215	0.069827
C	0.089627	0.000679	1.452724
C	1.402270	-0.000304	1.756036
N	2.088498	-0.001240	0.552360
C	1.234929	-0.001295	-0.511890
S	1.610787	-0.002455	-2.136970
H	3.085883	-0.001888	0.425681
H	1.903398	-0.000223	2.707979
H	-0.839825	-0.000129	-0.481473
H	-0.778664	0.001731	2.087813

$E(M06-2X/6-311+G^{**}) = -624.387712$

N	0.000997	0.000014	0.069711
C	0.088625	0.000351	1.453812
C	1.402409	0.000031	1.757701
N	2.088448	-0.001471	0.553090
C	1.235165	-0.001229	-0.511857
S	1.612177	-0.002427	-2.137368
H	3.087083	-0.002389	0.422488
H	1.900555	0.000356	2.710377
H	-0.839278	0.000339	-0.485620
H	-0.778366	0.001088	2.089753

2 X:S

$E(B3LYP/6-311+G^{**}) = -624.485224$

C	0.059070	-0.000393	-0.002244
N	-0.051214	-0.000448	1.327011
C	1.201865	-0.000275	1.916206
C	2.164235	0.000575	0.904544
N	1.373740	0.000611	-0.273239
H	1.330985	-0.000248	2.982474
H	-0.929767	-0.001074	1.822151
H	1.792554	0.001282	-1.192237
S	3.853624	0.001497	0.892635
H	-0.752674	-0.000822	-0.707565

$E(B3LYP/cc-pVTZ) = -624.511502$

N	0.003134	0.000041	0.001761
C	0.003594	-0.000104	1.340326
N	1.278784	0.000069	1.716400
C	2.107426	-0.000793	0.610928
C	1.312295	-0.000631	-0.533587
S	1.635468	-0.000966	-2.187995
H	3.175558	-0.001079	0.700460
H	1.583740	0.000244	2.674584
H	-0.808172	0.000397	-0.594978
H	-0.849872	0.000072	1.991045

$E(\omega B97X-D/6-311+G^{**}) = -624.383784$

N	0.006111	-0.000162	0.088290
C	0.096405	0.000566	1.420433
N	1.390569	-0.000247	1.711079
C	2.141359	-0.001308	0.551698
C	1.270211	-0.001361	-0.529862
S	1.477742	-0.002432	-2.205576
H	3.215643	-0.001985	0.566865
H	1.761808	-0.000033	2.646531

H	-0.845407	0.000056	-0.451991
H	-0.716625	0.001568	2.124619

$E(M06-2X/6-311+G^{**}) = -624.356766$

N	0.005784	-0.000137	0.088704
C	0.095331	0.000536	1.420681
N	1.390211	-0.000231	1.711926
C	2.142166	-0.001357	0.551780
C	1.271387	-0.001329	-0.530466
S	1.477162	-0.002364	-2.207004
H	3.215859	-0.002093	0.565586
H	1.760233	0.000009	2.649804
H	-0.844998	0.000153	-0.456291
H	-0.715317	0.001474	2.127365

3 X:S

$E(B3LYP/6-311+G^{**}) = -624.426486$

N	0.081267	0.027793	-0.047937
C	0.051375	0.035298	1.302740
N	1.340219	0.020717	1.679775
C	2.140825	-0.010082	0.544735
C	1.362578	-0.008628	-0.607929
S	-1.341183	0.158445	2.369045
H	3.213635	-0.026990	0.649886
H	1.632676	0.033311	2.646870
H	-0.764641	0.048173	-0.598832
H	-1.607031	-1.166514	2.472499

$E(B3LYP/cc-pVTZ) = -624.452987$

C	0.002002	-0.000838	0.001903
N	0.001730	0.001218	1.397389

C	1.224485	0.005106	1.964667
N	2.084594	0.018552	0.937714
C	1.367569	0.012365	-0.247008
S	1.643882	0.078852	3.666138
H	1.893319	0.021653	-1.185692
H	3.084723	0.031521	1.060211
H	-0.838023	0.000104	1.953294
H	1.642582	-1.249758	3.916747

$E(\omega B97X-D/6-311+G^{**}) = -624.325841$

N	-0.021349	0.040997	0.068786
C	-0.041494	-0.003954	1.463073
C	1.319367	-0.019250	1.728604
N	2.051094	0.012976	0.553647
C	1.205202	0.042848	-0.478601
S	1.638553	0.154629	-2.171499
H	3.053737	0.018583	0.449848
H	1.836550	-0.046976	2.674473
H	-0.856153	0.073140	-0.495328
H	1.619109	-1.167858	-2.435282

$E(M06-2X/6-311+G^{**}) = -624.299412$

N	-0.020370	0.039938	0.068449
C	-0.043514	-0.004288	1.464988
C	1.319074	-0.019038	1.729572
N	2.051899	0.012797	0.553717
C	1.205587	0.040921	-0.478333
S	1.640306	0.156093	-2.170589
H	3.055919	0.018080	0.444950
H	1.835121	-0.046114	2.675014
H	-0.854068	0.072050	-0.500236
H	1.614663	-1.165305	-2.429809

4 X:S

$$E(B3LYP/6-311+G^{**}) = -624.456554$$

N	-0.011462	0.019851	-0.008182
C	-0.005590	-0.008051	1.377531
C	1.302322	-0.044773	1.741845
N	2.019037	-0.025208	0.540908
C	1.237327	0.009079	-0.572415
S	2.035589	0.005693	3.344712
H	-0.893257	-0.001759	1.986611
H	-0.844434	0.050189	-0.572986
H	3.025811	-0.027669	0.495487
H	2.309488	-1.314610	3.459524

$$E(B3LYP/cc-pVTZ) = -624.482899$$

C	0.002711	0.001929	-0.000860
N	0.002106	-0.001958	1.394543
C	1.240187	-0.001299	1.951598
N	2.022531	0.011870	0.829999
C	1.310865	0.014713	-0.354712
S	-1.440812	0.093099	-1.001311
H	1.761478	0.024552	-1.329975
H	3.024972	0.022017	0.887288
H	-0.839514	0.002610	1.943930
H	-1.776142	-1.214133	-0.965135

$$E(\omega B97X-D/6-311+G^{**}) = -624.358252$$

N	-0.006449	0.014760	-0.001662
C	0.000872	-0.007114	1.379093
C	1.304333	-0.037096	1.739597
N	2.017507	-0.021412	0.543986

C	1.236860	0.006128	-0.564970
S	2.043021	0.004968	3.332006
H	-0.886888	-0.000249	1.988383
H	-0.838813	0.039889	-0.564413
H	3.022598	-0.020790	0.497205
H	2.281790	-1.316343	3.443812

$E(M06-2X/6-311+G^{**}) = -624.331865$

N	-0.006187	0.014733	-0.001666
C	-0.000652	-0.007237	1.379825
C	1.303882	-0.038568	1.740504
N	2.016564	-0.022463	0.545004
C	1.238024	0.004847	-0.566755
S	2.041100	0.006095	3.332681
H	-0.886252	0.000562	1.991480
H	-0.839261	0.040631	-0.566009
H	3.023434	-0.022383	0.502103
H	2.284180	-1.313475	3.435870

XYZ coordinates and total energies of 1-4 with R'=Me different X at B3LYP/6-311+G**

X: CH₂

1

$E(B3LYP/6-311+G^{**}) = -344.213323$

C	-0.103824	-0.036685	0.010192
N	-0.100043	-0.080600	1.401471
C	1.213822	-0.142212	1.870271
C	2.034399	-0.137884	0.800753
N	1.241141	-0.073464	-0.346579
C	-1.303027	-0.062697	2.195882
C	1.696820	-0.046528	-1.714130
C	-1.182189	0.027850	-0.816935

H	-2.184691	0.051098	-0.418977
H	-1.057499	0.057059	-1.888161
H	1.306069	-0.904264	-2.273356
H	1.369172	0.870278	-2.217355
H	2.785989	-0.084816	-1.729141
H	-1.940800	-0.921888	1.958930
H	-1.035262	-0.105219	3.251571
H	-1.877725	0.852684	2.014434
H	1.439579	-0.183432	2.921593
H	3.108487	-0.174374	0.746434

2

$E(B3LYP/6-311+G^{**}) = -344.178716$

C	-0.242409	-0.088568	-0.005736
C	-0.272104	-0.055997	1.419392
N	1.027502	-0.020854	1.877946
C	1.880968	-0.028529	0.858207
N	1.155069	-0.068930	-0.292032
H	-1.106504	-0.055976	2.096341
C	1.692494	-0.090062	-1.630434
C	-1.218466	-0.129246	-0.965780
H	-2.258687	-0.142051	-0.675639
H	-0.985052	-0.149064	-2.019582
H	1.368481	-0.995646	-2.153480
H	1.335560	0.777570	-2.194765
H	2.781940	-0.068861	-1.589872
C	1.411727	0.018648	3.279801
H	2.497905	0.041628	3.356919
H	0.997599	0.911642	3.752282
H	1.032298	-0.867298	3.792949
H	2.952938	-0.006687	0.932373

3

$$E(B3LYP/6-311+G^{**}) = -344.180913$$

N	0.009290	0.038927	-0.130651
C	0.039428	0.117946	1.269911
C	1.333265	0.105932	1.744787
N	2.058481	0.019073	0.536387
C	1.277937	-0.021663	-0.565300
C	3.514264	-0.029510	0.492868
C	1.729094	-0.084422	-1.983704
C	-1.185659	0.049325	-0.963471
H	0.907698	-0.357519	-2.647788
H	2.520518	-0.827769	-2.110159
H	2.126636	0.878523	-2.325701
H	3.866997	-0.982853	0.088350
H	3.919865	0.787349	-0.110748
H	3.857312	0.073040	1.519308
H	-1.241578	0.959328	-1.565882
H	-1.214382	-0.821813	-1.621675
H	-2.053726	0.012866	-0.307250
H	-0.894499	0.171498	1.807295

4

$$E(B3LYP/6-311+G^{**}) = -344.210274$$

C	-0.227633	-0.006931	-0.007722
C	-0.297714	-0.013431	1.348204
N	1.012653	-0.018008	1.817542
C	1.931786	-0.015444	0.811422
N	1.138520	-0.008193	-0.304996
H	-1.157685	-0.014621	1.998196
C	1.687588	-0.002447	-1.651558
C	-1.306871	0.000217	-1.037989

H	-2.285401	0.000297	-0.555226
H	-1.255649	-0.879499	-1.688193
H	1.371750	-0.888502	-2.209345
H	1.375589	0.890623	-2.200236
H	2.771400	-0.005288	-1.559383
C	1.375604	-0.025969	3.225103
H	2.461993	-0.023874	3.284443
H	0.984202	0.860373	3.732192
H	0.988356	-0.920317	3.721258
H	-1.251648	0.885468	-1.680270

X: SiH₂

1

*E(B3LYP/6-311+G**)* = -595.603590

C	-0.047283	0.003090	0.054029
N	-0.041776	-0.055244	1.419499
C	1.253989	-0.154972	1.902085
C	2.076384	-0.163157	0.826050
N	1.271273	-0.068293	-0.298498
C	-1.243056	0.018915	2.237579
C	1.745754	-0.010917	-1.673051
Si	-1.523895	0.486362	-1.078276
H	-2.532006	-0.410909	-0.386133
H	-1.127465	-0.425208	-2.223846
H	1.307522	-0.823066	-2.254935
H	1.456658	0.939185	-2.129373
H	2.831422	-0.099236	-1.675390
H	-1.925894	-0.790313	1.974714
H	-0.960987	-0.062203	3.286547
H	-1.751836	0.971552	2.069860
H	1.473255	-0.216986	2.953874

H 3.148359 -0.233691 0.762162

2

$E(B3LYP/6-311+G^{**}) = -595.580765$

C -0.156743 0.019691 0.015267

C -0.204807 0.027022 1.397713

N 1.085258 0.000405 1.901625

C 1.938165 -0.035753 0.873580

N 1.220202 -0.024761 -0.260231

H -1.057117 0.048651 2.054698

C 1.770283 -0.047859 -1.608674

Si -1.500701 0.355442 -1.340393

H -2.640295 -0.178784 -0.487169

H -1.202971 -0.915409 -2.133147

H 1.523963 -0.993672 -2.093294

H 1.314332 0.763253 -2.182006

H 2.851617 0.082008 -1.566493

C 1.453479 -0.008677 3.313029

H 2.538298 -0.040265 3.404091

H 1.079548 0.893483 3.799145

H 1.027730 -0.886546 3.801234

H 3.011018 -0.076512 0.949914

3

$E(B3LYP/6-311+G^{**}) = -595.573014$

C -0.031175 -0.022275 0.030391

N -0.041685 0.026055 1.383093

C 1.269676 0.101408 1.830347

C 2.166129 0.103574 0.772446

N 1.291290 0.024944 -0.311751

C -1.221204 0.004549 2.244421

C 1.760032 -0.003930 -1.693761

Si -1.492733 -0.131593 -1.133772

H	-2.740978	-0.160448	-0.333977
H	-1.402710	-1.363571	-1.957298
H	1.458671	-0.929910	-2.191155
H	1.375814	0.851296	-2.256436
H	2.845240	0.047898	-1.655792
H	1.459571	0.148395	2.891676
H	-1.513949	1.041014	-2.044028
H	-1.867874	0.860519	2.044832
H	-1.789762	-0.916680	2.107500
H	-0.881889	0.055867	3.277715

