

Supporting Information

Pnicogen– π complexes: theoretical study and biological implications..

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Cartesian Coordinates

1.

As	0.0000000	0.0000000	2.2108352
Cl	0.9782933	1.6944538	3.2523150
Cl	0.9782933	-1.6944538	3.2523150
Cl	-1.9565867	0.0000000	3.2523150
C	-0.0002072	1.3990489	-0.9995218
C	-1.2115083	0.6997039	-0.9995218
C	-1.2115083	-0.6997039	-0.9995218
C	-0.0002072	-1.3990489	-0.9995218
C	1.2117155	-0.6993450	-0.9995218
C	1.2117155	0.6993450	-0.9995218
H	0.0001895	2.4897913	-0.9951082
H	-2.1563172	1.2447316	-0.9951082
H	-2.1563172	-1.2447316	-0.9951082
H	0.0001895	-2.4897913	-0.9951082
H	2.1561278	-1.2450597	-0.9951082
H	2.1561278	1.2450597	-0.9951082

2.

Cl	1.0354838	1.7935106	3.5383034
Cl	1.0354838	-1.7935106	3.5383034
Cl	-2.0709677	0.0000000	3.5383034
C	-0.0001472	1.3992964	-1.0815990
C	-1.2117526	0.6997757	-1.0815990
C	-1.2117526	-0.6997757	-1.0815990
C	-0.0001472	-1.3992964	-1.0815990
C	1.2118999	-0.6995207	-1.0815990
C	1.2118999	0.6995207	-1.0815990
H	0.0002093	2.4900869	-1.0816997
H	-2.1565832	1.2448622	-1.0816997
H	-2.1565832	-1.2448622	-1.0816997
H	0.0002093	-2.4900869	-1.0816997
H	2.1563739	-1.2452248	-1.0816997
H	2.1563739	1.2452248	-1.0816997
Sb	0.0000000	0.0000000	2.3648823

3.

Cl	1.0805661	1.8715954	3.4709919
Cl	1.0805661	-1.8715954	3.4709919
Cl	-2.1611323	0.0000000	3.4709919
C	-0.0001491	1.4001242	-1.0567977
C	-1.2124686	0.7001912	-1.0567977
C	-1.2124686	-0.7001912	-1.0567977
C	-0.0001491	-1.4001242	-1.0567977
C	1.2126177	-0.6999330	-1.0567977
C	1.2126177	0.6999330	-1.0567977
H	0.0005795	2.4907785	-1.0572383
H	-2.1573672	1.2448873	-1.0572383
H	-2.1573672	-1.2448873	-1.0572383
H	0.0005795	-2.4907785	-1.0572383
H	2.1567876	-1.2458911	-1.0572383
H	2.1567876	1.2458911	-1.0572383

