Electronic Supplementary Information (ESI)

Computational Design of Boron-Free Triangular Molecules with Inverted Singlet-Triplet Energy Gap

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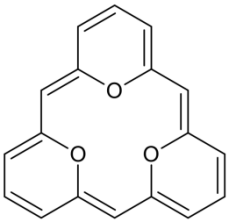
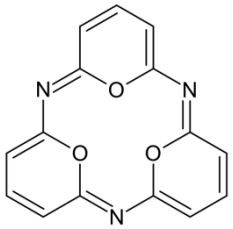
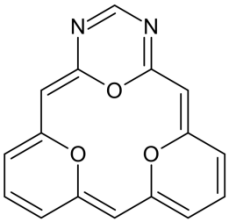
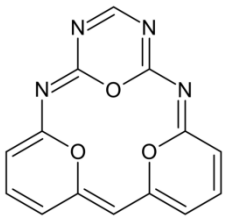
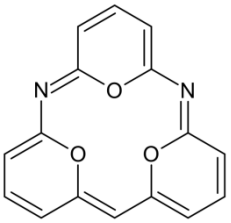
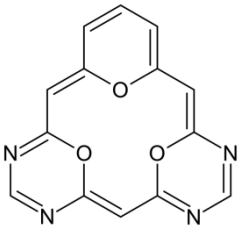
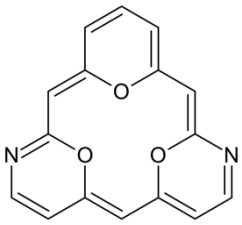
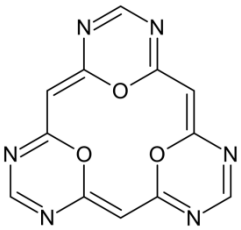
Table S1. Vertical absorption energy of the lowest singlet ($E(S_1)$), and lowest triplet ($E(T_1)$) states (spatial symmetry labels in parenthesis), energy gap between the lowest singlet and lowest triplet states ($\Delta_{ST} = E(S_1)-E(T_1)$, in eV), and oscillator strength (f), determined with the ADC(2)/cc-pVDZ method at the ground-state equilibrium geometry optimized at the MP2/cc-pVDZ level of theory for **PO** and its derivatives with nitrogen substitutions within the external rim.

abbreviation	molecule	$E(S_1)$ $E(T_1)$ Δ_{ST} f	abbreviation	molecule	$E(S_1)$ $E(T_1)$ Δ_{ST} f
PO		1.597 ($^1B_1$) 1.911 ($^3A_1$) - 0.314 0.000	**PO-3N**		2.049 ($^1B_1$) 2.398 ($^3B_1$) -0.349 0.000
PO-2Na		1.689 ($^1B_1$) 1.862 ($^3B_1$) -0.173 0.025	**PO-4Na**		1.953 ($^1B_1$) 1.981 ($^3B_1$) -0.028 0.072
PO-2Nb		1.873 ($^1B_1$) 2.051 ($^3B_1$) -0.178 0.014	**PO-4Nb**		1.888 ($^1B_1$) 2.043 ($^3B_1$) -0.155 0.021
PO-2Nc		1.720 ($^1B_1$) 1.989 ($^3B_1$) -0.269 0.002	**PO-6N**		2.124 ($^1B_1$) 2.518 ($^3B_1$) -0.394 0.000

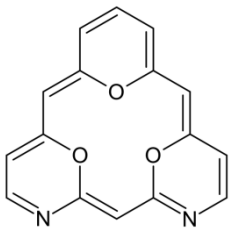
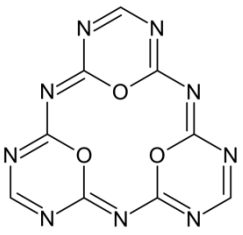
PO-2Nd		1.732 ($^1B_1$) 1.976 ($^3B_1$) -0.235 0.011	**PO-9N**		2.731 ($^1B_1$) 3.196 ($^3B_1$) -0.465 0.000

Table S2. Vertical absorption energy of the lowest singlet ($E(S_1)$), and lowest triplet ($E(T_1)$) states (spatial symmetry labels in parenthesis), energy gap between the lowest singlet and lowest triplet states ($\Delta_{ST} = E(S_1)-E(T_1)$, in eV), and oscillator strength (f), determined with the ADC(2)/cc-pVDZ method at the ground-state equilibrium geometry optimized at the MP2/cc-pVDZ level of theory for **PO** derivatives with amino and nitro substitutions.

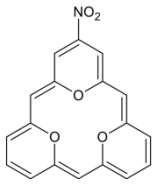
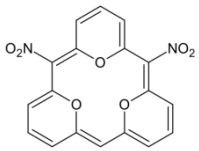
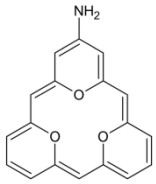
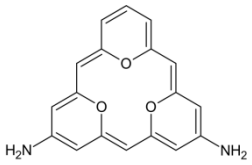
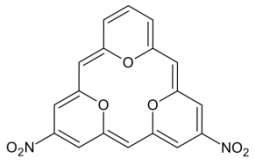
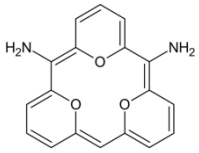
abbreviation	molecule	$E(S_1)$ $E(T_1)$ Δ_{ST} f	abbreviation	molecule	$E(S_1)$ $E(T_1)$ Δ_{ST} f
PO-NO_2		1.499 ($^1B_1$) 1.548 ($^3B_1$) -0.049 0.010	**PO-2NO_2b**		1.870 ($^1B_1$) 1.969 ($^3B_1$) -0.099 0.017
PO-NH_2		1.669 (^1A") 1.893 (^3A") -0.224 0.014	**PO-2NH_2a**		1.772 (^1A") 1.965 (^3A") -0.193 0.017
PO-2NO_2a		1.434 ($^1B_1$) 1.442 ($^3A_1$) -0.008 0.007	**PO-2NH_2b**		1.763 (^1A) 1.790 (^3A) -0.027 0.001

Table S3. Vertical absorption energy of the lowest singlet ($E(S_1)$), and lowest triplet ($E(T_1)$) states (spatial symmetry labels in parenthesis), energy gap between the lowest singlet and lowest triplet states ($\Delta_{ST} = E(S_1)-E(T_1)$, in eV), and oscillator strength (f), determined with the ADC(2)/cc-pVDZ method at the ground-state equilibrium geometry optimized at the MP2/cc-pVDZ level of theory for **PNH** derivatives with nitrogen substitutions to the external rim.