4

$E(B3LYP/6-311+G^{**}) = -595.604561$

C	-0.139361	-0.009361	0.030029
C	-0.204277	-0.016213	1.393053
N	1.094913	-0.014892	1.870152
C	2.021682	-0.007964	0.862823
N	1.239155	-0.005053	-0.252154
H	-1.065525	-0.021124	2.042383
C	1.799538	0.002785	-1.595854
Si	-1.554715	-0.009667	-1.182484
H	-2.813074	-0.010955	-0.396503
H	-1.517455	-1.209426	-2.059216
H	1.489311	-0.886006	-2.152036
H	1.485451	0.895647	-2.143237
H	2.882996	0.004609	-1.499563
C	1.453321	-0.021170	3.281016
H	2.539209	-0.011963	3.344457
H	1.054164	0.862667	3.785298
H	1.070129	-0.918576	3.773660
H	-1.518623	1.191116	-2.058382

X:NH

1

$E(B3LYP/6-311+G^{**}) = -360.286176$

C	0.120769	-0.060491	0.090044
N	0.036219	-0.013294	1.480402
C	1.318960	0.066748	2.031767
C	2.202180	0.046676	1.012142
N	1.483274	-0.051685	-0.176272
N	-0.790242	-0.097691	-0.822541
H	1.480553	0.111276	3.094807
C	-1.217201	0.030895	2.197926
H	-1.724684	-0.113350	-0.427054
C	2.015856	-0.017337	-1.522545
H	3.277964	0.074300	1.025714
H	-1.778325	0.942916	1.965708
H	-1.838884	-0.834792	1.948772
H	-1.014497	0.010943	3.268459
H	1.359829	-0.598085	-2.170506
H	2.063877	1.005916	-1.910370
H	3.016437	-0.452723	-1.527295

2

$E(B3LYP/6-311+G^{**}) = -360.255412$

N	-0.005196	0.000000	0.000559
C	-0.005262	-0.000038	1.388167
C	1.344351	-0.000008	1.831541
N	2.080354	0.000166	0.604607
C	1.244555	0.000143	-0.454951
N	1.999955	-0.000073	2.956277
C	3.528954	0.000252	0.573677
C	-1.196663	0.000069	-0.831056

H	1.532606	0.000427	-1.491390
H	1.357602	-0.000242	3.743075
H	-0.921883	-0.000529	1.949358
H	3.907623	0.881987	1.094063
H	3.907648	-0.880781	1.095217
H	3.870250	-0.000409	-0.462227
H	-1.795268	-0.889729	-0.624634
H	-1.795139	0.889968	-0.624691
H	-0.905628	0.000000	-1.881119

3

$E(B3LYP/6-311+G^{**}) = -360.225028$

C	0.004894	-0.081828	0.022175
N	-0.013989	-0.060243	1.433794
C	1.220879	-0.034296	1.984545
N	2.097458	-0.038800	0.967596
C	1.364432	-0.080812	-0.222036
N	1.590539	0.012558	3.332476
C	-1.244983	-0.039586	2.211460
C	3.546408	-0.010029	1.102133
H	1.629236	-0.892851	3.789618
H	1.028435	0.649300	3.883372
H	1.893096	-0.109823	-1.162027
H	3.957127	0.707354	0.390521
H	3.802425	0.293258	2.116367
H	3.972356	-0.995919	0.899592
H	-2.055528	-0.229093	1.512084
H	-1.236951	-0.814094	2.983385
H	-1.403806	0.935819	2.682167

4

$E(B3LYP/6-311+G^{**}) = -360.250579$

C	-0.006950	0.000012	-0.002036
C	-0.005149	0.000012	1.358185
N	1.327255	0.000011	1.747654
C	2.190856	0.000205	0.687654
N	1.339266	0.000136	-0.380018
C	1.775061	-0.000123	3.130454
C	1.799630	0.000265	-1.761328
N	-1.038725	-0.000093	-0.966847
H	-0.829434	-0.000075	2.053001
H	-1.622726	-0.826595	-0.930603
H	-1.622675	0.826456	-0.930844
H	2.887072	-0.000042	-1.735404
H	1.441788	-0.885344	-2.290093
H	1.442313	0.886284	-2.289771
H	1.418091	0.890289	3.655645
H	1.418299	-0.890751	3.655423
H	2.863231	0.000003	3.121390

X:PH

1

$E(B3LYP/6-311+G^{**}) = -646.881596$

C	0.165237	0.007336	0.093383
N	0.072113	0.015657	1.469591
C	1.343318	-0.001188	2.036120
C	2.238033	-0.019724	1.024181
N	1.520133	-0.014583	-0.163855
P	-1.064738	0.019790	-1.174489
H	1.492502	0.001938	3.101746
C	-1.172701	0.036160	2.210830

H	-2.152838	0.041485	-0.259322
C	2.075898	-0.028557	-1.502405
H	3.313830	-0.035763	1.041144
H	-1.750737	0.931471	1.967487
H	-1.776204	-0.843833	1.973516
H	-0.943780	0.036561	3.276136
H	1.730218	-0.912073	-2.046793
H	1.758712	0.861399	-2.053626
H	3.163091	-0.045854	-1.434486

2

$E(B3LYP/6-311+G^{**}) = -646.852790$

C	-0.018107	0.009545	-0.020895
N	0.023534	-0.059630	1.392621
C	1.302984	-0.045867	1.833189
N	2.102445	0.029139	0.769167
C	1.337799	0.064727	-0.375142
P	-1.432282	0.023847	-1.104034
C	3.558534	0.067527	0.811418
H	1.622757	-0.088455	2.858996
C	-1.139455	-0.134361	2.255502
H	-2.397016	-0.052790	-0.058245
H	1.788909	0.126516	-1.349472
H	-1.772191	0.743132	2.105192
H	-1.723459	-1.026152	2.017630
H	-0.811860	-0.176739	3.294506
H	3.966623	-0.785787	0.267490
H	3.917277	0.992104	0.356428
H	3.890617	0.024896	1.847682

3

$E(B3LYP/6-311+G^{**}) = -646.823544$

C	0.019170	-0.109097	0.006715
N	0.027729	-0.097027	1.405671
C	1.274890	-0.023936	1.950299
N	2.126054	0.016080	0.898331
C	1.377545	-0.039915	-0.265579
P	1.811047	0.036518	3.694928
C	-1.199689	-0.146196	2.191481
C	3.585329	0.044444	0.949382
H	1.091531	-1.099048	4.163137
H	0.836322	0.962425	4.158287
H	1.884323	-0.021354	-1.218191
H	3.949909	0.726932	0.181318
H	3.922537	0.391408	1.924229
H	3.990973	-0.952700	0.764091
H	-2.016590	-0.230765	1.479596
H	-1.204112	-1.010812	2.859939
H	-1.324939	0.763958	2.783588

4

$E(B3LYP/6-311+G^{**}) = -646.854344$

N	0.072137	-0.002910	-0.062385
C	0.054890	-0.115449	1.302241
N	1.379973	-0.065393	1.619497
C	2.208774	0.074279	0.492616
C	1.353449	0.111885	-0.567734
C	1.851345	-0.150634	2.993571
P	4.023101	0.187565	0.379224
H	1.569882	0.210262	-1.619432
H	4.360173	-0.903773	1.230404

H	4.242001	1.157717	1.399038
C	-1.136290	-0.005993	-0.873805
H	0.974666	-0.252731	3.628998
H	2.501609	-1.018056	3.130555
H	2.400294	0.751276	3.275058
H	-1.128584	-0.843551	-1.576063
H	-1.983664	-0.109236	-0.199463
H	-1.229892	0.929099	-1.432000

X: O

1

$E(B3LYP/6-311+G^{**}) = -380.194319$

N	0.227782	-0.017760	-0.145100
C	0.085792	0.012235	1.237506
N	1.389550	0.020986	1.720027
C	2.292159	-0.002594	0.659455
C	1.577995	-0.026365	-0.487113
O	-0.953531	0.027574	1.884580
H	3.357402	-0.000934	0.814175
C	1.707044	0.051492	3.133803
C	-0.901285	-0.034383	-1.053633
H	1.909005	-0.048926	-1.511126
H	2.276439	-0.835135	3.426140
H	2.280693	0.947475	3.386571
H	0.764430	0.065811	3.679825
H	-0.891976	0.843737	-1.705238
H	-0.895674	-0.938921	-1.668075
H	-1.807251	-0.019914	-0.448756

2

$E(B3LYP/6-311+G^{**}) = -380.161092$

N	-0.021914	-0.002695	0.001338
C	0.005649	-0.015887	1.345570
N	1.277947	0.002630	1.740520
C	2.120658	0.028618	0.640429
C	1.336379	0.026076	-0.532101
O	1.570616	0.041748	-1.740922
H	3.190052	0.044442	0.744956
C	1.720720	-0.002860	3.125097
C	-1.192976	-0.016154	-0.854043
H	-0.844637	-0.035561	2.005950
H	2.337365	-0.883423	3.316096
H	2.304797	0.895746	3.333621
H	0.851316	-0.025312	3.781750
H	-0.820301	0.004666	-1.878773
H	-1.782472	-0.923808	-0.703082
H	-1.819710	0.861896	-0.679961

3

$E(B3LYP/6-311+G^{**}) = -380.093700$

C	0.014655	0.179635	0.020704
N	-0.007947	0.046015	1.444738
C	1.224186	-0.051201	1.959062
N	2.110551	0.009632	0.970068
C	1.364839	0.159561	-0.225940
O	1.592817	-0.156801	3.253857
H	1.899217	0.236603	-1.159282
C	3.557524	-0.041179	1.119001
C	-1.227835	0.017384	2.235997
H	0.848949	-0.461482	3.785477
H	3.968734	-0.751639	0.400451

H	3.994529	0.943949	0.939529
H	3.809156	-0.365170	2.128027
H	-2.049406	0.138796	1.533739
H	-1.350408	-0.940025	2.755513
H	-1.253085	0.836515	2.961811

4

$E(B3LYP/6-311+G^{**}) = -380.121700$

C	-0.000203	-0.010053	0.003297
N	-0.017919	-0.021703	1.382565
C	1.251548	-0.000365	1.915816
N	2.032958	0.024725	0.806194
C	1.299860	0.019380	-0.387926
O	-1.181161	-0.029194	-0.666578
H	1.745434	0.036658	-1.368140
C	3.484363	0.054080	0.858520
C	-1.232072	-0.052848	2.184792
H	-1.016759	-0.009953	-1.614633
H	3.909140	-0.823027	0.361856
H	3.872609	0.957717	0.379802
H	3.773356	0.049481	1.907565
H	-1.850395	0.825636	1.987108
H	-1.816277	-0.950369	1.969707
H	-0.923433	-0.057109	3.227696

X:S

1

$E(B3LYP/6-311+G^{**}) = -703.155979$

C	0.164308	-0.002110	0.071138
N	0.060655	0.022489	1.442293
C	1.322069	0.023958	2.019307
C	2.226198	0.000088	1.011901

N	1.516475	-0.015870	-0.179750
S	-1.085365	-0.012863	-1.050258
H	1.464429	0.041357	3.085765
C	-1.208919	0.044111	2.149234
C	2.082490	-0.042846	-1.518010
H	3.301914	-0.007048	1.038489
H	-1.782710	0.927786	1.864610
H	-1.795625	-0.840495	1.895527
H	-1.009753	0.061370	3.220412
H	1.746223	-0.934170	-2.050537
H	1.758371	0.834117	-2.081049
H	3.169019	-0.048878	-1.435520

2

$E(B3LYP/6-311+G^{**}) = -703.128533$

N	-0.008221	-0.003288	0.010202
C	0.000970	-0.014755	1.353398
N	1.269494	0.002603	1.766119
C	2.103611	0.025883	0.664202
C	1.328165	0.022921	-0.493252
S	1.740380	0.043653	-2.136886
H	3.173824	0.042403	0.762977
C	1.705321	-0.001629	3.156110
C	-1.202665	-0.016632	-0.823281
H	-0.862318	-0.034207	1.996165
H	2.317425	-0.883887	3.350148
H	2.289138	0.896412	3.364343
H	0.832286	-0.020714	3.807364
H	-0.855126	0.006102	-1.857214
H	-1.780102	-0.926818	-0.650611
H	-1.818692	0.862076	-0.623341

3

$$E(B3LYP/6-311+G^{**}) = -703.065526$$

C	0.004264	0.059073	-0.007516
N	-0.041159	0.097387	1.391584
C	1.185980	0.057958	1.970394
N	2.083031	0.009581	0.961989
C	1.372675	0.014769	-0.229331
S	1.578617	0.162278	3.683128
H	1.913346	-0.011460	-1.162850
C	3.536317	0.008063	1.084998
C	-1.294354	0.122877	2.138845
H	1.288161	-1.118618	4.018484
H	3.949279	-0.697020	0.363323
H	3.935854	1.004441	0.883208
H	3.821135	-0.293616	2.091029
H	-2.073170	0.385616	1.427771
H	-1.513812	-0.859824	2.564821
H	-1.249688	0.859087	2.942876

4

$$E(B3LYP/6-311+G^{**}) = -703.095027$$

C	0.036153	0.015884	0.018161
N	0.030064	-0.023035	1.418794
C	1.288687	-0.020498	1.945193
N	2.079057	0.039285	0.827868
C	1.346432	0.061352	-0.344220
S	-1.386284	0.147766	-1.019150
H	1.785043	0.105865	-1.327324
C	3.532893	0.074660	0.889679