Bi	0.0000000	0.0000000	2.2712398
4.			
C	-0.7075902	-1.2255822	1.0123053
C	-1.3711164	0.0000000	1.0144411
C	-0.7075902	1.2255822	1.0123053
C	0.6855582	1.1874216	1.0144411
C	1.4151804	0.0000000	1.0123053
C	0.6855582	-1.1874216	1.0144411
F	1.3605736	2.3565826	1.0142775
F	-2.7211472	0.0000000	1.0142775
F	1.3605736	-2.3565826	1.0142775
As	0.0000000	0.0000000	-2.2720121
Cl	-1.9572420	0.0000000	-3.2961975
Cl	0.9786210	1.6950213	-3.2961975
Cl	0.9786210	-1.6950213	-3.2961975
H	-1.2512667	2.1672576	1.0125110
H	-1.2512667	-2.1672576	1.0125110
H	2.5025335	0.0000000	1.0125110
5.			
C	-0.7076319	-1.2256544	1.1021481
C	-1.3715423	0.0000000	1.1030384
C	-0.7076319	1.2256544	1.1021481
C	0.6857712	1.1877905	1.1030384
C	1.4152638	0.0000000	1.1021481
C	0.6857712	-1.1877905	1.1030384
F	1.3606197	2.3566625	1.1041414
F	-2.7212394	0.0000000	1.1041414
F	1.3606197	-2.3566625	1.1041414
Sb	0.0000000	0.0000000	-2.4492751
Cl	-2.0760605	0.0000000	-3.5993591
Cl	1.0380303	1.7979212	-3.5993591
Cl	1.0380303	-1.7979212	-3.5993591
H	-1.2513578	2.1674153	1.1064563
H	-1.2513578	-2.1674153	1.1064563
H	2.5027156	0.0000000	1.1064563
6.			
C	-0.7079759	-1.2262502	1.0843995
C	-1.3727304	0.0000000	1.0889031
C	-0.7079759	1.2262502	1.0843995
C	0.6863652	1.1888194	1.0889031
C	1.4159517	0.0000000	1.0843995
C	0.6863652	-1.1888194	1.0889031
F	1.3602726	2.3560613	1.0945182
F	-2.7205452	0.0000000	1.0945182
F	1.3602726	-2.3560613	1.0945182
Bi	0.0000000	0.0000000	-2.3871545
Cl	-2.1651455	0.0000000	-3.5616816
Cl	1.0825727	1.8750710	-3.5616816
Cl	1.0825727	-1.8750710	-3.5616816
H	-1.2517553	2.1681037	1.0895789
H	-1.2517553	-2.1681037	1.0895789
H	2.5035105	0.0000000	1.0895789
7.			
As	0.0000000	0.0000000	2.3476975
Cl	0.9779086	1.6937874	3.3631711
Cl	0.9779086	-1.6937874	3.3631711
Cl	-1.9558172	0.0000000	3.3631711
C	-0.0000458	1.3990899	-1.0348513
C	-1.2116245	0.6995846	-1.0348513
C	-1.2116245	-0.6995846	-1.0348513
C	-0.0000458	-1.3990899	-1.0348513
C	1.2116703	-0.6995053	-1.0348513
C	1.2116703	0.6995053	-1.0348513
F	2.3709081	1.3685937	-1.0380172
F	-0.0002171	2.7375635	-1.0380172

F	-2.3706910	1.3689698	-1.0380172
F	-2.3706910	-1.3689698	-1.0380172
F	-0.0002171	-2.7375635	-1.0380172
F	2.3709081	-1.3685937	-1.0380172

8.

C	-1.2116692	-0.6995422	1.1763778
C	-1.2116692	0.6995422	1.1763778
C	0.0000133	1.3991074	1.1763778
C	1.2116559	0.6995652	1.1763778
C	1.2116559	-0.6995652	1.1763778
C	0.0000133	-1.3991074	1.1763778
F	2.3709133	1.3691410	1.1812807
F	0.0002543	2.7378416	1.1812807
F	-2.3711676	1.3687006	1.1812807
F	-2.3711676	-1.3687006	1.1812807
F	0.0002543	-2.7378416	1.1812807
F	2.3709133	-1.3691410	1.1812807
Sb	0.0000000	0.0000000	-2.6741439
Cl	-1.0344139	1.7916575	-3.8239355
Cl	2.0688278	0.0000000	-3.8239355
Cl	-1.0344139	-1.7916575	-3.8239355

9.

C	-1.2122765	-0.6999089	1.1837174
C	-1.2122765	0.6999089	1.1837174
C	-0.0000006	1.3998167	1.1837174
C	1.2122772	0.6999078	1.1837174
C	1.2122772	-0.6999078	1.1837174
C	-0.0000006	-1.3998167	1.1837174
F	2.3707629	1.3691323	1.1930624
F	0.0003219	2.7377070	1.1930624
F	-2.3710848	1.3685747	1.1930624
F	-2.3710848	-1.3685747	1.1930624
F	0.0003219	-2.7377070	1.1930624
F	2.3707629	-1.3691323	1.1930624
Bi	0.0000000	0.0000000	-2.6758553
Cl	-1.0753043	1.8624816	-3.8616078
Cl	2.1506085	0.0000000	-3.8616078
Cl	-1.0753043	-1.8624816	-3.8616078

10a.