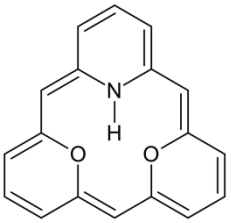
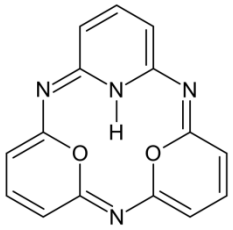
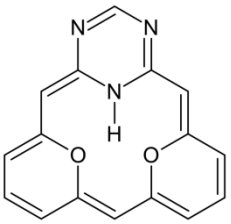
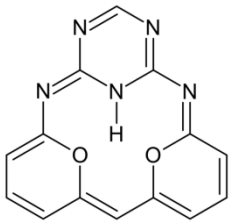
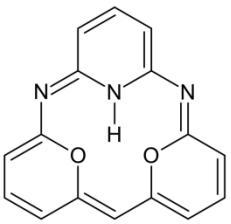
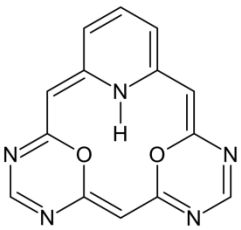
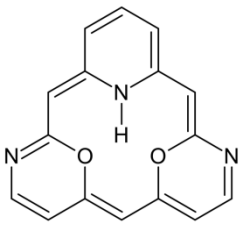
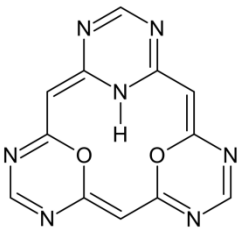
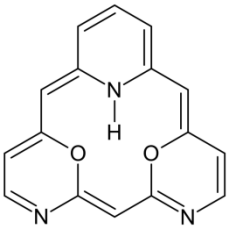
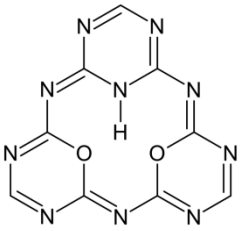
abbreviation	molecule	$E(S_1)$ $E(T_1)$ Δ_{ST} f	abbreviation	molecule	$E(S_1)$ $E(T_1)$ Δ_{ST} f
PNH		1.620 ($^1B_1$) 1.734 ($^3B_1$) -0.114 0.037	**PNH-3N**		2.096 ($^1B_1$) 2.192 ($^3B_1$) -0.096 0.045
PNH-2Na		1.477 ($^1B_1$) 1.606 ($^3B_1$) -0.129 0.042	**PNH-4Na**		1.761 ($^1B_1$) 1.796 ($^3B_1$) -0.035 0.086
PNH-2Nb		1.869 ($^1B_1$) 1.890 ($^3B_1$) -0.021 0.079	**PNH-4Nb**		2.218 ($^1B_1$) 2.387 ($^3A_1$) -0.169 0.009
PNH-2Nc		1.869 ($^1B_1$) 2.016 ($^3B_1$) -0.147 0.034	**PNH-6N**		2.163 ($^1B_1$) 2.393 ($^3B_1$) -0.230 0.026
PNH-2Nd		1.939 ($^1B_1$) 2.138 ($^3B_1$) -0.199 0.014	**PNH-9N**		2.778 ($^1B_1$) 3.060 ($^3B_1$) -0.282 0.032

Table S4. Vertical absorption energy of the lowest singlet ($E(S_1)$), and lowest triplet ($E(T_1)$) states (spatial symmetry labels in parenthesis), energy gap between the lowest singlet and lowest triplet states ($\Delta_{ST} = E(S_1)-E(T_1)$, in eV), and oscillator strength (f), determined with the ADC(2)/cc-pVDZ method at the ground-state equilibrium geometry optimized at the MP2/cc-pVDZ level of theory for **PNH** derivatives with amino and nitro substitutions.

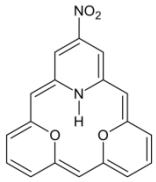
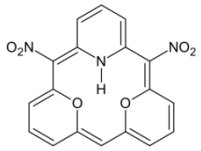
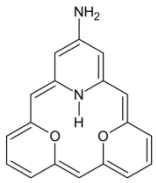
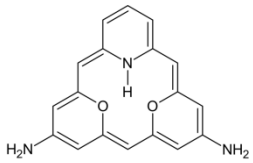
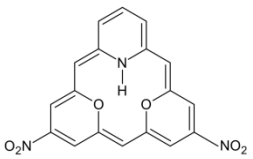
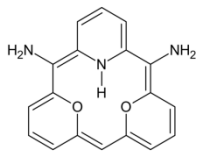
abbreviation	molecule	$E(S_1)$ $E(T_1)$ Δ_{ST} f	abbreviation	molecule	$E(S_1)$ $E(T_1)$ Δ_{ST} f
PNH-NO_2		1.533 ($^1B_1$) 1.731 ($^3B_1$) -0.198 0.012	**PNH-2NO_2b**		1.792 ($^1B_1$) 1.796 ($^3B_1$) -0.004 0.132
PNH-NH_2		1.634 (^1A") 1.703 (^3A") -0.069 0.058	**PNH-2NH_2a**		1.905 (^1B) 2.161 (^3B) -0.256 0.008
PNH-2NO_2a		1.432 ($^1B_1$) 1.348 ($^3B_1$) 0.084 0.064	**PNH-2NH_2b**		1.635 ($^1B_2$) 1.726 ($^3B_2$) -0.091 0.049

Table S5. Vertical absorption energy of the lowest singlet ($E(S_1)$), and lowest triplet ($E(T_1)$) states (spatial symmetry labels in parenthesis), energy gap between the lowest singlet and lowest triplet states ($\Delta_{ST} = E(S_1)-E(T_1)$, in eV), and oscillator strength (f), determined with the ADC(2)/cc-pVDZ method at the ground-state equilibrium geometry optimized at the MP2/cc- pVDZ level of theory for **PS** derivatives with nitrogen substitutions to the external rim.