C	-1.166464	-0.084065	2.246431
H	-1.787289	-1.143532	-0.956822
H	3.963631	-0.792077	0.381766
H	3.917053	0.988308	0.428952
H	3.815339	0.053763	1.940134
H	-1.835813	0.746998	2.017071
H	-1.703916	-1.022943	2.090792
H	-0.841707	-0.023003	3.282455

XYZ coordinates and total energies of 2 and 4 with different X:N-R at different level of theory

4 X: N-CH₃

$E(B3LYP/6-311+G^{**}) = -399.567773$

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.401393
C	1.312316	0.000000	1.768020
N	2.045790	-0.006540	0.583441
C	1.245419	-0.013986	-0.535010
N	1.926731	0.079939	3.013447
C	1.055582	0.044663	4.180694
C	3.496357	0.004165	0.520977
C	-1.210116	0.013602	-0.802346
H	-0.898682	0.004731	1.993054
H	1.666998	0.101422	5.082093
H	0.395357	0.915364	4.164422
H	0.432095	-0.860125	4.231014
H	3.773888	0.087233	-0.527504
H	3.901326	0.854040	1.076706
H	3.921985	-0.921317	0.924536
H	-1.824053	-0.868005	-0.595452
H	-1.800060	0.912384	-0.599814
H	-0.911759	0.006683	-1.848771
H	2.726095	-0.534834	3.100838

$$E(\omega B97X-D/6-311+G^{**}) = -399.433852$$

C	0.005588	-0.000035	0.002529
N	0.009624	-0.002720	1.353023
C	1.293070	-0.000114	1.901431
C	2.139402	0.018209	0.841731
N	1.343165	0.020403	-0.291600
C	-1.196000	-0.005259	2.151452
N	3.522523	0.104357	0.764035
C	4.233933	0.063089	2.027428
C	1.862654	0.043613	-1.640751
H	1.485258	-0.003324	2.960716
H	5.305668	0.124729	1.836169
H	3.947492	0.929903	2.628388
H	4.026674	-0.845900	2.610809
H	1.016911	0.171474	-2.313014
H	2.563455	0.872832	-1.765974
H	2.369663	-0.895339	-1.887440
H	-1.236277	-0.893548	2.787858
H	-1.244084	0.888157	2.780044
H	-2.044023	-0.012114	1.469393
H	3.913758	-0.520455	0.072632

2 X: N-CH₃

$$E(B3LYP/6-311+G^{**}) = -399.570844$$

C	-0.004644	-0.044581	-0.208507
C	-0.115104	-0.014809	1.208459
N	1.246771	0.056638	1.640712
C	2.076948	0.068685	0.579193
N	1.345218	0.008764	-0.530126
N	-1.070071	-0.036184	2.083609
C	1.878017	-0.000983	-1.882054

H	3.151070	0.117708	0.616035
C	1.615490	0.108095	3.040894
C	-2.401837	-0.110927	1.522834
H	-0.760800	-0.096644	-0.969181
H	-3.138743	-0.124766	2.329593
H	-2.644137	0.749668	0.872791
H	-2.563168	-1.020889	0.916329
H	2.702121	0.141914	3.129194
H	1.173229	0.990924	3.506570
H	1.223416	-0.771053	3.555479
H	1.497458	0.858491	-2.438055
H	2.965785	0.049990	-1.843656
H	1.579055	-0.918674	-2.393049

$E(\omega B97X-D/6-311+G^{**}) = -399.432043$

C	0.003153	0.062399	0.017730
N	0.010262	0.037382	1.339623
C	1.313759	-0.003152	1.806396
C	2.170976	-0.001299	0.680335
N	1.272568	0.040253	-0.416599
C	-1.166378	0.041430	2.181979
N	3.447037	-0.026088	0.470343
C	4.231498	-0.066610	1.679300
C	1.731089	0.057407	-1.785044
H	-0.876806	0.093996	-0.601746
H	1.534747	-0.026456	2.857780
H	5.294685	-0.086077	1.428376
H	4.062738	0.811946	2.328643
H	4.022447	-0.960218	2.295532
H	0.871084	0.087686	-2.455220
H	2.367112	0.929742	-1.944641
H	2.331224	-0.833326	-1.978252

H	-1.137835	0.904290	2.849517
H	-2.058845	0.098393	1.559253
H	-1.198939	-0.874067	2.775292

4 X: N-Cl

$E(B3LYP/6-311+G^{**}) = -819.834215$

N	-0.036697	-0.034378	0.067703
C	0.007545	-0.040127	1.463528
C	1.335492	-0.048054	1.797260
N	2.028300	-0.019624	0.609651
C	1.201424	-0.021159	-0.493318
N	-1.141819	0.042439	2.225741
Cl	-1.915898	-1.640687	2.557728
C	-1.272593	-0.033383	-0.706186
H	1.804619	-0.070176	2.767851
H	-0.915977	0.329860	3.172813
C	3.479842	0.022779	0.502060
H	3.727627	-0.005365	-0.556757
H	3.874302	0.942219	0.942156
H	3.928535	-0.838336	1.003257
H	-0.998080	0.093625	-1.750662
H	-1.808981	-0.975374	-0.576616
H	-1.916734	0.785842	-0.383263

$E(\omega B97X-D/6-311+G^{**}) = -819.692441$

C	0.003023	0.000425	-0.000218
N	0.005777	-0.002864	1.357692
C	1.288178	-0.010866	1.884793
C	2.136465	-0.022987	0.825520
N	1.337084	-0.000924	-0.295547
C	-1.199207	0.003529	2.165917
N	1.507096	0.066756	3.259434

Cl	1.481290	-1.533278	4.059501
C	1.843066	0.027759	-1.653233
H	3.213905	-0.044130	0.792563
H	2.438649	0.414917	3.449536
H	0.984028	0.020143	-2.321105
H	2.429316	0.933266	-1.827888
H	2.463912	-0.849088	-1.851274
H	-2.041101	0.120595	1.487247
H	-1.298517	-0.933537	2.717640
H	-1.170141	0.831124	2.876365

2 X: N-Cl

$E(B3LYP/6-311+G^{**}) = -819.847445$

N	-0.033340	-0.000026	0.006167
C	-0.086974	-0.000029	1.393106
C	1.239866	-0.000092	1.865676
N	2.029212	-0.000132	0.687782
C	1.231249	-0.000092	-0.401329
N	1.882123	-0.000072	3.017500
Cl	0.719023	0.000470	4.358036
C	-1.197562	0.000006	-0.866945
H	1.563909	-0.000145	-1.424161
C	3.481309	-0.000129	0.708405
H	-1.015267	0.000055	1.931135
H	3.855151	-0.000166	-0.315641
H	3.840553	0.883239	1.239038
H	3.840554	-0.883456	1.239101
H	-0.870578	0.000047	-1.906019
H	-1.800874	-0.889966	-0.678849
H	-1.800872	0.889963	-0.678780

$E(\omega B97X-D/6-311+G^{**}) = -819.704340$

C	0.003753	-0.000014	0.003414
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N	0.002315	0.000020	1.324261
C	1.301942	0.000074	1.799694
C	2.151894	0.000111	0.683965
N	1.279126	0.000042	-0.419440
C	-1.179266	-0.000033	2.162888
N	3.442693	0.000187	0.426123
Cl	4.347054	0.000252	1.921817
C	1.746635	0.000066	-1.788190
H	-0.868206	-0.000087	-0.627687
H	1.528082	0.000120	2.849443
H	0.888244	-0.000007	-2.460459
H	2.362207	0.883739	-1.962732
H	2.362342	-0.883516	-1.962713
H	-2.069485	-0.000030	1.534750
H	-1.182646	-0.890568	2.793007
H	-1.182685	0.890460	2.793066

4 X: N-F

$E(B3LYP/6-311+G^{**}) = -459.451015$

N	-0.050991	-0.030392	0.070101
C	-0.009106	-0.044001	1.465803
C	1.316008	-0.055513	1.803545
N	2.011975	-0.026349	0.619752
C	1.186956	-0.025681	-0.487083
N	-1.160672	0.020798	2.229521
F	-1.660735	-1.379700	2.439691
C	-1.286451	-0.048637	-0.705005
H	1.782037	-0.076707	2.775870
H	-0.933623	0.261720	3.190926
C	3.464500	0.006752	0.515237
H	3.713323	0.002561	-0.543648
H	3.865131	0.911931	0.978341
H	3.905962	-0.870107	0.995001

H	-1.012139	0.068306	-1.750672
H	-1.813439	-0.993651	-0.561992
H	-1.937830	0.768772	-0.392441

$E(\omega B97X-D/6-311+G^{**}) = -459.298018$

C	0.003188	0.002283	0.000128
N	0.005214	-0.004520	1.354985
C	1.287862	-0.009116	1.883070
C	2.136754	-0.009163	0.823130
N	1.341386	0.013862	-0.295441
C	-1.198699	-0.022994	2.165587
N	1.507482	0.042626	3.255941
F	1.489996	-1.314947	3.766429
C	1.844977	0.047480	-1.654689
H	3.214749	-0.018473	0.793625
H	2.468963	0.310398	3.442067
H	0.984099	0.035536	-2.319878
H	2.424915	0.956877	-1.829069
H	2.470789	-0.825235	-1.855001
H	-2.046334	0.030090	1.486166
H	-1.249235	-0.941199	2.752877
H	-1.208457	0.831881	2.843549

2 X: N-F

$E(B3LYP/6-311+G^{**}) = -459.460549$

N	-0.037120	0.000018	0.031469
C	-0.087776	-0.000226	1.417447
C	1.243670	0.000087	1.876813
N	2.030297	-0.000128	0.705664
C	1.224795	-0.000394	-0.383390
N	1.856662	0.000083	3.042847
F	0.777989	0.000413	4.019630
C	-1.204774	0.000296	-0.837739

H	1.554052	-0.000548	-1.406944
C	3.482375	-0.000152	0.721140
H	-1.010638	-0.000515	1.963829
H	3.853468	-0.000324	-0.303681
H	3.845009	0.884185	1.248860
H	3.844934	-0.884362	1.249123
H	-0.881906	0.000273	-1.877936
H	-1.806914	-0.889659	-0.646482
H	-1.806643	0.890429	-0.646426

$E(\omega B97X-D/6-311+G^{**}) = -459.305102$

C	0.002467	0.000505	0.003576
N	0.000650	0.000000	1.323888
C	1.297380	0.000422	1.804644
C	2.144352	0.000823	0.685934
N	1.282635	0.000834	-0.418740
C	-1.183034	-0.000650	2.160063
N	3.439630	0.001240	0.463956
F	4.032583	0.001318	1.769187
C	1.754788	0.001174	-1.785747
H	-0.867511	0.000500	-0.629710
H	1.525212	0.000247	2.853316
H	0.900058	0.001201	-2.462287
H	2.370683	0.885573	-1.958970
H	2.370940	-0.882974	-1.959356
H	-2.072308	-0.000813	1.530753
H	-1.186288	-0.891508	2.789498
H	-1.186917	0.889905	2.789921

4 X: N-CF₃

$E(B3LYP/6-311+G^{**}) = -697.399732$

C	0.044393	0.500354	-0.363763
C	-0.177757	0.408075	0.973820
N	1.017833	-0.039102	1.538794
C	1.991418	-0.233963	0.604268
N	1.355707	0.110741	-0.560704
N	-1.316660	0.694615	1.756857
C	-2.415547	-0.174672	1.724185
F	-2.062061	-1.426679	2.064359
C	1.217000	-0.288301	2.960897
C	2.009074	0.058390	-1.860748
F	-3.357430	0.263284	2.583014
F	-3.028225	-0.276267	0.506513
H	1.498166	-0.645587	-2.522435
H	2.021782	1.046438	-2.327905
H	3.031042	-0.276904	-1.697417
H	2.249857	-0.604357	3.086503
H	1.036155	0.618282	3.541925
H	0.545936	-1.073750	3.313077
H	-0.621613	0.796994	-1.157376
H	-1.600293	1.664961	1.804934

$$E(\omega B97X-D/6-3II+G^{**}) = -697.188955$$

N	0.006279	-0.000775	0.007743
C	0.004065	0.013096	1.384922
C	1.304947	0.018202	1.757003
N	2.047695	0.003637	0.584538
C	1.263669	-0.009653	-0.524366
N	1.920045	0.039870	3.022554
C	1.906756	-1.129973	3.791522
F	0.670412	-1.544783	4.162414
C	3.497438	-0.021473	0.540090
C	-1.193276	-0.013724	-0.806033

F	2.457275	-2.149188	3.127363
F	2.590917	-0.925287	4.923386
H	-1.790856	-0.904116	-0.596700
H	-1.795817	0.878414	-0.619586
H	-0.878846	-0.026541	-1.847620
H	3.785794	0.001840	-0.508444
H	3.913691	0.844942	1.057252
H	3.879148	-0.930807	1.007075
H	-0.890997	0.007192	1.985260
H	1.761921	0.866848	3.580259