C	-0.6500313	1.1258873	-1.2858845
C	-0.6500313	-1.1258873	-1.2858845
C	1.3000626	0.0000000	-1.2858845
H	-1.1968646	2.0730303	-1.2814599
H	-1.1968646	-2.0730303	-1.2814599
H	2.3937292	0.0000000	-1.2814599
N	0.6899724	-1.1950672	-1.2849807
N	-1.3799448	0.0000000	-1.2849807
N	0.6899724	1.1950672	-1.2849807
Cl	-0.9772373	1.6926247	3.1435801
Cl	-0.9772373	-1.6926247	3.1435801
Cl	1.9544747	0.0000000	3.1435801
As	0.0000000	0.0000000	2.1262350

11a.

C	-0.6501279	1.1260546	-1.3957741
C	-0.6501279	-1.1260546	-1.3957741
C	1.3002559	0.0000000	-1.3957741
H	-1.1969906	2.0732485	-1.3919591
H	-1.1969906	-2.0732485	-1.3919591
H	2.3939812	0.0000000	-1.3919591
N	0.6899874	-1.1950932	-1.3937576
N	-1.3799748	0.0000000	-1.3937576
N	0.6899874	1.1950932	-1.3937576
Cl	-1.0387936	1.7992433	3.4254909
Cl	-1.0387936	-1.7992433	3.4254909

Cl	2.0775872	0.0000000	3.4254909
Sb	0.0000000	0.0000000	2.2679996

12a.

C	-0.6506434	1.1269474	-1.3826480
C	-0.6506434	-1.1269474	-1.3826480
C	1.3012867	0.0000000	-1.3826480
H	-1.1974826	2.0741007	-1.3784961
H	-1.1974826	-2.0741007	-1.3784961
H	2.3949652	0.0000000	-1.3784961
N	0.6901116	-1.1953083	-1.3792461
N	-1.3802232	0.0000000	-1.3792461
N	0.6901116	1.1953083	-1.3792461
Cl	-1.0821149	1.8742780	3.3983283
Cl	-1.0821149	-1.8742780	3.3983283
Cl	2.1642298	0.0000000	3.3983283
Bi	0.0000000	0.0000000	2.2261854

10b.

C	0.6498943	-1.1256500	-1.3005023
C	0.6498943	1.1256500	-1.3005023
C	-1.2997887	0.0000000	-1.3005023
H	1.1967981	-2.0729152	-1.2978172
H	1.1967981	2.0729152	-1.2978172
H	-2.3935963	0.0000000	-1.2978172
N	-0.6899773	1.1950757	-1.2996216
N	1.3799546	0.0000000	-1.2996216
N	-0.6899773	-1.1950757	-1.2996216
Cl	-0.9766179	-1.6915519	3.1781358
Cl	1.9532359	0.0000000	3.1781358
Cl	-0.9766179	1.6915519	3.1781358
As	0.0000000	0.0000000	2.1594160

11b.

C	0.6500058	-1.1258431	-1.4113499
C	0.6500058	1.1258431	-1.4113499
C	-1.3000117	0.0000000	-1.4113499
H	1.1969230	-2.0731314	-1.4092500
H	1.1969230	2.0731314	-1.4092500
H	-2.3938460	0.0000000	-1.4092500
N	-0.6899835	1.1950865	-1.4094191
N	1.3799670	0.0000000	-1.4094191
N	-0.6899835	-1.1950865	-1.4094191
Cl	2.0760926	0.0000000	3.4623296
Cl	-1.0380463	1.7979489	3.4623296
Cl	-1.0380463	-1.7979489	3.4623296
Sb	0.0000000	0.0000000	2.3030685

12b.

C	0.6504575	-1.1266255	-1.4013530
C	0.6504575	1.1266255	-1.4013530
C	-1.3009151	0.0000000	-1.4013530
H	1.1973651	-2.0738972	-1.3996826
H	1.1973651	2.0738972	-1.3996826
H	-2.3947302	0.0000000	-1.3996826
N	-0.6901006	1.1952894	-1.3980398
N	1.3802013	0.0000000	-1.3980398
N	-0.6901006	-1.1952894	-1.3980398
Cl	-1.0804675	-1.8714246	3.4434625
Cl	2.1609350	0.0000000	3.4434625
Cl	-1.0804675	1.8714246	3.4434625
Bi	0.0000000	0.0000000	2.2668388