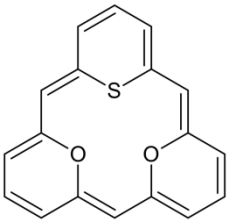
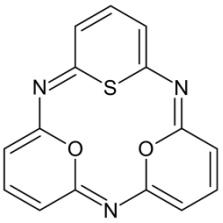
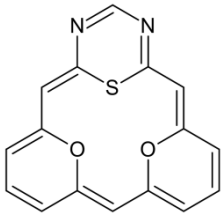
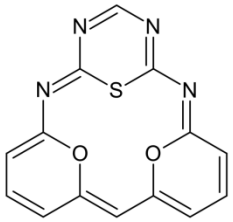
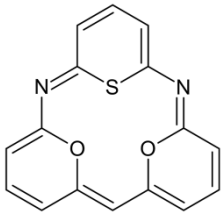
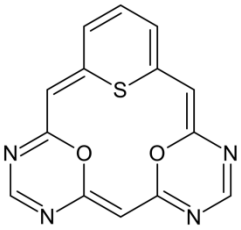
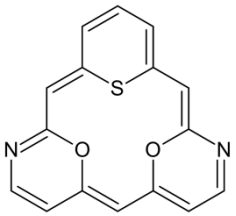
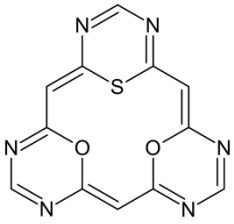
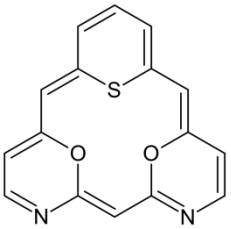
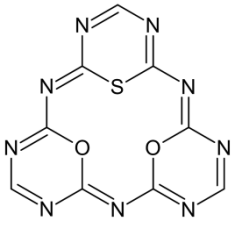
abbreviation	molecule	$E(S_1)$ $E(T_1)$ Δ_{ST} f	abbreviation	molecule	$E(S_1)$ $E(T_1)$ Δ_{ST} f
PS		1.446 (^{1}A") 1.550 (^{3}A") -0.104 0.023	**PS-3N**		1.691 (^{1}A") 1.823 (^{3}A") -0.132 0.024
PS-2Na		1.612 (^{1}A") 1.751 (^{3}A') -0.139 0.003	**PS-4Na**		1.948 (^{1}A") 1.870 (^{3}A") 0.078 0.013
PS-2Nb		1.749 (^{1}A") 1.747 (^{3}A') 0.002 0.001	**PS-4Nb**		1.656(^{1}A") 1.732 (^{3}A") -0.076 0.040
PS-2Nc		1.501 (^{1}A") 1.624 (^{3}A") -0.123 0.022	**PS-6N**		1.759(^{1}A") 1.927 (^{3}A") -0.168 0.026
PS-2Nd		1.519 (^{1}A") 1.623 (^{3}A") -0.104 0.039	**PS-9N**		2.437(^{1}A") 2.660 (^{3}A") -0.223 0.017

Table S6. Vertical absorption energy of the lowest singlet ($E(S_1)$), and lowest triplet ($E(T_1)$) states (spatial symmetry labels in parenthesis), energy gap between the lowest singlet and lowest triplet states ($\Delta_{ST} = E(S_1)-E(T_1)$, in eV), and oscillator strength (f), determined with the ADC(2)/cc-pVDZ method at the ground-state equilibrium geometry optimized at the MP2/cc-pVDZ level of theory for **PS** derivatives with amino and nitro substitutions.

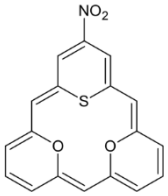
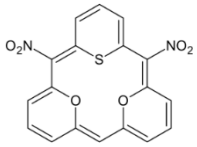
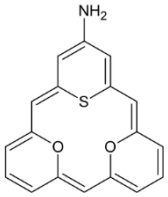
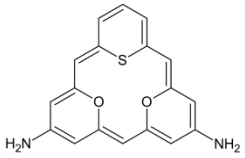
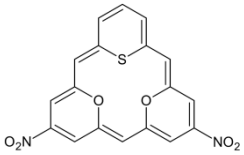
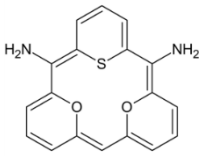
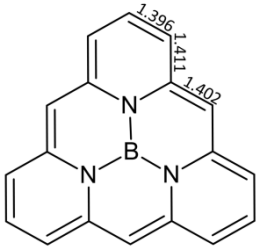
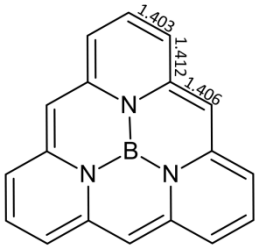
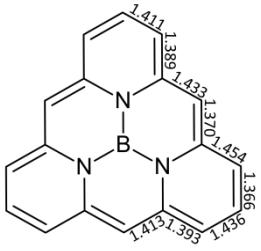
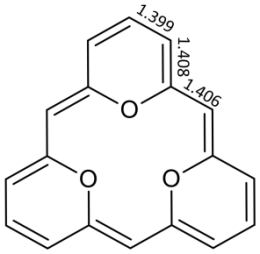
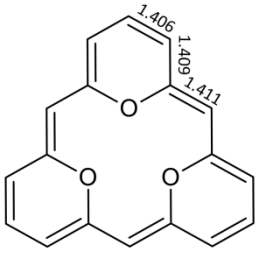
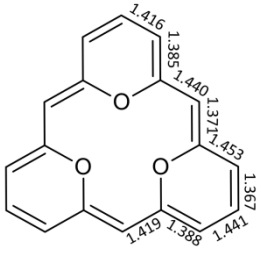
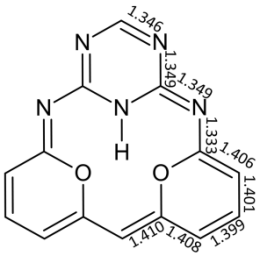
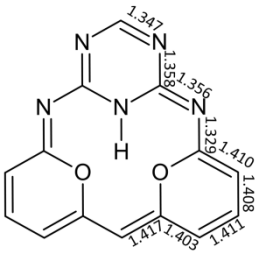
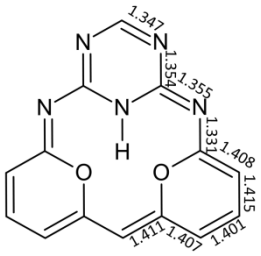
abbreviation	molecule	$E(S_1)$ $E(T_1)$ Δ_{ST} f	abbreviation	molecule	$E(S_1)$ $E(T_1)$ Δ_{ST} f
PS-NO_2		1.415 (^{1}A) 1.266 (^{3}A) 0.149 0.055	**PS-2NO_2b**		1.805 (^{1}A) 1.938 (^{3}A) - 0.133 0.008
PS-NH_2		1.525 (^{1}A) 1.688 (^{3}A) - 0.163 0.004	**PS-2NH_2a**		1.517 (^{1}A) 1.551 (^{3}A) - 0.034 0.058
PS-2NO_2a		1.577 (^{1}A) 1.317 (^{3}A) 0.260 0.012	**PS-2NH_2b**		1.391 (^{1}A") 1.191 (^{3}A') 0.200 0.055

Table S7. Lengths of the external CC/CN bonds in the optimized molecular geometries of the ground (S_0), and of the lowest excited singlet (S_1) and triplet (T_1) states, their adiabatic energy ($E_{0\text{-}0}$), energy of the $S_1 \rightarrow S_0$ or $T_1 \rightarrow S_0$ vertical emission fluorescence and phosphorescence (E_{em}), the adiabatic energy difference between the lowest excited singlet and triplet states ($\Delta_{ST} = S_1\text{-}T_1$), and oscillator strength (f_{em}) from the S_1 state of selected PX molecules. Molecular symmetry in a given state is in parentheses, and energies are in electronvolts.