2 X: N-CF₃

E(B3LYP/6-311+G**) = -697.425215

C	-0.044806	0.000448	-0.162843
C	-0.129504	0.000136	1.233580
N	1.214823	-0.000118	1.663462
C	2.041002	0.000013	0.600660
N	1.297752	0.000316	-0.503882
N	-1.077976	0.000124	2.153621
C	-2.368699	-0.000510	1.737642
F	-2.738665	-1.091410	0.953073
C	1.597528	-0.000670	3.067424
C	1.811643	0.000856	-1.867246
F	-3.228601	0.000802	2.780935
F	-2.738936	1.088155	0.950047
H	1.462945	-0.888780	-2.393985
H	1.464504	0.891831	-2.392763
H	2.900534	-0.000136	-1.841503
H	2.684881	-0.000834	3.141191
H	1.186678	0.882333	3.557527
H	1.186452	-0.883927	3.556883

H	-0.821734	0.000839	-0.904243
H	3.115936	-0.000108	0.635474

$E(\omega B97X-D/6-311+G^{**}) = -697.209242$

N	0.006316	0.000026	0.007213
C	0.009037	0.000086	1.388335
C	1.338105	0.000119	1.805703
N	2.077050	0.000062	0.615121
C	1.252024	0.000015	-0.440607
N	2.000703	0.000246	2.947209
C	1.264136	-0.000941	4.086693
F	0.415374	1.078967	4.234771
C	3.525860	-0.000150	0.592522
C	-1.186611	0.000359	-0.817932
F	0.419707	-1.084152	4.235101
F	2.045848	0.000791	5.178143
H	-1.779758	-0.889916	-0.606087
H	-1.778352	0.891909	-0.607490
H	-0.897286	-0.000721	-1.868129
H	3.866979	-0.000211	-0.442684
H	3.895515	0.883083	1.113558
H	3.895247	-0.883492	1.113567
H	-0.898730	0.000214	1.963253
H	1.550032	-0.000002	-1.474797

4 X: N-'Bu

$E(B3LYP/6-311+G^{**}) = -517.541691$

C	-0.251778	-0.026786	0.412397
C	0.010484	0.066772	1.747668
N	1.407697	0.087017	1.865427
C	2.046009	-0.002915	0.675520
N	0.998865	-0.065772	-0.213114
C	2.101503	0.195038	3.135933

C	1.192987	-0.149170	-1.649419
N	-1.408750	-0.019228	-0.362226
C	-2.780713	-0.018216	0.196069
C	-3.020042	1.284887	0.976742
C	-3.722123	-0.050121	-1.018851
C	-3.054121	-1.251269	1.082049
H	-1.334862	-0.638933	-1.159222
H	0.682730	0.672062	-2.159879
H	2.263165	-0.084369	-1.832800
H	0.826583	-1.100855	-2.050941
H	1.841344	1.129192	3.642790
H	1.849907	-0.645091	3.790280
H	3.169913	0.182787	2.929875
H	-0.640977	0.120874	2.600437
H	-4.077831	-1.228069	1.466300
H	-2.929823	-2.173198	0.506363
H	-2.374809	-1.297374	1.934410
H	-4.057266	1.328413	1.318824
H	-2.375513	1.366762	1.852472
H	-2.828311	2.149138	0.336888
H	-4.764954	-0.048021	-0.694235
H	-3.556030	0.818709	-1.660288
H	-3.563418	-0.955376	-1.615054

$E(\omega B97X-D/6-311+G^{**}) = -517.377735$

N	-0.002996	0.010444	0.010215
C	-0.008969	-0.007457	1.400171
C	1.297044	-0.019988	1.772090
N	2.031124	-0.002247	0.584900
C	1.258848	0.006463	-0.520456
N	-1.219996	0.052153	2.077673
C	-1.319840	0.032532	3.545093

C	-0.712456	-1.240526	4.155209
C	3.476257	0.007692	0.546614
C	-1.198958	0.042387	-0.801455
C	-0.656341	1.287343	4.120693
C	-2.817988	0.074543	3.859910
H	-1.918587	-0.542042	1.651429
H	-1.838614	0.879584	-0.510723
H	-0.884287	0.162026	-1.835872
H	-1.767953	-0.889655	-0.713356
H	3.869886	0.898178	1.044654
H	3.883154	-0.883284	1.033127
H	3.778383	0.016546	-0.498939
H	1.765117	-0.035850	2.739967
H	-0.829978	-1.236732	5.242481
H	-1.214361	-2.129291	3.761319
H	0.351072	-1.331991	3.930272
H	-0.795158	1.316525	5.204561
H	0.415017	1.316420	3.918036
H	-1.105373	2.183145	3.685747
H	-2.980471	0.080359	4.940119
H	-3.275176	0.970583	3.432976
H	-3.329382	-0.804351	3.452104

2 X: N-^tBu

*E(B3LYP/6-311+G**)* = -517.544733

N	0.427156	-0.302986	-0.051841
C	0.158526	0.041970	1.221789
N	1.308875	0.285428	1.841366
C	2.370677	0.100119	0.965937
C	1.843947	-0.289550	-0.298287
C	1.441687	0.688293	3.231057
N	2.249496	-0.603570	-1.489092
C	3.671407	-0.618046	-1.836267

C	4.316800	0.779790	-1.694311
C	-0.533216	-0.652142	-1.078412
C	4.460331	-1.654921	-1.003878
C	3.743034	-1.033726	-3.317220
H	3.380858	0.252429	1.293426
H	-0.817838	0.110713	1.668404
H	-1.541367	-0.590012	-0.666267
H	-0.429245	0.028126	-1.925593
H	-0.334954	-1.662918	-1.439605
H	4.777848	-1.073814	-3.672845
H	3.287336	-2.018218	-3.452162
H	3.187752	-0.321484	-3.933236
H	5.359968	0.765880	-2.026909
H	3.771804	1.504552	-2.305353
H	4.300809	1.136540	-0.661454
H	5.505924	-1.702822	-1.325541
H	4.450127	-1.418461	0.063050
H	4.017361	-2.646766	-1.129232
H	0.453138	0.756808	3.684322
H	2.036717	-0.046996	3.777017
H	1.932709	1.661958	3.291693

$E(\omega B97X-D/6-311+G^{**}) = -517.375524$

C	-0.010617	-0.000145	0.002291
N	-0.003520	-0.000314	1.426912
C	1.251148	-0.000091	1.899657
N	2.082934	0.000464	0.873472
C	1.371251	0.000614	-0.314141
C	-1.222673	-0.001699	2.198750
C	3.526787	0.001747	0.966002
N	-1.161509	-0.000735	-0.590579
C	-1.246065	-0.000320	-2.044219

C	-2.741804	-0.000748	-2.382134
C	-0.612904	1.262037	-2.657893
C	-0.612013	-1.261916	-2.658537
H	1.883076	0.000762	-1.257895
H	1.537589	-0.000114	2.937438
H	-0.976500	0.002221	3.261570
H	-1.816705	0.877126	1.942960
H	-1.811835	-0.885427	1.948489
H	-2.907991	-0.000655	-3.464730
H	-3.220340	-0.884716	-1.951880
H	-3.220908	0.882812	-1.951665
H	-0.753874	1.281385	-3.743603
H	-1.080866	2.154230	-2.232517
H	0.460219	1.321276	-2.458725
H	-0.752695	-1.280682	-3.744295
H	0.461093	-1.320633	-2.459117
H	-1.079556	-2.154639	-2.233817
H	3.822468	-0.000371	2.014891
H	3.929318	-0.887216	0.477153
H	3.927595	0.893674	0.481129

4 X: N-Ph

$E(B3LYP/6-311+G^{**}) = -591.356516$

N	0.318154	-0.543583	0.595446
C	0.462625	0.449914	1.573595
C	1.744933	0.888743	1.467728
N	2.322137	0.162061	0.438268
C	1.462225	-0.744517	-0.120714
N	-0.580841	0.854769	2.409895
C	-0.956446	0.196086	3.587805
C	-0.324535	-0.982446	4.007799

C	-0.741083	-1.619702	5.174592
C	-1.779659	-1.100544	5.944486
C	-2.404592	0.075962	5.528595
C	-2.004277	0.717930	4.362872
C	3.694189	0.331949	-0.014309
C	-0.916782	-1.274213	0.345594
H	2.268007	1.636819	2.040741
H	-2.504614	1.627325	4.043988
H	-3.214139	0.497495	6.114403
H	-2.096365	-1.600497	6.851844
H	-0.239786	-2.530261	5.484281
H	0.494723	-1.389668	3.427532
H	-0.737070	-1.926444	-0.505957
H	-1.200110	-1.873678	1.213632
H	-1.731070	-0.583780	0.115512
H	3.861369	-0.377181	-0.822435
H	3.857802	1.347697	-0.384319
H	4.398732	0.128963	0.796683
H	-0.932620	1.791499	2.288216

$E(\omega B97X-D/6-311+G^{**}) = -591.154191$

C	-0.010646	0.007937	0.012662
C	-0.036729	-0.007736	1.411171
C	1.171470	0.009165	2.113245
C	2.375695	0.046999	1.421627
C	2.402767	0.060571	0.032991
C	1.198580	0.037000	-0.664125
N	-1.262729	-0.019713	2.076850
C	-1.378813	-0.041472	3.464296
N	-1.215454	1.099453	4.245936
C	-1.376139	0.852025	5.573094
N	-1.654048	-0.482052	5.587585

C	-1.650651	-1.047915	4.327182
C	-0.925604	2.412750	3.704236
C	-1.929939	-1.216721	6.804986
H	-1.827563	-2.094297	4.138944
H	-0.944263	0.000714	-0.541708
H	1.199349	0.046453	-1.748605
H	3.345333	0.087466	-0.500287
H	3.303837	0.060807	1.982561
H	1.164713	-0.015241	3.197141
H	-0.856196	3.100343	4.544288
H	0.017895	2.405892	3.153676
H	-1.723600	2.732665	3.030899
H	-1.824340	-0.522912	7.636744
H	-2.947624	-1.615186	6.792953
H	-1.222589	-2.040641	6.927978
H	-2.079293	-0.244342	1.535106

2 X: N-Ph

$E(B3LYP/6-311+G^{**}) = -591.366364$

N	0.070098	-0.123687	0.102274
C	0.198883	-0.161854	1.524868
C	1.598347	-0.116540	1.721995
N	2.203689	-0.014940	0.477704
C	1.278693	-0.024044	-0.478052
N	-0.902885	-0.172327	2.229072
C	-0.919994	-0.315298	3.605177
C	0.092672	-0.910669	4.391505
C	-0.049688	-1.040730	5.772302
C	-1.192640	-0.581832	6.422871
C	-2.209801	-0.000659	5.659183
C	-2.080205	0.123862	4.283551
C	3.639801	0.059266	0.256323

C	-1.217156	-0.135723	-0.569053
H	1.471940	0.019206	-1.535536
H	2.178228	-0.069281	2.623456
H	-2.872320	0.566408	3.689933
H	-3.113463	0.355546	6.143724
H	-1.294212	-0.679668	7.497608
H	0.744152	-1.512252	6.343795
H	0.976524	-1.317807	3.916970
H	-1.059156	-0.111143	-1.647760
H	-1.766184	-1.035471	-0.289331
H	-1.804948	0.727498	-0.253506
H	3.836394	0.147890	-0.811604
H	4.048978	0.931557	0.769366
H	4.122690	-0.842176	0.638541

$E(\omega B97X-D/6-311+G^{**}) = -591.157453$

C	0.002023	-0.135548	0.018439
C	-0.036551	0.037831	1.413834
C	1.195724	0.177346	2.078185
C	2.397570	0.121371	1.382115
C	2.416504	-0.074244	0.006932
C	1.203389	-0.196594	-0.668102
N	-1.278502	0.120327	2.021086
C	-1.446755	-0.287704	3.250203
N	-2.706700	-0.064701	3.854320
C	-2.748741	-0.619487	5.073522
N	-1.576082	-1.180060	5.315896
C	-0.732267	-0.992855	4.236643
C	-3.780841	0.625169	3.175436
C	-1.211983	-1.874294	6.534056
H	-3.585379	-0.598375	5.750612
H	0.256150	-1.412970	4.222706

H	-0.942605	-0.224859	-0.506741
H	1.196274	-0.340663	-1.743957
H	3.356449	-0.123620	-0.530800
H	3.330621	0.240290	1.924485
H	1.209723	0.370668	3.145103
H	-4.638024	0.701897	3.845263
H	-3.441991	1.618383	2.879679
H	-4.052436	0.078270	2.271549
H	-2.051923	-1.853759	7.227813
H	-0.957773	-2.910732	6.306997
H	-0.352960	-1.383530	6.993870

4 X: N-Si(CH₃)₃

E(B3LYP/6-311+G**) = -769.011523

C	0.096479	-0.545549	0.195953
N	0.099440	-0.363003	1.554918
C	1.194409	0.387928	2.001267
C	1.905332	0.695344	0.881218
N	1.211363	0.131467	-0.189650
C	-0.926832	-0.907476	2.426882
N	1.377520	0.739887	3.337237
Si	1.782886	2.329986	3.982384
C	1.670282	2.133052	5.851862
C	1.631169	0.243641	-1.575713
C	3.526712	2.860751	3.498652
C	0.545536	3.593585	3.340450
H	1.313072	-0.032675	3.986481
H	-1.357215	-0.121873	3.052543
H	-1.698836	-1.334708	1.790733
H	-0.526856	-1.695191	3.073785
H	1.654671	1.290813	-1.891214
H	2.624066	-0.192653	-1.718479