BCN				
	$S_0(D_{3h})$	$S_1(D_{3h})$	$T_1(C_{2v})$	Δ_{ST}
				
$E_{0\text{-}0}$	-	1.591	1.613	-0.022
E_{em}	-	1.582	1.270	0.312
f_{em}	-	0.0	-	
PO				
	$S_0(D_{3h})$	$S_1(D_{3h})$	$T_1(C_{2v})$	Δ_{ST}
				
$E_{0\text{-}0}$	-	1.552	1.559	-0.007
E_{em}	-	1.540	1.170	0.370
f_{em}	-	0.0	-	
PNH-4N				
	$S_0(C_{2v})$	$S_1(C_{2v})$	$T_1(C_{2v})$	Δ_{ST}
				
$E_{0\text{-}0}$	-	1.685	1.727	-0.042
E_{em}	-	1.641	1.671	-0.030
f_{em}	-	0.081	-	

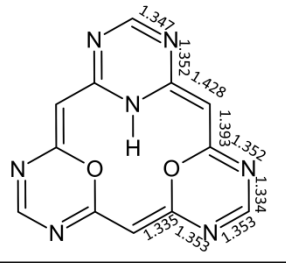
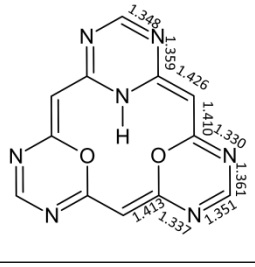
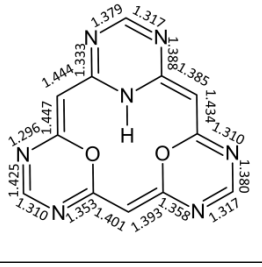
PNH-6N				
	$S_0(C_{2v})$	$S_1(C_{2v})$	$S_1(C_s)$	Δ_{ST}
				
E_{0-0}	-	2.061	2.164	-0.103
E_{em}	-	1.975	1.435	0.540
f_{em}	-	0.024	-	

Table S7. Cartesian coordinates of the selected **PX** molecules in its ground electronic state (S_0), optimized with the MP2/cc-pVDZ method, and in the lowest excited (S_1) and triplet (T_1) states optimized with the ADC(2)/cc-pVDZ method.

BCN, S_0

N	1.2564454	0.7256701	0.0000000
C	1.2394698	2.1394983	0.0000000
C	2.4719096	2.8255166	0.0000000
C	3.6792706	2.1249730	0.0000000
C	3.6827041	0.7291169	0.0000000
C	2.4725837	0.0044097	0.0000000
C	-0.0004335	2.7936692	0.0000000
C	-1.2401091	2.1391123	0.0000000
C	-2.4727852	2.8247554	0.0000000
C	-3.6799141	2.1238550	0.0000000
C	-3.6829219	0.7279768	0.0000000
C	-2.4725940	0.0036616	0.0000000
N	-1.2566723	0.7252783	0.0000000
C	2.4196068	-1.3964586	0.0000000
C	1.2331277	-2.1431630	0.0000000
C	1.2110136	-3.5534950	0.0000000
C	0.0006423	-4.2488288	0.0000000
C	-1.2099189	-3.5538749	0.0000000
C	-1.2324712	-2.1435238	0.0000000
N	0.0002270	-1.4509473	0.0000000
C	-2.4191697	-1.3972122	0.0000000
H	2.4470454	3.9175233	0.0000000
H	4.6271556	2.6724254	0.0000000
H	4.6161588	0.1618770	0.0000000
H	2.1691435	-4.0779779	0.0000000
H	0.0008096	-5.3434468	0.0000000
H	-2.1678959	-4.0786387	0.0000000
H	-4.6161978	0.1604440	0.0000000
H	-4.6279656	2.6710194	0.0000000
H	-2.4482547	3.9167706	0.0000000
H	-3.3645158	-1.9431916	0.0000000
H	-0.0006150	3.8853534	0.0000000

H	3.3651207	-1.9421473	0.0000000
B	0.0000007	-0.0000003	0.0000000

BCN, S_1

N	-1.2509954	0.0000000	-0.7222699
C	-2.4763206	0.0000000	-0.0077341
C	-3.6886504	0.0000000	-0.7315861
C	-3.6975103	0.0000000	-2.1347679
C	-2.4778913	0.0000000	-2.8286840
C	-1.2448494	0.0000000	-2.1406994
C	-2.4205313	0.0000000	1.3974920
C	-1.2314732	0.0000000	2.1484218
N	0.0000000	0.0000000	1.4445301
C	1.2314732	0.0000000	2.1484218
C	1.2107544	0.0000000	3.5602621
C	0.0000000	0.0000000	4.2695092
C	-1.2107544	0.0000000	3.5602621
B	0.0000000	0.0000000	0.0000035
N	1.2509954	0.0000000	-0.7222699
C	2.4763206	0.0000000	-0.0077341
C	3.6886504	0.0000000	-0.7315861
C	3.6975103	0.0000000	-2.1347679
C	2.4778913	0.0000000	-2.8286840
C	1.2448494	0.0000000	-2.1406994
C	2.4205313	0.0000000	1.3974920
C	0.0000000	0.0000000	-2.7949899
H	2.1718342	0.0000000	4.0808544
H	0.0000000	0.0000000	5.3632157
H	-2.1718342	0.0000000	4.0808544
H	-4.6200402	0.0000000	-0.1595642
H	-4.6446888	0.0000000	-2.6816228
H	-2.4482021	0.0000000	-3.9213026
H	2.4482021	0.0000000	-3.9213026
H	4.6446888	0.0000000	-2.6816228
H	4.6200402	0.0000000	-0.1595642
H	0.0000000	0.0000000	-3.8876363
H	3.3668025	0.0000000	1.9438060
H	-3.3668025	0.0000000	1.9438060

BCN, T_1

N	-1.2484450	0.0000000	-0.7257774
C	-2.4656653	0.0000000	0.0147373
C	-3.7002670	0.0000000	-0.7540757
C	-3.7038403	0.0000000	-2.1200490
C	-2.4542417	0.0000000	-2.8278805
C	-1.2493071	0.0000000	-2.1292020
C	-2.4352187	0.0000000	1.3847296
C	-1.2347247	0.0000000	2.1679807
N	0.0000000	0.0000000	1.4409470
C	1.2347247	0.0000000	2.1679807
C	1.2096173	0.0000000	3.5565670
C	0.0000000	0.0000000	4.2832704
C	-1.2096173	0.0000000	3.5565670

B	0.0000000	0.0000000	0.0096880
N	1.2484450	0.0000000	-0.7257774
C	2.4656653	0.0000000	0.0147373
C	3.7002670	0.0000000	-0.7540757
C	3.7038403	0.0000000	-2.1200490
C	2.4542417	0.0000000	-2.8278805
C	1.2493071	0.0000000	-2.1292020
C	2.4352187	0.0000000	1.3847296
C	0.0000000	0.0000000	-2.7901435
H	2.1742515	0.0000000	4.0752940
H	0.0000000	0.0000000	5.3767269
H	-2.1742515	0.0000000	4.0752940
H	-4.6350543	0.0000000	-0.1858127
H	-4.6457935	0.0000000	-2.6762418
H	-2.4223180	0.0000000	-3.9198372
H	2.4223180	0.0000000	-3.9198372
H	4.6457935	0.0000000	-2.6762418
H	4.6350543	0.0000000	-0.1858127
H	0.0000000	0.0000000	-3.8829863
H	3.3883771	0.0000000	1.9207377
H	-3.3883771	0.0000000	1.9207377

PO, S_0

O	1.2983169	0.7495852	0.0000000
C	1.2679782	2.1230487	0.0000000
C	2.4837136	2.8327726	0.0000000
C	3.6960166	2.1338978	0.0000000
C	3.6951085	0.7345752	0.0000000
C	2.4726018	0.0365793	0.0000000
C	0.0000000	2.7315997	0.0000000
C	-1.2679782	2.1230487	0.0000000
O	-1.2983169	0.7495852	0.0000000
C	-2.4726018	0.0365793	0.0000000
C	-3.6951085	0.7345752	0.0000000
C	-3.6960166	2.1338978	0.0000000
C	-2.4837136	2.8327726	0.0000000
C	-2.3656333	-1.3657974	0.0000000
C	-1.2046237	-2.1596233	0.0000000
O	0.0000000	-1.4991657	0.0000000
C	1.2046237	-2.1596233	0.0000000
C	1.2113949	-3.5673430	0.0000000
C	0.0000000	-4.2677907	0.0000000
C	-1.2113949	-3.5673430	0.0000000
C	2.3656333	-1.3657974	0.0000000
H	3.3126706	-1.9125697	0.0000000
H	4.6446020	2.6815638	0.0000000
H	0.0000000	3.8251441	0.0000000
H	-3.3126706	-1.9125697	0.0000000
H	-4.6446020	2.6815638	0.0000000
H	0.0000000	-5.3631758	0.0000000
H	2.1742400	-4.0844621	0.0000000
H	-2.4501293	3.9251806	0.0000000
H	-2.1742400	-4.0844621	0.0000000

H	-4.6243693	0.1592864	0.0000000
H	2.4501293	3.9251806	0.0000000
H	4.6243693	0.1592864	0.0000000

PO, S_1

O	1.2858584	0.7423906	0.0000000
C	1.2721647	2.1210177	0.0000000
C	2.4879982	2.8340844	0.0000000
C	3.7134041	2.1439297	0.0000000
C	3.6983863	0.7376196	0.0000000
C	2.4729345	0.0412164	0.0000000
C	0.0000000	2.7319629	0.0000000
C	-1.2721647	2.1210177	0.0000000
O	-1.2858584	0.7423906	0.0000000
C	-2.4729345	0.0412164	0.0000000
C	-3.6983863	0.7376196	0.0000000
C	-3.7134041	2.1439297	0.0000000
C	-2.4879982	2.8340844	0.0000000
C	-2.3659468	-1.3659824	0.0000000
C	-1.2007728	-2.1622360	0.0000000
O	0.0000000	-1.4847802	0.0000000
C	1.2007728	-2.1622360	0.0000000
C	1.2103915	-3.5717019	0.0000000
C	0.0000000	-4.2878561	0.0000000
C	-1.2103915	-3.5717019	0.0000000
C	2.3659468	-1.3659824	0.0000000
H	3.3136263	-1.9131241	0.0000000
H	4.6611744	2.6911227	0.0000000
H	0.0000000	3.8262498	0.0000000
H	-3.3136263	-1.9131241	0.0000000
H	-4.6611744	2.6911227	0.0000000
H	0.0000000	-5.3822492	0.0000000
H	2.1774244	-4.0822741	0.0000000
H	-2.4466512	3.9268485	0.0000000
H	-2.1774244	-4.0822741	0.0000000
H	-4.6240705	0.1554251	0.0000000
H	2.4466512	3.9268485	0.0000000
H	4.6240705	0.1554251	0.0000000

PO, T_1

O	-0.0267253	1.4755496	0.0000000
C	1.1956503	2.1406980	0.0000000
C	1.1706015	3.5935751	0.0000000
C	-0.0089846	4.2841744	0.0000000
C	-1.2453631	3.5422274	0.0000000
C	-1.2105242	2.1554512	0.0000000
C	2.3479099	1.3969055	0.0000000
H	3.2833035	1.9665883	0.0000000
H	2.1349430	4.1117210	0.0000000
H	-0.0238124	5.3785017	0.0000000
H	-2.2147009	4.0474938	0.0000000
O	-1.2806001	-0.7332281	0.0000000
O	1.2881673	-0.7321420	0.0000000

C	-2.4705596	-0.0640604	0.0000000
C	1.3075750	-2.1217317	0.0000000
C	-3.6799308	-0.7454002	0.0000000
C	2.5063393	-2.8144051	0.0000000
C	-3.6836246	-2.1864547	0.0000000
C	3.7443888	-2.1257077	0.0000000
C	-2.4862718	-2.8461831	0.0000000
C	3.7012869	-0.7115100	0.0000000
C	-1.2255572	-2.1232207	0.0000000
C	2.4914303	-0.0354765	0.0000000
C	-2.3811939	1.3519241	0.0000000
C	0.0025752	-2.7323502	0.0000000
H	-3.3331320	1.8921158	0.0000000
H	-0.0079083	-3.8274796	0.0000000
H	-4.6104484	-0.1717754	0.0000000
H	2.4666044	-3.9093124	0.0000000
H	-4.6310332	-2.7343849	0.0000000
H	4.6956335	-2.6659444	0.0000000
H	-2.4372821	-3.9397802	0.0000000
H	4.6212437	-0.1163784	0.0000000