H	0.909206	-0.299307	-2.182489
H	2.832673	1.230943	0.770795
H	3.794834	3.804846	3.984693
H	4.265853	2.110136	3.793635
H	3.617133	3.014559	2.419462
H	0.812382	4.605420	3.661665
H	0.511704	3.591863	2.247078
H	-0.462771	3.378171	3.705119
H	1.907766	3.076254	6.353106
H	0.664538	1.838003	6.165292
H	2.375384	1.382367	6.222461

$E(\omega B97X-D/6-311+G^{**}) = -768.834$

C	1.428630	-0.960825	-0.522327
N	2.647194	-0.547117	-0.010001
C	2.686990	0.785288	0.255739
N	1.433385	1.186247	-0.095819
C	0.644531	0.142120	-0.580295
C	3.767411	-1.433105	0.223313
C	0.976247	2.554441	0.015385
N	-0.694140	0.290124	-0.938161
Si	-2.018684	-0.255561	0.068828
C	-1.969166	-2.121238	0.236054
C	-1.864779	0.512162	1.772694
C	-3.581757	0.301885	-0.799322
H	-0.869209	0.867577	-1.746251
H	0.040053	2.598539	0.576025
H	1.747571	3.113763	0.540729
H	0.818724	3.000817	-0.970556
H	3.501475	-2.209658	0.945370
H	4.089379	-1.905151	-0.708627
H	4.582624	-0.833006	0.623319
H	1.213406	-1.977907	-0.805688

H	-2.790538	-2.482744	0.862839
H	-2.047368	-2.606563	-0.740947
H	-1.032416	-2.442874	0.700833
H	-2.592501	0.089635	2.472346
H	-0.866021	0.333351	2.184079
H	-2.023023	1.594085	1.735735
H	-4.465562	0.016908	-0.220852
H	-3.605955	1.388732	-0.923252
H	-3.672775	-0.156805	-1.788275

2 X: N-Si(CH₃)₃

$E(B3LYP/6-311+G^{**}) = -769.019276$

C	-0.009718	-0.228062	0.033640
C	0.000352	-0.009064	1.431833
N	1.408960	0.135500	1.709847
C	2.132983	0.008918	0.584082
N	1.297246	-0.208971	-0.429534
N	-0.857702	0.080328	2.397787
Si	-2.568743	-0.041240	2.379837
C	-3.172910	0.195081	4.152371
C	1.911421	0.375153	3.048148
C	1.694180	-0.395575	-1.815548
C	-3.381924	1.287756	1.290936
C	-3.170864	-1.736363	1.765794
H	-0.835275	-0.391599	-0.634773
H	3.204312	0.072196	0.503058
H	2.991034	0.525016	3.010199
H	1.422493	1.256741	3.464883
H	1.673965	-0.473536	3.692396
H	-4.474753	1.219305	1.325586
H	-3.099696	2.290626	1.626817
H	-3.079601	1.196014	0.242483

H	-4.263385	-1.809325	1.800978
H	-2.861306	-1.928753	0.733210
H	-2.762627	-2.540916	2.385661
H	-4.263538	0.129292	4.224867
H	-2.743913	-0.566593	4.810688
H	-2.867188	1.172959	4.536938
H	2.779525	-0.334928	-1.891641
H	1.364216	-1.374451	-2.169357
H	1.246952	0.380819	-2.439657
$E(\omega B97X-D/6-311+G^{**}) = -768.835979$			
N	0.006207	0.010885	0.072338
C	0.048547	0.020833	1.454412
C	1.398037	0.006734	1.859049
N	2.095834	-0.008949	0.614315
C	1.237673	-0.006035	-0.413172
N	2.066924	0.004084	2.969116
Si	1.403895	-0.003104	4.544454
C	0.361829	-1.547326	4.866629
C	3.538124	-0.034021	0.548989
C	-1.205214	0.042917	-0.719857
C	2.820872	0.031091	5.775271
C	0.297670	1.496277	4.867811
H	-0.851444	0.034014	2.042921
H	1.496695	-0.013911	-1.458383
H	3.855101	-0.038345	-0.494547
H	3.939172	0.840430	1.063161
H	3.909470	-0.922682	1.061347
H	-0.082572	1.494541	5.895000
H	0.853172	2.427028	4.716457
H	-0.566347	1.515788	4.195382
H	-0.039707	-1.553505	5.885626
H	-0.485249	-1.609814	4.175342

H	0.961809	-2.453149	4.735242
H	2.459746	0.006126	6.808547
H	3.482350	-0.827241	5.624645
H	3.419466	0.937886	5.646067
H	-0.947353	-0.034384	-1.775863
H	-1.846521	-0.795908	-0.445146
H	-1.738475	0.979098	-0.545682

XYZ coordinates and total energies of 2 and 4 with different P-R substituent at different level of theory

4 X: P-CF₃

*E(B3LYP/6-311+G**)* = -983.996579

C	0.031657	0.005652	0.003442
N	0.014253	0.002159	1.379206
C	1.275290	0.038962	1.920067
N	2.074311	0.047203	0.818611
C	1.341835	0.026611	-0.383018
C	-1.195116	-0.033108	2.191197
C	3.525881	0.139754	0.923734
P	1.874381	0.051818	-2.112076
C	2.547396	-1.718594	-2.349453
H	3.172009	0.599179	-1.940435
F	3.246347	-1.771946	-3.508780
F	3.368639	-2.183350	-1.377803
F	1.529281	-2.600058	-2.450185
H	3.886562	1.078222	0.494624
H	3.769051	0.117384	1.983298
H	4.006926	-0.698049	0.419373
H	-1.835372	0.822994	1.965506
H	-1.751766	-0.956523	2.014347
H	-0.889440	0.009488	3.234156
H	-0.860550	-0.006635	-0.602476

$E(\omega B97X-D/6-311+G^{**}) = -983.778645$

N	0.006401	-0.000079	0.012278
C	-0.000296	0.023341	1.385358
C	1.297985	0.024928	1.783818
N	2.043497	0.003237	0.603548
C	1.269199	-0.020611	-0.509505
P	2.021986	0.140779	3.435954
C	1.981653	-1.689747	3.918270
F	0.803112	-2.302347	3.731572
C	3.493969	-0.032465	0.547399
C	-1.188538	-0.014156	-0.809909
F	2.897824	-2.377247	3.213128
F	2.290876	-1.821224	5.220545
H	-1.776673	-0.914138	-0.616907
H	-1.800944	0.868801	-0.613562
H	-0.869373	-0.008313	-1.849935
H	3.775681	-0.017731	-0.503050
H	3.921745	0.837083	1.051528
H	3.875543	-0.944170	1.012387
H	-0.904440	0.031890	1.973081
H	0.818834	0.430555	4.119339

2 X: P-CF₃

$E(B3LYP/6-311+G^{**}) = -984.013698$

C	0.036592	-0.039473	0.018603
N	-0.020426	0.001123	1.349972
C	1.246697	-0.059185	1.907341
C	2.153287	-0.143257	0.840272
N	1.333305	-0.126244	-0.313180
C	1.411918	-0.027657	3.389058
P	3.930315	-0.258398	0.543173
C	4.579067	-0.248617	2.295868
F	4.181054	-1.289436	3.102810

C	1.836725	-0.194828	-1.676674
F	5.934031	-0.332250	2.235148
F	4.312141	0.875961	3.042227
H	-0.874738	0.067090	1.882324
H	-0.795865	-0.008014	-0.660731
H	0.997239	-0.163033	-2.370438
H	2.507105	0.647191	-1.861798
H	2.399593	-1.120778	-1.812655
H	2.015145	0.824638	3.708480
H	0.434821	0.045448	3.875159
H	1.908632	-0.927487	3.757760

$$E(\omega B97X-D/6-311+G^{**}) = -983.787617$$

N	0.005638	-0.000019	0.009486
C	0.007612	0.000087	1.386369
C	1.323695	0.000080	1.821239
N	2.068426	0.000003	0.637755
C	1.256164	-0.000052	-0.428126
P	2.162586	0.000070	3.401231
C	0.604224	-0.000535	4.426737
F	-0.219971	1.074159	4.250292
C	3.516981	-0.000142	0.592840
C	-1.185332	0.000480	-0.821775
F	-0.219260	-1.075719	4.250030
F	0.935571	-0.000586	5.733673
H	-1.778610	-0.889302	-0.609669
H	-1.775695	0.892991	-0.612991
H	-0.893801	-0.002017	-1.871191
H	3.846415	-0.000188	-0.445709
H	3.896099	0.887303	1.103910
H	3.895926	-0.887640	1.103947
H	-0.908978	0.000111	1.948027

H 1.565323 -0.000085 -1.459123

4 X: P-Cl

$E(B3LYP/6-311+G^{**}) = -1106.502735$

N -0.003106 -0.006524 0.003052

C -0.005568 0.032274 1.378972

N 1.319297 0.065906 1.677964

C 2.137401 0.048768 0.534587

C 1.266592 0.007304 -0.520438

C 1.807142 0.117398 3.051009

P 3.927219 0.054763 0.355837

Cl 4.487056 1.955818 1.186062

C -1.225699 -0.058279 -0.788490

H 1.475102 -0.011800 -1.578581

H 4.219661 -0.665576 1.544866

H -2.063981 -0.032163 -0.096031

H -1.284395 0.800053 -1.461760

H -1.267778 -0.979953 -1.373825

H 0.935421 0.161967 3.699446

H 2.387629 -0.776885 3.290396

H 2.427600 1.001734 3.205209

$E(\omega B97X-D/6-311+G^{**}) = -1106.360198$

C 0.001593 0.002792 0.001575

N 0.005936 0.004131 1.371195

C 1.272231 0.002624 1.893368

N 2.047256 -0.003055 0.783249

C 1.302498 -0.004547 -0.399566

C -1.188101 -0.000751 2.195319

C 3.497216 -0.000673 0.845247

P 1.836739 -0.024340 -2.110468

Cl 2.882203 1.799050 -2.280248

H	-0.901397	0.006923	-0.588988
H	2.998858	-0.811083	-1.916600
H	-0.869242	0.067999	3.233201
H	-1.823212	0.853945	1.953091
H	-1.752318	-0.924811	2.050698
H	3.773840	0.014719	1.896975
H	3.905692	-0.900057	0.378150
H	3.900610	0.881466	0.344824

4 X: P-Cl

$E(B3LYP/6-311+G^{**}) = -1106.507333$

N	-0.016952	-0.000005	-0.014958
C	-0.034229	0.000009	1.366275
C	1.286995	0.000047	1.819923
N	2.052434	-0.000104	0.635997
C	1.243918	-0.000195	-0.445014
P	2.069773	0.000165	3.422908
Cl	0.239269	0.000095	4.573123
C	-1.200094	0.000051	-0.867817
H	1.561988	-0.000349	-1.472509
C	3.503575	-0.000122	0.617425
H	-0.951209	0.000083	1.925649
H	3.858923	-0.000277	-0.412443
H	3.875431	0.887832	1.136432
H	3.875402	-0.887941	1.136681
H	-0.892327	0.000030	-1.912349
H	-1.797746	-0.890271	-0.667542
H	-1.797670	0.890428	-0.667558

$E(\omega B97X-D/6-311+G^{**}) = -1106.361483$

C	0.005313	0.000222	0.004259
N	0.001374	-0.000005	1.328783

C	1.299758	0.000122	1.790875
C	2.148979	0.000158	0.691175
N	1.282649	0.000224	-0.407268
C	-1.181373	-0.000226	2.170639
P	3.912785	0.000228	0.459146
Cl	4.399326	0.000355	2.533289
C	1.736153	0.000328	-1.780889
H	-0.862631	0.000265	-0.632434
H	1.532513	0.000098	2.840351
H	0.877682	0.000337	-2.451647
H	2.347530	0.888839	-1.959857
H	2.347607	-0.888107	-1.959973
H	-2.071002	-0.000171	1.542352
H	-1.182535	-0.891306	2.798964
H	-1.182630	0.890655	2.799244

2 X: P-F

$E(B3LYP/6-311+G^{**}) = -746.150539$

N	-0.003632	-0.011210	0.001029
C	-0.007418	0.018611	1.377773
N	1.316468	0.061915	1.676627
C	2.136397	0.068170	0.533907
C	1.266530	0.028414	-0.521318
C	1.810377	0.124707	3.046937
P	3.927451	0.107946	0.376717
F	4.296259	1.523305	1.168726
C	-1.224903	-0.072040	-0.791659
H	1.475555	0.026480	-1.579590
H	4.208591	-0.731699	1.493894
H	-2.063967	-0.065810	-0.099625
H	-1.296728	0.792616	-1.455623
H	-1.253442	-0.987757	-1.387124
H	0.943037	0.172726	3.701048

H	2.395635	-0.765790	3.289070
H	2.431386	1.011070	3.188165

$E(\omega B97X-D/6-311+G^{**}) = -745.995903$

C	0.001499	-0.011619	0.002671
N	0.005146	-0.008059	1.372112
C	1.272354	0.003964	1.895009
N	2.045990	-0.008092	0.785083
C	1.302519	-0.019591	-0.398938
C	-1.188988	0.006356	2.196046
C	3.496216	0.009658	0.837179
P	1.855609	-0.055748	-2.101467
F	2.764415	1.318303	-2.171929
H	-0.901638	-0.010073	-0.587932
H	2.958410	-0.927068	-1.891016
H	-0.870144	-0.049676	3.234707
H	-1.752310	0.929226	2.040880
H	-1.824628	-0.851061	1.964488
H	3.782495	0.101081	1.882503
H	3.908348	-0.917061	0.430408
H	3.886029	0.856720	0.270227