PNH, S_0

C	-2.5343937	0.0000000	-0.0361462
O	-1.3413611	0.0000000	-0.7469227
C	-1.2798636	0.0000000	-2.1321530
C	-2.4870455	0.0000000	-2.8480250
C	-3.7114059	0.0000000	-2.1605008
C	-3.7440353	0.0000000	-0.7661750
C	0.0000000	0.0000000	-2.7177337
C	1.2798636	0.0000000	-2.1321530
O	1.3413611	0.0000000	-0.7469227
C	2.5343937	0.0000000	-0.0361462
C	3.7440353	0.0000000	-0.7661750
C	3.7114059	0.0000000	-2.1605008
C	2.4870455	0.0000000	-2.8480250
C	2.4244237	0.0000000	1.3587371
C	1.2300152	0.0000000	2.1348845
N	0.0000000	0.0000000	1.5185155
C	-1.2300152	0.0000000	2.1348845
C	-1.2198563	0.0000000	3.5483812
C	0.0000000	0.0000000	4.2380875
C	1.2198563	0.0000000	3.5483812
C	-2.4244237	0.0000000	1.3587371
H	-3.3673712	0.0000000	1.9116146
H	-2.1726582	0.0000000	4.0845779
H	0.0000000	0.0000000	5.3336886
H	2.1726582	0.0000000	4.0845779
H	3.3673712	0.0000000	1.9116146
H	0.0000000	0.0000000	-3.8117977
H	4.6852585	0.0000000	-0.2109735
H	-2.4429628	0.0000000	-3.9397355
H	4.6500451	0.0000000	-2.7255031
H	-4.6500451	0.0000000	-2.7255031

H	2.4429628	0.0000000	-3.9397355
H	-4.6852585	0.0000000	-0.2109735
H	0.0000000	0.0000000	0.4952557

PNH, S_1

C	-2.5271431	0.0000000	-0.0448491
O	-1.3154811	0.0000000	-0.7400018
C	-1.2780018	0.0000000	-2.1325096
C	-2.4874936	0.0000000	-2.8517940
C	-3.7241942	0.0000000	-2.1808077
C	-3.7308045	0.0000000	-0.7710333
C	0.0000000	0.0000000	-2.7309986
C	1.2780018	0.0000000	-2.1325096
O	1.3154811	0.0000000	-0.7400018
C	2.5271431	0.0000000	-0.0448491
C	3.7308045	0.0000000	-0.7710333
C	3.7241942	0.0000000	-2.1808077
C	2.4874936	0.0000000	-2.8517940
C	2.4173020	0.0000000	1.3575226
C	1.2294678	0.0000000	2.1444304
N	0.0000000	0.0000000	1.5249090
C	-1.2294678	0.0000000	2.1444304
C	-1.2233067	0.0000000	3.5668117
C	0.0000000	0.0000000	4.2542532
C	1.2233067	0.0000000	3.5668117
C	-2.4173020	0.0000000	1.3575226
H	-3.3634318	0.0000000	1.9069126
H	-2.1766692	0.0000000	4.1019705
H	0.0000000	0.0000000	5.3501851
H	2.1766692	0.0000000	4.1019705
H	3.3634318	0.0000000	1.9069126
H	0.0000000	0.0000000	-3.8257795
H	4.6675713	0.0000000	-0.2063373
H	-2.4314495	0.0000000	-3.9442657
H	4.6630567	0.0000000	-2.7424839
H	-4.6630567	0.0000000	-2.7424839
H	2.4314495	0.0000000	-3.9442657
H	-4.6675713	0.0000000	-0.2063373
H	0.0000000	0.0000000	0.5003004

PNH, T_1

C	-2.5567888	0.0000000	-0.0576348
O	-1.3392769	0.0000000	-0.7237751
C	-1.2742206	0.0000000	-2.1289631
C	-2.5087409	0.0000000	-2.8485437
C	-3.7212569	0.0000000	-2.2000608
C	-3.7357652	0.0000000	-0.7511350
C	0.0000000	0.0000000	-2.7116613
C	1.2742206	0.0000000	-2.1289631
O	1.3392769	0.0000000	-0.7237751
C	2.5567888	0.0000000	-0.0576348
C	3.7357652	0.0000000	-0.7511350
C	3.7212569	0.0000000	-2.2000608

C	2.5087409	0.0000000	-2.8485437
C	2.4192828	0.0000000	1.3850698
C	1.2337267	0.0000000	2.1124899
N	0.0000000	0.0000000	1.4965070
C	-1.2337267	0.0000000	2.1124899
C	-1.2158164	0.0000000	3.5501259
C	0.0000000	0.0000000	4.2436631
C	1.2158164	0.0000000	3.5501259
C	-2.4192828	0.0000000	1.3850698
H	-3.3544988	0.0000000	1.9529906
H	-2.1699175	0.0000000	4.0851811
H	0.0000000	0.0000000	5.3390449
H	2.1699175	0.0000000	4.0851811
H	3.3544988	0.0000000	1.9529906
H	0.0000000	0.0000000	-3.8076638
H	4.6750219	0.0000000	-0.1907620
H	-2.4489523	0.0000000	-3.9422239
H	4.6617932	0.0000000	-2.7594527
H	-4.6617932	0.0000000	-2.7594527
H	2.4489523	0.0000000	-3.9422239
H	-4.6750219	0.0000000	-0.1907620
H	0.0000000	0.0000000	0.4734980

PS, S_0

C	-0.0593146	-3.5218802	-1.2393100
C	0.3753474	-2.1895380	-1.3751159
S	1.2403185	-1.4969073	0.0000000
C	0.3753474	-2.1895380	1.3751159
C	-0.0593146	-3.5218802	1.2393100
C	-0.1722747	-4.1825402	0.0000000
C	0.2232096	-1.3919393	-2.5316111
C	0.1161555	0.0118842	-2.5716513
O	-0.0015119	0.6717987	-1.3578518
C	-0.0731424	2.0435172	-1.2772290
C	-0.1194658	2.7959946	-2.4650531
C	-0.0768885	2.1557110	-3.7092469
C	0.0485327	0.7611428	-3.7568642
C	-0.1125661	2.6306541	0.0000000
C	-0.0731424	2.0435172	1.2772290
O	-0.0015119	0.6717987	1.3578518
C	0.1161555	0.0118842	2.5716513
C	0.0485327	0.7611428	3.7568642
C	-0.0768885	2.1557110	3.7092469
C	-0.1194658	2.7959946	2.4650531
C	0.2232096	-1.3919393	2.5316111
H	0.1081615	-1.8986918	3.4984085
H	-0.1157861	2.7399076	4.6342425
H	-0.1979153	3.7216644	0.0000000
H	0.1081615	-1.8986918	-3.4984085
H	-0.1157861	2.7399076	-4.6342425
H	-0.5635667	-5.2065501	0.0000000
H	-0.4536866	-4.0230616	2.1342525
H	-0.1829119	3.8849780	-2.3865003