4 X: P-F

$E(B3LYP/6-311+G^{**}) = -746.146584$

N	-0.047387	-0.031365	-0.126521
C	-0.116222	-0.232286	1.264967
C	1.222683	-0.249102	1.673769
N	2.013104	-0.064686	0.557204
C	1.242604	0.065545	-0.522616
P	-1.640099	-0.406941	2.156559
F	-0.882913	-0.598922	3.666259

C	-1.218690	0.053300	-0.975704
H	1.637895	-0.375445	2.656507
C	3.470489	-0.020359	0.560558
H	3.829891	0.137555	-0.455176
H	3.812410	0.798371	1.195401
H	3.866663	-0.963045	0.940888
H	-0.917105	0.210116	-2.010796
H	-1.795224	-0.873485	-0.896257
H	-1.849818	0.884271	-0.645861
H	1.585869	0.219575	-1.530033

$E(\omega B97X-D/6-311+G^{**}) = -745.987823$

C	0.004162	-0.000288	0.002558
N	0.006632	-0.000179	1.347502
C	1.316810	0.000023	1.831306
C	2.104990	-0.000090	0.683237
N	1.264056	-0.000197	-0.407630
C	-1.151770	-0.000012	2.210968
P	1.712060	0.000392	3.555548
F	3.381739	0.000449	3.294280
C	1.699787	-0.000749	-1.792294
H	3.175321	0.000284	0.584499
H	0.828082	0.000775	-2.445185
H	2.299224	0.889136	-1.986936
H	2.296364	-0.892501	-1.987215
H	-2.061871	-0.000518	1.612211
H	-1.126672	-0.888456	2.848631
H	-1.127103	0.889044	2.847795
H	-0.868505	-0.000633	-0.627262

4 X: P-CH₃

$E(B3LYP/6-311+G^{**}) = -686.183688$

N	0.080641	0.066061	0.036636
C	0.233151	-0.045015	1.405873
C	1.533286	-0.379520	1.644625
N	2.119140	-0.463285	0.366601
C	1.240104	-0.197401	-0.641416
P	2.254230	-0.616301	3.302715
C	3.481549	0.789218	3.434923
C	3.496953	-0.847745	0.097475
C	-1.166782	0.411197	-0.628994
H	-0.571873	0.111358	2.106069
H	4.087493	0.629254	4.330587
H	4.144118	0.890152	2.574685
H	2.928041	1.721012	3.565178
H	3.621207	-0.860340	-0.982960
H	4.199577	-0.132647	0.531350
H	3.710087	-1.842029	0.496897
H	-1.943788	-0.322572	-0.399482
H	-1.508551	1.402853	-0.321278
H	-0.977672	0.412087	-1.700325
H	3.185393	-1.636946	2.962723

$E(\omega B97X-D/6-311+G^{**}) = -686.046411$

C	0.019767	0.013358	0.000216
N	0.016738	0.009773	1.363264
C	1.287447	-0.009851	1.894210
C	2.157424	-0.005911	0.852360
N	1.347175	0.009591	-0.288862
C	-1.198089	0.008752	2.153297
P	3.965618	0.035008	0.993652
C	4.369379	1.713894	0.311318
C	1.832884	-0.040233	-1.653187

H	1.483472	-0.029269	2.954747
H	5.452731	1.789740	0.190406
H	3.891142	1.932655	-0.643963
H	4.058231	2.465249	1.039515
H	0.961253	-0.059452	-2.303819
H	2.438441	0.837339	-1.889292
H	2.428994	-0.940189	-1.820842
H	-1.274946	-0.907849	2.743202
H	-1.220943	0.871254	2.823611
H	-2.038367	0.064701	1.464198
H	4.261961	-0.716707	-0.171807

4 X: P-CH₃

*E(B3LYP/6-311+G**)* = -686.178692

C	0.058471	0.000072	-0.078727
C	0.018800	0.000541	1.324329
N	1.386036	0.000774	1.687204
C	2.172109	0.000898	0.588658
N	1.380889	0.000389	-0.484191
P	-1.279364	0.001138	2.533089
C	1.839532	-0.000574	-1.870313
H	3.247784	0.000336	0.580108
C	1.844384	0.002142	3.062124
C	-2.723277	0.000210	1.326666
H	-0.741799	0.000274	-0.795510
H	-3.640876	0.000484	1.919991
H	-2.744461	0.890544	0.687956
H	-2.744266	-0.890935	0.689084
H	2.934063	0.001433	3.086099
H	1.458298	0.887735	3.574398
H	1.457160	-0.881760	3.576423

H	0.966701	0.000851	-2.519724
H	2.434443	0.890681	-2.075376
H	2.431450	-0.893866	-2.075226

$E(\omega B97X-D/6-311+G^{**}) = -686.038478$

N	0.002061	0.009439	0.015064
C	0.005620	-0.032561	1.394417
C	1.331639	-0.006023	1.832454
N	2.068829	0.052435	0.637863
C	1.250610	0.060265	-0.424362
P	2.113079	-0.030499	3.416271
C	0.536449	-0.108321	4.417288
C	3.512849	0.096840	0.599805
C	-1.185616	-0.001126	-0.816783
H	1.554665	0.100574	-1.456331
H	-0.911463	-0.076829	1.954139
H	0.811481	-0.132243	5.474372
H	-0.103069	0.768607	4.263300
H	-0.049726	-1.010953	4.209103
H	3.851718	0.137345	-0.435436
H	3.861295	0.977632	1.144867
H	3.914191	-0.791960	1.093014
H	-1.806368	0.864601	-0.581900
H	-0.893573	0.039479	-1.865497
H	-1.752733	-0.915244	-0.635822

4 X: P-Bu

$E(B3LYP/6-311+G^{**}) = -804.152940$

C	-0.005596	-0.498049	0.394431
C	0.385152	-0.962531	1.616614
N	1.554288	-0.304263	1.952253

C	1.952277	0.582362	0.988346
N	0.981963	0.440657	0.041081
C	2.296935	-0.521777	3.184630
C	1.014083	1.189797	-1.208975
P	-1.379451	-1.005747	-0.701345
C	-2.920093	-0.093017	-0.025150
C	-2.772502	1.406120	-0.335546
C	-4.113069	-0.672503	-0.808290
C	-3.130686	-0.297760	1.480155
H	-1.625336	-2.243812	-0.048408
H	0.186167	1.900594	-1.266049
H	1.955303	1.734325	-1.232479
H	0.957565	0.513070	-2.064003
H	1.687671	-0.265911	4.055640
H	2.616122	-1.564218	3.265364
H	3.173345	0.122173	3.157304
H	-0.073446	-1.704356	2.250236
H	-4.023623	0.245395	1.812557
H	-3.275158	-1.354145	1.725142
H	-2.280992	0.072971	2.057821
H	-3.679729	1.941095	-0.033679
H	-1.934087	1.848299	0.209718
H	-2.622031	1.584914	-1.404085
H	-5.038870	-0.172684	-0.502636
H	-3.996215	-0.530994	-1.886375
H	-4.240117	-1.743116	-0.619859

$E(\omega B97X-D/6-311+G^{**}) = -803.985765$

N	-0.039201	0.009071	0.042885
C	-0.018285	-0.030885	1.440371
C	1.299502	-0.009637	1.767133
N	2.008822	0.044944	0.586892

C	1.200561	0.061240	-0.510378
P	-1.507050	-0.168022	2.476703
C	-1.794125	1.607984	3.058309
C	-0.571182	2.218515	3.744189
C	3.455021	0.079206	0.505815
C	-1.244266	-0.013980	-0.765265
C	-2.180566	2.455407	1.840588
C	-2.968846	1.543798	4.043657
H	-0.827649	-0.622450	3.635075
H	-1.824127	0.902045	-0.630770
H	-0.933757	-0.092788	-1.804913
H	-1.867945	-0.870047	-0.499731
H	3.847931	0.973970	0.995038
H	3.888719	-0.807560	0.974435
H	3.724319	0.097889	-0.548304
H	1.771250	-0.034283	2.736685
H	-0.795093	3.242214	4.066142
H	-0.281628	1.645964	4.630628
H	0.285960	2.260437	3.067621
H	-2.440755	3.469608	2.162148
H	-1.350563	2.535487	1.132040
H	-3.046274	2.039617	1.316001
H	-3.207528	2.549310	4.406727
H	-3.866797	1.133106	3.573218
H	-2.729200	0.926714	4.915688

2 X: P-Bu

$E(B3LYP/6-311+G^{**}) = -804.145778$

N	0.149249	-0.245053	0.053597
C	0.010609	0.112302	1.344598
N	1.225239	0.302276	1.855045

C	2.174945	0.064206	0.877847
C	1.522089	-0.295458	-0.313162
C	1.512570	0.699451	3.226506
P	1.949657	-0.747980	-1.981509
C	3.866899	-0.677121	-1.990063
C	4.411711	0.736574	-1.716396
C	-0.940492	-0.543044	-0.856683
C	4.504846	-1.699321	-1.031734
C	4.246764	-1.068158	-3.432970
H	3.219818	0.166754	1.099554
H	-0.918976	0.225338	1.873975
H	-1.890422	-0.432251	-0.333335
H	-0.899070	0.137337	-1.711052
H	-0.833730	-1.563846	-1.232394
H	5.336892	-1.060426	-3.553602
H	3.885920	-2.070623	-3.681262
H	3.820953	-0.369694	-4.159351
H	5.507330	0.749760	-1.800200
H	4.008393	1.452504	-2.436745
H	4.154227	1.099468	-0.718397
H	5.600093	-1.676582	-1.118248
H	4.253925	-1.507119	0.014255
H	4.167606	-2.711945	-1.266214
H	0.577704	0.814191	3.773397
H	2.121938	-0.064141	3.713013
H	2.050980	1.648774	3.232081

$$E(\omega B97X-D/6-311+G^{**}) = -803.973428$$

C	-0.008312	-0.000107	-0.008135
N	-0.002688	0.000000	1.401500
C	1.250209	0.000018	1.875262
N	2.081054	0.000006	0.845359

C	1.352219	0.000014	-0.326250
C	-1.202906	-0.000156	2.208268
C	3.528977	0.000912	0.924172
P	-1.567973	-0.000448	-0.854414
C	-1.048905	-0.000562	-2.679866
C	-2.378459	-0.000730	-3.452095
C	-0.270871	1.260737	-3.079213
C	-0.270655	-1.261779	-3.079044
H	1.852091	-0.000213	-1.276779
H	1.532910	0.000109	2.914033
H	-0.930281	0.000090	3.263838
H	-1.798618	0.884412	1.970693
H	-1.798244	-0.885057	1.971010
H	-2.187916	-0.000680	-4.532152
H	-2.975755	-0.885741	-3.212607
H	-2.975977	0.884111	-3.212553
H	-0.043521	1.246380	-4.153738
H	-0.857923	2.158007	-2.867469
H	0.675917	1.358579	-2.541965
H	-0.043408	-1.247585	-4.153593
H	0.676225	-1.359289	-2.541898
H	-0.857485	-2.159137	-2.867052
H	3.834641	-0.002556	1.969749
H	3.923669	-0.888107	0.430607
H	3.922418	0.893876	0.436737

4 X: P-Ph

$E(B3LYP/6-311+G^{**}) = -877.963436$

C	-0.007689	0.315242	0.103850
C	0.093338	0.039841	1.473100
C	1.326660	-0.383068	1.985148
C	2.434521	-0.516665	1.150002

C	2.326869	-0.229057	-0.209551
C	1.102280	0.188554	-0.728881
P	-1.413569	0.072003	2.552517
C	-2.177259	1.675658	2.161060
C	-3.455577	1.835706	1.711998
N	-3.655872	3.188423	1.521798
C	-2.546457	3.930695	1.834605
N	-1.651947	2.979294	2.221622
C	-4.898185	3.781120	1.048139
C	-0.309424	3.316849	2.675160
H	-4.213065	1.090996	1.526196
H	1.429407	-0.602866	3.043158
H	3.383441	-0.839236	1.564349
H	3.189775	-0.327656	-0.858246
H	1.009445	0.416666	-1.785034
H	-0.954123	0.643359	-0.313157
H	-0.740482	0.441644	3.749421
H	-0.199084	4.394518	2.578492
H	-0.170551	3.032915	3.721398
H	0.443391	2.812790	2.066650
H	-4.750532	4.857924	1.002146
H	-5.150810	3.407766	0.052354
H	-5.719742	3.557738	1.733613

$$E(\omega B97X-D/6-3II+G^{**}) = -877.757904$$

C	0.005673	0.004172	0.002153
C	-0.003022	0.011236	1.359985
N	1.345783	0.026813	1.729565
C	2.186927	0.034460	0.664910
N	1.323755	0.016395	-0.392564
P	-1.474203	-0.090449	2.407062
C	-1.115724	-1.617462	3.379020

C	-1.480998	-1.696252	4.723869
C	-1.270653	-2.865266	5.445057
C	-0.694547	-3.971257	4.830794
C	-0.334484	-3.902499	3.490067
C	-0.547760	-2.734997	2.767060
C	1.825713	0.052426	3.098294
C	1.763764	0.028687	-1.773566
H	-0.820917	-0.011321	-0.690831
H	-1.925933	-0.838007	5.218616
H	-1.551789	-2.908359	6.491527
H	-0.524095	-4.881482	5.394403
H	0.120615	-4.758537	3.004440
H	-0.249089	-2.687224	1.724474
H	-1.077303	0.829884	3.410641
H	2.912372	0.081425	3.058021
H	1.459132	0.940561	3.618536
H	1.500708	-0.838471	3.639501
H	2.847429	-0.069630	-1.774225
H	1.323197	-0.806734	-2.322549
H	1.486628	0.966471	-2.261310