H	-0.4536866	-4.0230616	-2.1342525
H	0.1143033	0.2270164	-4.7092356
H	-0.1829119	3.8849780	2.3865003
H	0.1143033	0.2270164	4.7092356

PS, S_1

O	-0.2571384	0.6364857	-1.3384726
C	0.0530444	0.0498243	-2.5527304
C	-0.3559011	0.6662229	-3.7501386
C	-1.0331668	1.8936189	-3.7166675
C	-1.2944080	2.4883460	-2.4721240
C	-0.9058515	1.8464473	-1.2775950
C	0.7404570	-1.1815535	-2.4902570
C	1.3257194	-1.7834348	-1.3490649
C	1.5250103	-3.1764467	-1.2299301
C	1.7558134	-3.8327660	0.0000000
C	1.5250103	-3.1764467	1.2299301
C	1.3257194	-1.7834348	1.3490649
S	1.8787057	-0.7724022	0.0000000
C	-1.1751796	2.3721118	0.0000000
C	-0.9058515	1.8464473	1.2775950
C	-1.2944080	2.4883460	2.4721240
C	-1.0331668	1.8936189	3.7166675
C	-0.3559011	0.6662229	3.7501386
C	0.0530444	0.0498243	2.5527304
O	-0.2571384	0.6364857	1.3384726
C	0.7404570	-1.1815535	2.4902570
H	-0.1144534	0.1700843	-4.6936087
H	-1.3429095	2.3844774	-4.6434164
H	-1.8099093	3.4488028	-2.3962202
H	-1.8099093	3.4488028	2.3962202
H	-1.3429095	2.3844774	4.6434164
H	-0.1144534	0.1700843	4.6936087
H	1.3652810	-3.7902438	2.1270907
H	1.8896082	-4.9190074	0.0000000
H	1.3652810	-3.7902438	-2.1270907
H	0.7802678	-1.7420759	3.4331560
H	0.7802678	-1.7420759	-3.4331560
H	-1.7010317	3.3309543	0.0000000

PS, T_1

O	-0.4291527	0.4986292	-1.3456624
C	0.0472887	0.0013056	-2.5624993
C	-0.3567540	0.6866660	-3.7741043
C	-1.0209139	1.8807969	-3.7294915
C	-1.2923609	2.4534418	-2.4388327
C	-0.9697445	1.7548744	-1.2845201
C	0.8366539	-1.1147123	-2.5452128
C	1.3599820	-1.7775719	-1.3636309
C	1.4641025	-3.1580827	-1.2296812
C	1.6787161	-3.8309105	0.0000000
C	1.4641025	-3.1580827	1.2296812
C	1.3599820	-1.7775719	1.3636309

S	1.8736952	-0.7653375	0.0000000
C	-1.2231226	2.2938083	0.0000000
C	-0.9697445	1.7548744	1.2845201
C	-1.2923609	2.4534418	2.4388327
C	-1.0209139	1.8807969	3.7294915
C	-0.3567540	0.6866660	3.7741043
C	0.0472887	0.0013056	2.5624993
O	-0.4291527	0.4986292	1.3456624
C	0.8366539	-1.1147123	2.5452128
H	-0.0800837	0.2225672	-4.7256056
H	-1.3110412	2.4074514	-4.6422695
H	-1.7488413	3.4414327	-2.3419733
H	-1.7488413	3.4414327	2.3419733
H	-1.3110412	2.4074514	4.6422695
H	-0.0800837	0.2225672	4.7256056
H	1.2582236	-3.7657312	2.1230880
H	1.7405228	-4.9236965	0.0000000
H	1.2582236	-3.7657312	-2.1230880
H	1.0570385	-1.5576113	3.5249494
H	1.0570385	-1.5576113	-3.5249494
H	-1.6986058	3.2792244	0.0000000

PNH-4N, S_0

C	-2.4713931	0.0000000	0.4320629
O	-1.3160564	0.0000000	-0.3464311
C	-1.2753746	0.0000000	-1.7223130
C	-2.5101698	0.0000000	-2.3988328
C	-3.6989843	0.0000000	-1.6616343
C	-3.6949197	0.0000000	-0.2602965
C	0.0000000	0.0000000	-2.3241599
C	1.2753746	0.0000000	-1.7223130
O	1.3160564	0.0000000	-0.3464311
C	2.4713931	0.0000000	0.4320629
C	3.6949197	0.0000000	-0.2602965
C	3.6989843	0.0000000	-1.6616343
C	2.5101698	0.0000000	-2.3988328
N	2.3831169	0.0000000	1.7619776
C	1.2157778	0.0000000	2.4374337
N	0.0000000	0.0000000	1.8012753
C	-1.2157778	0.0000000	2.4374337
N	-1.2224888	0.0000000	3.7866397
C	0.0000000	0.0000000	4.3509960
N	1.2224888	0.0000000	3.7866397
N	-2.3831169	0.0000000	1.7619776
H	0.0000000	0.0000000	5.4481071
H	0.0000000	0.0000000	-3.4177322
H	4.6091976	0.0000000	0.3347874
H	-2.5120681	0.0000000	-3.4912045
H	4.6572949	0.0000000	-2.1925278
H	-4.6572949	0.0000000	-2.1925278
H	2.5120681	0.0000000	-3.4912045
H	-4.6091976	0.0000000	0.3347874
H	0.0000000	0.0000000	0.7821793

PNH-4N, S_1

C	-2.4595596	0.0000000	0.4297101
O	-1.2851706	0.0000000	-0.3366545
C	-1.2777993	0.0000000	-1.7265861
C	-2.5087267	0.0000000	-2.3996947
C	-3.7190241	0.0000000	-1.6738893
C	-3.6859232	0.0000000	-0.2666505
C	0.0000000	0.0000000	-2.3398444
C	1.2777993	0.0000000	-1.7265861
O	1.2851706	0.0000000	-0.3366545
C	2.4595596	0.0000000	0.4297101
C	3.6859232	0.0000000	-0.2666505
C	3.7190241	0.0000000	-1.6738893
C	2.5087267	0.0000000	-2.3996947
N	2.3788068	0.0000000	1.7565772
C	1.2112415	0.0000000	2.4455512
N	0.0000000	0.0000000	1.8082671
C	-1.2112415	0.0000000	2.4455512
N	-1.2251606	0.0000000	3.8037872
C	0.0000000	0.0000000	4.3647456
N	1.2251606	0.0000000	3.8037872
N	-2.3788068	0.0000000	1.7565772
H	0.0000000	0.0000000	5.4623540
H	0.0000000	0.0000000	-3.4346232
H	4.5935498	0.0000000	0.3410541
H	-2.5017390	0.0000000	-3.4934970
H	4.6769523	0.0000000	-2.2023683
H	-4.6769523	0.0000000	-2.2023683
H	2.5017390	0.0000000	-3.4934970
H	-4.5935498	0.0000000	0.3410541
H	0.0000000	0.0000000	0.7844218