4 X: P-Ph

$E(B3LYP/6-311+G^{**}) = -877.963331$

N	0.085331	0.170085	-0.008361
H	-0.057421	-0.157235	2.127115
C	0.540583	-0.081022	1.236355
C	2.741821	-0.490507	2.302082
N	1.865475	-0.213637	1.170969
C	2.278664	-0.052849	-0.136822
C	1.154640	0.193360	-0.934061
P	0.851173	0.447437	-2.673418

C	2.610537	0.491467	-3.258810
C	3.534250	1.460997	-2.827535
C	4.824874	1.516581	-3.348406
C	5.223344	0.617614	-4.339780
C	4.316691	-0.336299	-4.797239
C	3.031104	-0.401425	-4.258231
C	-1.303503	0.375764	-0.375969
H	3.313732	-0.135567	-0.413534
H	2.339055	-1.158597	-4.611611
H	4.611266	-1.038512	-5.570542
H	6.224203	0.667319	-4.754592
H	5.515633	2.276481	-2.996306
H	3.227306	2.190552	-2.085070
H	-1.921780	0.376141	0.521719
H	-1.399988	1.330892	-0.898397
H	-1.629968	-0.417699	-1.053080
H	2.146936	-0.560212	3.211691
H	3.265900	-1.434037	2.141652
H	3.470928	0.314017	2.409971

$E(\omega B97X-D/6-311+G^{**}) = -877.753111$

C	0.036638	-0.440116	0.351137
C	0.055185	0.161407	1.614981
C	1.294441	0.562974	2.125636
C	2.470944	0.361666	1.409981
C	2.432362	-0.248272	0.161189
C	1.209615	-0.648085	-0.367588
P	-1.507372	0.424616	2.580310
C	-1.488114	-1.188847	3.325164
N	-2.480195	-1.599885	4.225495
C	-2.245103	-2.851766	4.648145
N	-1.136559	-3.281083	4.061666

C	-0.640926	-2.290816	3.242397
C	-3.587143	-0.760463	4.627349
C	-0.538573	-4.590448	4.243014
H	-2.849208	-3.410896	5.341802
H	0.258053	-2.426848	2.667154
H	-0.915605	-0.749543	-0.067842
H	1.168958	-1.117258	-1.345396
H	3.347718	-0.404519	-0.399787
H	3.419005	0.684952	1.827630
H	1.329280	1.038303	3.100600
H	-4.206387	-1.293866	5.348404
H	-3.198378	0.158595	5.072711
H	-4.178519	-0.493717	3.748141
H	-1.130864	-5.163335	4.955466
H	-0.512526	-5.117171	3.288438
H	0.476630	-4.479563	4.625370

4 X: P-^tBu

$E(B3LYP/6-311+G^{**}) = -804.152940$

C	-0.005596	-0.498049	0.394431
C	0.385152	-0.962531	1.616614
N	1.554288	-0.304263	1.952253
C	1.952277	0.582362	0.988346
N	0.981963	0.440657	0.041081
C	2.296935	-0.521777	3.184630
C	1.014083	1.189797	-1.208975
P	-1.379451	-1.005747	-0.701345
C	-2.920093	-0.093017	-0.025150
C	-2.772502	1.406120	-0.335546
C	-4.113069	-0.672503	-0.808290
C	-3.130686	-0.297760	1.480155

H	-1.625336	-2.243812	-0.048408
H	0.186167	1.900594	-1.266049
H	1.955303	1.734325	-1.232479
H	0.957565	0.513070	-2.064003
H	1.687671	-0.265911	4.055640
H	2.616122	-1.564218	3.265364
H	3.173345	0.122173	3.157304
H	-0.073446	-1.704356	2.250236
H	-4.023623	0.245395	1.812557
H	-3.275158	-1.354145	1.725142
H	-2.280992	0.072971	2.057821
H	-3.679729	1.941095	-0.033679
H	-1.934087	1.848299	0.209718
H	-2.622031	1.584914	-1.404085
H	-5.038870	-0.172684	-0.502636
H	-3.996215	-0.530994	-1.886375
H	-4.240117	-1.743116	-0.619859

$E(\omega B97X-D/6-311+G^{**}) = -803.985765$

N	-0.039201	0.009071	0.042885
C	-0.018285	-0.030885	1.440371
C	1.299502	-0.009637	1.767133
N	2.008822	0.044944	0.586892
C	1.200561	0.061240	-0.510378
P	-1.507050	-0.168022	2.476703
C	-1.794125	1.607984	3.058309
C	-0.571182	2.218515	3.744189
C	3.455021	0.079206	0.505815
C	-1.244266	-0.013980	-0.765265
C	-2.180566	2.455407	1.840588
C	-2.968846	1.543798	4.043657
H	-0.827649	-0.622450	3.635075

H	-1.824127	0.902045	-0.630770
H	-0.933757	-0.092788	-1.804913
H	-1.867945	-0.870047	-0.499731
H	3.847931	0.973970	0.995038
H	3.888719	-0.807560	0.974435
H	3.724319	0.097889	-0.548304
H	1.771250	-0.034283	2.736685
H	-0.795093	3.242214	4.066142
H	-0.281628	1.645964	4.630628
H	0.285960	2.260437	3.067621
H	-2.440755	3.469608	2.162148
H	-1.350563	2.535487	1.132040
H	-3.046274	2.039617	1.316001
H	-3.207528	2.549310	4.406727
H	-3.866797	1.133106	3.573218
H	-2.729200	0.926714	4.915688

2 X: P-^tBu

$E(B3LYP/6-311+G^{**}) = -804.145778$

N	0.149249	-0.245053	0.053597
C	0.010609	0.112302	1.344598
N	1.225239	0.302276	1.855045
C	2.174945	0.064206	0.877847
C	1.522089	-0.295458	-0.313162
C	1.512570	0.699451	3.226506
P	1.949657	-0.747980	-1.981509
C	3.866899	-0.677121	-1.990063
C	4.411711	0.736574	-1.716396
C	-0.940492	-0.543044	-0.856683
C	4.504846	-1.699321	-1.031734
C	4.246764	-1.068158	-3.432970
H	3.219818	0.166754	1.099554

H	-0.918976	0.225338	1.873975
H	-1.890422	-0.432251	-0.333335
H	-0.899070	0.137337	-1.711052
H	-0.833730	-1.563846	-1.232394
H	5.336892	-1.060426	-3.553602
H	3.885920	-2.070623	-3.681262
H	3.820953	-0.369694	-4.159351
H	5.507330	0.749760	-1.800200
H	4.008393	1.452504	-2.436745
H	4.154227	1.099468	-0.718397
H	5.600093	-1.676582	-1.118248
H	4.253925	-1.507119	0.014255
H	4.167606	-2.711945	-1.266214
H	0.577704	0.814191	3.773397
H	2.121938	-0.064141	3.713013
H	2.050980	1.648774	3.232081

$E(\omega B97X-D/6-311+G^{**}) = -803.973428$

C	-0.008312	-0.000107	-0.008135
N	-0.002688	0.000000	1.401500
C	1.250209	0.000018	1.875262
N	2.081054	0.000006	0.845359
C	1.352219	0.000014	-0.326250
C	-1.202906	-0.000156	2.208268
C	3.528977	0.000912	0.924172
P	-1.567973	-0.000448	-0.854414
C	-1.048905	-0.000562	-2.679866
C	-2.378459	-0.000730	-3.452095
C	-0.270871	1.260737	-3.079213
C	-0.270655	-1.261779	-3.079044
H	1.852091	-0.000213	-1.276779
H	1.532910	0.000109	2.914033

H	-0.930281	0.000090	3.263838
H	-1.798618	0.884412	1.970693
H	-1.798244	-0.885057	1.971010
H	-2.187916	-0.000680	-4.532152
H	-2.975755	-0.885741	-3.212607
H	-2.975977	0.884111	-3.212553
H	-0.043521	1.246380	-4.153738
H	-0.857923	2.158007	-2.867469
H	0.675917	1.358579	-2.541965
H	-0.043408	-1.247585	-4.153593
H	0.676225	-1.359289	-2.541898
H	-0.857485	-2.159137	-2.867052
H	3.834641	-0.002556	1.969749
H	3.923669	-0.888107	0.430607
H	3.922418	0.893876	0.436737

4 X: P-Si(CH₃)₃

$E(B3LYP/6-311+G^{**}) = -1055.599404$

N	0.368679	0.483969	0.647801
C	0.463281	-0.644405	1.483202
C	1.722003	-1.125402	1.273869
N	2.333171	-0.288472	0.353455
C	1.510047	0.715707	-0.067338
P	-0.763690	-1.366539	2.633369
Si	-0.529808	-0.079418	4.529191
C	1.115411	-0.588560	5.301153
C	3.692110	-0.460018	-0.136447
C	-0.828615	1.287950	0.451874
C	-0.542117	1.786445	4.232776
C	-1.966403	-0.559251	5.659534
H	-1.929766	-0.737721	2.121045

H	-1.176318	1.713651	1.394400
H	-0.565321	2.091161	-0.232669
H	-1.632691	0.691859	0.012276
H	4.412332	-0.387918	0.682998
H	3.806553	-1.429771	-0.628095
H	3.884473	0.332948	-0.856054
H	2.206114	-1.991074	1.696492
H	1.278277	-0.054595	6.243045
H	1.141907	-1.660743	5.514873
H	1.953900	-0.355883	4.638600
H	-0.361500	2.314053	5.175860
H	0.237631	2.090127	3.529455
H	-1.505417	2.128295	3.844225
H	-1.881893	-0.044829	6.622523
H	-2.931785	-0.286161	5.223496
H	-1.979568	-1.634797	5.856496

$E(\omega B97X-D/6-311+G^{**}) = -1055.420455$

C	-0.000497	0.124318	0.105386
N	0.008232	0.022581	1.463413
C	1.298437	-0.036836	1.999289
C	2.125351	0.037724	0.925738
N	1.324791	0.145907	-0.194849
C	-1.215741	-0.119274	2.226083
P	1.822289	-0.078782	3.744802
Si	1.711610	2.156183	4.191632
C	1.906313	2.374211	6.047230
C	1.830452	0.251633	-1.548096
C	3.164333	2.908714	3.272104
C	0.117637	2.953387	3.600282
H	0.588013	-0.463609	4.323555
H	-1.294093	0.654998	2.991039

H	-2.042826	-0.020833	1.526294
H	-1.262774	-1.100848	2.704308
H	2.447429	1.146705	-1.660214
H	2.423539	-0.628747	-1.807665
H	0.973035	0.318039	-2.214807
H	3.202732	0.016527	0.880981
H	3.195940	3.992298	3.422358
H	4.114717	2.490856	3.615734
H	3.078768	2.721745	2.197587
H	0.177420	4.040280	3.719221
H	-0.059827	2.742523	2.541765
H	-0.746662	2.604713	4.172191
H	1.939861	3.437461	6.305325
H	1.071125	1.926254	6.593277
H	2.830349	1.913095	6.406878

2 X: P-Si(CH₃)₃

E(B3LYP/6-311+G**) = -1055.603722

N	-0.048697	-0.235215	0.166011
C	-0.092276	0.166778	1.449059
N	1.158529	0.363056	1.865115
C	2.029149	0.081951	0.828906
C	1.292755	-0.310287	-0.293801
C	1.546291	0.803904	3.198756
P	1.628001	-0.822832	-1.974831
Si	3.872134	-0.725319	-2.041588
C	4.601159	1.012373	-1.763408
C	-1.206883	-0.553240	-0.652128
C	4.756459	-1.910433	-0.840474
C	4.330670	-1.257466	-3.801994
H	3.090554	0.178934	0.963022

H	-0.979735	0.307088	2.040718
H	-2.113189	-0.413807	-0.062424
H	-1.224310	0.096642	-1.529428
H	-1.137598	-1.586587	-0.998094
H	5.416739	-1.240686	-3.942873
H	3.980264	-2.272015	-4.012639
H	3.885036	-0.590836	-4.545938
H	5.692985	0.997180	-1.860565
H	4.205019	1.712599	-2.504296
H	4.363205	1.416802	-0.775002
H	5.843570	-1.857466	-0.971376
H	4.539211	-1.688406	0.208636
H	4.442938	-2.941703	-1.025682
H	0.653175	0.945512	3.805824
H	2.182946	0.051598	3.667208
H	2.089565	1.748052	3.133838

$E(\omega B97X-D/6-311+G^{**}) = -1055.420301$

C	-0.033630	-0.000452	-0.015465
N	-0.006274	0.000058	1.392073
C	1.253108	0.000486	1.843988
N	2.067514	0.000417	0.798819
C	1.315114	-0.000035	-0.356038
C	-1.192575	0.000093	2.223183
C	3.517164	0.001360	0.853753
P	-1.598657	-0.001385	-0.875197
Si	-0.862054	0.000789	-2.976662
C	-2.395215	0.000254	-4.072707
C	0.157027	1.529618	-3.437743
C	0.159499	-1.525526	-3.440664
H	1.789802	-0.000280	-1.320744
H	1.556618	0.000894	2.876919

H	-0.895154	0.000912	3.272038
H	-1.792277	0.884147	1.999067
H	-1.791588	-0.884723	2.000246
H	-2.111778	0.004481	-5.130444
H	-3.009302	-0.886254	-3.890364
H	-3.014404	0.881973	-3.884523
H	0.498994	1.470984	-4.477200
H	-0.455225	2.429764	-3.331546
H	1.037676	1.661764	-2.802325
H	0.499644	-1.465243	-4.480626
H	1.041516	-1.656436	-2.806885
H	-0.450632	-2.427082	-3.334252
H	3.839372	-0.001135	1.894330
H	3.904258	-0.888217	0.355422
H	3.903116	0.893928	0.359888

XYZ coordinates and total energies of the thiazol analogues (1'-4')

1' X:O

$E(B3LYP/6-311+G^{**}) = -644.391221$

C	-0.252187	-0.000505	-0.030244
N	-0.064473	-0.000608	1.337974
C	1.247068	0.000209	1.796448
C	2.161642	0.001299	0.813996
S	1.405024	0.001157	-0.774894
O	-1.303583	-0.001376	-0.621946
H	3.233639	0.002221	0.922153
H	1.433997	0.000078	2.859532
H	-0.873763	-0.002051	1.941374

2' X:O

$E(B3LYP/6-311+G^{**}) = -644.356500$

C	-0.290559	0.000421	-0.045588
C	0.058409	0.000292	1.309096

N	1.409655	-0.000398	1.569517
C	2.255482	-0.000661	0.548315
S	1.457349	-0.000218	-0.953621
H	3.323341	-0.001104	0.698896
H	1.745445	-0.000380	2.523199
O	-1.317979	0.000864	-0.674482
H	-0.647417	0.000031	2.122315

3' X:O

$E(B3LYP/6-311+G^{**}) = -644.293258$

S	-0.033421	0.165166	0.103612
C	-0.036172	0.166876	1.828214
N	1.210784	0.050536	2.257337
C	2.172638	-0.039095	1.219135
C	1.717903	0.002622	-0.066612
O	-1.034753	0.260522	2.721925
H	1.429214	0.031542	3.247027
H	-1.881046	0.338877	2.267227
H	3.202310	-0.135459	1.535575

4' X:O

$E(B3LYP/6-311+G^{**}) = -644.318933$

C	-0.207801	-0.125964	0.095482
C	0.043270	-0.132129	1.421787
N	1.397643	0.016451	1.704125
C	2.287943	0.145353	0.697148
S	1.329498	0.072931	-0.738938
O	-0.761988	-0.253407	2.505223
H	1.706911	0.026661	2.668431
H	-1.157616	-0.222599	-0.404590
H	-1.678151	-0.351262	2.226186

1' X:S

$$E(B3LYP/6-311+G^{**}) = -967.348393$$

C	-0.186473	-0.000544	-0.013851
N	-0.017136	-0.000924	1.345152
C	1.281132	0.000195	1.828115
C	2.205354	0.001411	0.851131
S	1.438539	0.001178	-0.727448
S	-1.626516	-0.001501	-0.830129
H	3.277516	0.002300	0.960210
H	1.450897	-0.000079	2.894138
H	-0.835947	-0.001610	1.937077

2' X:S

$$E(B3LYP/6-311+G^{**}) = -967.317690$$

C	-0.145764	0.000208	-0.096477
C	-0.030991	-0.000100	1.294238
N	1.359702	-0.000468	1.586648
C	2.210694	-0.000568	0.565151
S	1.380609	-0.000074	-0.902574
S	-1.187765	0.000097	2.522560
H	3.283516	-0.000884	0.670089
H	1.645408	-0.000654	2.559534
H	-1.059776	0.000578	-0.664602

3' X:S

$$E(B3LYP/6-311+G^{**}) = -967.262691$$

S	0.065531	0.029050	0.043576
C	0.008532	0.013734	1.768937
N	1.272565	-0.006167	2.203470
C	2.245532	-0.004504	1.198432
C	1.795477	0.038949	-0.099470
S	-1.345803	-0.116285	2.895894

H	1.490221	0.013017	3.193792
H	-2.060872	0.907411	2.383024
H	3.276276	-0.033619	1.525785

4' X:S

$E(B3LYP/6-311+G^{**}) = -967.289103$

C	-0.133261	-0.006628	-0.063167
C	0.002167	0.044578	1.279670
N	1.359058	0.029799	1.648630
C	2.320269	-0.045256	0.713966
S	1.453016	-0.086825	-0.793787
S	-1.277034	0.226642	2.497664
H	1.610372	0.085645	2.628174
H	-1.054421	-0.003541	-0.622488
H	-1.320457	-1.068379	2.886192

1' X:NH

$E(B3LYP/6-311+G^{**}) = -624.485092$

C	-0.278450	0.000235	0.010074
N	-0.071087	-0.000241	1.386394
C	1.252621	0.000328	1.814784
C	2.142976	0.001266	0.813370
S	1.343297	0.001417	-0.761238
N	-1.352148	-0.000963	-0.672647
H	3.217227	0.001658	0.891729
H	1.463158	-0.000152	2.873850
H	-0.851950	-0.001927	2.023728
H	-2.187228	-0.002135	-0.089157

2' X:NH

$E(B3LYP/6-311+G^{**}) = -624.447919$

C	-0.240603	0.000616	-0.207760
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C	-0.003522	0.000038	1.194840
N	1.323337	-0.000258	1.525908
C	2.215397	-0.000627	0.543717
S	1.431479	-0.000275	-0.989617
H	3.277967	-0.001030	0.714173
H	1.616569	-0.000416	2.494267
N	-1.269665	0.001283	-0.972228
H	-0.750990	-0.000099	1.970311
H	-2.132667	0.000764	-0.430824

3' X:NH

$E(B3LYP/6-311+G^{**}) = -624.425790$

S	-0.120006	0.171794	0.142896
C	0.013165	0.079413	1.840281
N	1.296059	-0.046991	2.209086
C	2.314318	-0.087567	1.229334
C	1.702343	0.018971	0.032012
N	-1.032514	0.071372	2.724304
H	2.105760	0.023592	-0.967330
H	1.537715	-0.135179	3.187875
H	-0.839250	0.356672	3.673698
H	-1.930406	0.371595	2.379321

4' X:NH

$E(B3LYP/6-311+G^{**}) = -624.448862$

C	-0.186945	-0.183228	0.149104
C	0.061823	-0.053025	1.472305
N	1.431499	0.129825	1.708308
C	2.310457	0.148366	0.684729
S	1.333271	-0.059641	-0.725220
N	-0.804391	-0.000960	2.569760
H	1.762292	0.290865	2.651567

H	-0.603001	-0.686769	3.288933
H	-1.137028	-0.359317	-0.328454
H	-1.779325	-0.049569	2.307990

1' X:PH

$E(B3LYP/6-311+G^{**}) = -911.078787$

C	-0.157163	-0.000257	-0.030739
N	-0.007005	-0.000661	1.338672
C	1.288207	0.000213	1.832404
C	2.222172	0.001258	0.869272
S	1.475043	0.001176	-0.727436
P	-1.609441	-0.000939	-0.982768
H	3.293185	0.001996	0.982590
H	1.447367	-0.000047	2.900360
H	-0.819475	-0.001244	1.936077
H	-2.454475	-0.002012	0.172453

2' X:PH

$E(B3LYP/6-311+G^{**}) = -911.047335$

C	-0.088950	0.000183	-0.266877
C	0.052131	0.000116	1.130675
N	1.346663	-0.000371	1.560855
C	2.298510	-0.000832	0.630301
S	1.581508	-0.000700	-0.939666
H	3.351794	-0.001222	0.848903
H	1.574805	-0.000362	2.547232
P	-1.499438	0.000993	-1.314355
H	-0.746786	0.000485	1.853587
H	-2.402936	0.001709	-0.207870

3' X:PH

$E(B3LYP/6-311+G^{**}) = -911.021444$

S	0.059469	-0.361237	-0.023237
C	-0.010884	-0.020314	1.636826
N	1.237428	0.258399	2.073318
C	2.322397	0.239596	1.202473
C	1.803364	-0.093691	-0.025160
P	-1.576768	-0.060044	2.602196
H	2.323250	-0.207551	-0.963983
H	1.381736	0.483326	3.050266
H	-1.020712	-0.671513	3.762262
H	-1.472095	1.256701	3.136516

4' X:PH

$E(B3LYP/6-311+G^{**}) = -911.049475$

C	0.036077	0.061213	0.017043
C	0.029035	-0.117401	1.358924
S	1.715879	-0.308549	1.864803
C	2.391529	-0.147019	0.284099
N	1.322210	0.038680	-0.519797
P	-1.487691	-0.143453	2.384689
H	-1.040488	0.735900	3.409868
H	-0.817119	0.210079	-0.629766
H	-1.189328	-1.313177	3.137577
H	1.468675	0.160603	-1.513358

1' X:CH₂

$E(B3LYP/6-311+G^{**}) = -608.418996$

C	-0.284749	-0.163559	0.074334
N	-0.048831	0.014132	1.437502
C	1.280153	0.077364	1.826429
C	2.152581	-0.038960	0.816956
S	1.312507	-0.242385	-0.733073

C	-1.480367	-0.258883	-0.532316
H	3.227939	-0.018967	0.864076
H	1.515472	0.210991	2.872053
H	-0.813393	0.078087	2.089088
H	-2.397689	-0.198716	0.039599
H	-1.555830	-0.396522	-1.600257

2' X:CH₂

$E(B3LYP/6-311+G^{**}) = -608.380110$

S	-0.090186	-0.287608	0.222111
C	0.066807	-0.146390	2.028687
C	1.457006	0.050166	2.293949
N	2.219473	0.075126	1.171893
C	1.623497	-0.079855	-0.007631
C	-0.989810	-0.225630	2.874572
H	2.141862	-0.079432	-0.948960
H	3.220891	0.207732	1.230965
H	1.915863	0.177277	3.259768
H	-0.832433	-0.133963	3.941371
H	-2.000076	-0.378929	2.523722

3' X:CH₂

$E(B3LYP/6-311+G^{**}) = -608.380265$

S	-0.090980	-0.127796	0.182534
C	-0.106548	-0.011798	1.898000
N	1.162891	0.100025	2.287580
C	2.114746	0.093306	1.252283
C	1.638828	-0.026006	-0.027978
C	-1.271325	-0.026088	2.833203
H	1.417007	0.183750	3.265411
H	-1.209746	-0.864097	3.535166
H	-2.201587	-0.127478	2.274346
H	-1.329031	0.900563	3.413553

H 3.150174 0.183378 1.553823

4' X:CH₂

$E(B3LYP/6-311+G^{**}) = -608.406146$

C -0.246280 0.085002 0.097758

C -0.051170 -0.065490 1.425176

N 1.323062 -0.136453 1.707641

C 2.242503 -0.056824 0.725438

S 1.305958 0.128217 -0.720022

C -1.051621 -0.156291 2.533826

H 1.639993 -0.249814 2.662430

H -0.913196 0.649962 3.261604

H -1.189671 0.167858 -0.417983

H -0.967240 -1.107733 3.069393

H -2.064848 -0.081979 2.139348

1' X:SiH₂

$E(B3LYP/6-311+G^{**}) = -859.794689$

C -0.164735 -0.102114 0.097383

N 0.052042 0.102132 1.427318

C 1.363316 0.125086 1.873417

C 2.247814 -0.090629 0.883340

S 1.405835 -0.337204 -0.637842

Si -1.788511 0.222345 -0.801824

H 3.322133 -0.133684 0.950263

H 1.569525 0.294903 2.919385

H -0.732646 0.237573 2.049780

H -2.684143 -0.404787 0.244052

H -1.682837 -0.851039 -1.850881

2' X:SiH₂

$E(B3LYP/6-311+G^{**}) = -859.768439$

S	0.038244	-0.463913	0.238268
C	0.163004	-0.063254	1.960349
C	1.502633	0.199288	2.200102
N	2.308799	0.127996	1.092725
C	1.705296	-0.191064	-0.052806
Si	-1.334912	0.266872	3.095890
H	2.216647	-0.250246	-0.998813
H	3.303180	0.314167	1.138105
H	1.940846	0.479336	3.145630
H	-0.822386	-0.507450	4.291802
H	-2.288455	-0.733237	2.479195

3' X:SiH₂

$E(B3LYP/6-311+G^{**}) = -859.774557$

S	0.085439	0.531767	0.126690
C	0.020059	0.115734	1.803700
N	1.289152	-0.120568	2.168510
C	2.251778	0.022598	1.168929
C	1.799984	0.389120	-0.078960
Si	-1.464313	-0.000624	2.947241
H	1.528982	-0.388396	3.116790
H	-0.965820	-0.442951	4.275753
H	-2.433139	-0.986268	2.414808
H	-2.115580	1.324428	3.068656
H	3.277888	-0.167080	1.455803

4' X:SiH₂

$E(B3LYP/6-311+G^{**}) = -859.801180$

C	0.109679	0.190569	0.057508
C	0.164471	-0.082121	1.383253
S	1.845593	-0.520850	1.739674
C	2.430449	-0.331681	0.126323

N	1.344352	0.045087	-0.578799
Si	-1.239892	-0.018132	2.614079
H	-0.941139	0.961542	3.687294
H	-0.752435	0.493209	-0.520608
H	-1.446929	-1.351979	3.229787
H	1.437016	0.220085	-1.571044
H	-2.468242	0.394039	1.888701