PNH-4N, T_1

C	-2.4562529	0.0000000	0.4295081
O	-1.2888272	0.0000000	-0.3266541
C	-1.2758759	0.0000000	-1.7260778
C	-2.5117043	0.0000000	-2.3984319
C	-3.7148400	0.0000000	-1.6805883
C	-3.6805790	0.0000000	-0.2660504
C	0.0000000	0.0000000	-2.3294508
C	1.2758759	0.0000000	-1.7260778
O	1.2888272	0.0000000	-0.3266541
C	2.4562529	0.0000000	0.4295081
C	3.6805790	0.0000000	-0.2660504
C	3.7148400	0.0000000	-1.6805883
C	2.5117043	0.0000000	-2.3984319
N	2.3815517	0.0000000	1.7588914
C	1.2123477	0.0000000	2.4433169
N	0.0000000	0.0000000	1.8081683
C	-1.2123477	0.0000000	2.4433169
N	-1.2237662	0.0000000	3.7972713
C	0.0000000	0.0000000	4.3592300

N	1.2237662	0.0000000	3.7972713
N	-2.3815517	0.0000000	1.7588914
H	0.0000000	0.0000000	5.4566641
H	0.0000000	0.0000000	-3.4250582
H	4.5873877	0.0000000	0.3424433
H	-2.5026594	0.0000000	-3.4928107
H	4.6732233	0.0000000	-2.2076880
H	-4.6732233	0.0000000	-2.2076880
H	2.5026594	0.0000000	-3.4928107
H	-4.5873877	0.0000000	0.3424433
H	0.0000000	0.0000000	0.7841868

PNH-6N, S_0

N	0.0000000	0.0000000	-1.4710900
C	-1.2041591	0.0000000	-2.1117360
N	-1.2188032	0.0000000	-3.4634308
C	0.0000000	0.0000000	-4.0359510
N	1.2188032	0.0000000	-3.4634308
C	1.2041591	0.0000000	-2.1117360
C	-2.4096689	0.0000000	-1.3467818
C	-2.4928921	0.0000000	0.0435470
N	-3.6591963	0.0000000	0.7265953
C	-3.5325503	0.0000000	2.0544755
N	-2.4076555	0.0000000	2.8056787
C	-1.2673452	0.0000000	2.1122657
O	-1.2862762	0.0000000	0.7307509
C	0.0000000	0.0000000	2.7222968
C	1.2673452	0.0000000	2.1122657
O	1.2862762	0.0000000	0.7307509
C	2.4928921	0.0000000	0.0435470
N	3.6591963	0.0000000	0.7265953
C	3.5325503	0.0000000	2.0544755
N	2.4076555	0.0000000	2.8056787
H	4.4715839	0.0000000	2.6211388
C	2.4096689	0.0000000	-1.3467818
H	-4.4715839	0.0000000	2.6211388
H	-3.3510942	0.0000000	-1.8960163
H	0.0000000	0.0000000	3.8125824
H	3.3510942	0.0000000	-1.8960163
H	0.0000000	0.0000000	-5.1325932
H	0.0000000	0.0000000	-0.4482160

PNH-6N, S_1

N	0.0000000	0.0000000	-1.4750442
C	-1.2040283	0.0000000	-2.1210942
N	-1.2214559	0.0000000	-3.4802947
C	0.0000000	0.0000000	-4.0511188
N	1.2214559	0.0000000	-3.4802947
C	1.2040283	0.0000000	-2.1210942
C	-2.4062468	0.0000000	-1.3545301
C	-2.4963688	0.0000000	0.0528791
N	-3.6468656	0.0000000	0.7203546
C	-3.5475615	0.0000000	2.0779526

N	-2.4117125	0.0000000	2.8099767
C	-1.2680374	0.0000000	2.1170327
O	-1.2696555	0.0000000	0.7235523
C	0.0000000	0.0000000	2.7407415
C	1.2680374	0.0000000	2.1170327
O	1.2696555	0.0000000	0.7235523
C	2.4963688	0.0000000	0.0528791
N	3.6468656	0.0000000	0.7203546
C	3.5475615	0.0000000	2.0779526
N	2.4117125	0.0000000	2.8099767
H	4.4897750	0.0000000	2.6345188
C	2.4062468	0.0000000	-1.3545301
H	-4.4897750	0.0000000	2.6345188
H	-3.3483609	0.0000000	-1.9047698
H	0.0000000	0.0000000	3.8322508
H	3.3483609	0.0000000	-1.9047698
H	0.0000000	0.0000000	-5.1480439
H	0.0000000	0.0000000	-0.4499414

PNH-6N, T_1

N	2.4298179	-2.8070588	0.0000000
C	1.2584096	-2.1190735	0.0000000
O	1.2839343	-0.7088210	0.0000000
C	2.5064708	-0.0584102	0.0000000
N	3.6454406	-0.7061245	0.0000000
C	3.5289797	-2.0815202	0.0000000
C	0.0066045	-2.7310942	0.0000000
C	-1.2618781	-2.1362027	0.0000000
N	-2.4388129	-2.8033053	0.0000000
C	-3.5503221	-2.1105694	0.0000000
N	-3.6482644	-0.6887335	0.0000000
C	-2.5018407	-0.0846827	0.0000000
O	-1.2859230	-0.7064255	0.0000000
C	-2.4035379	1.3587320	0.0000000
C	-1.1796516	2.1242269	0.0000000
N	0.0022683	1.4665871	0.0000000
C	1.2260880	2.0956512	0.0000000
N	1.2033828	3.4832510	0.0000000
C	0.0130174	4.0466127	0.0000000
N	-1.2333766	3.4565828	0.0000000
C	2.4075257	1.3720613	0.0000000
H	4.4798654	-2.6253811	0.0000000
H	-4.5060556	-2.6399252	0.0000000
H	-3.3410276	1.9183324	0.0000000
H	0.0175416	-3.8226971	0.0000000
H	3.3449620	1.9264301	0.0000000
H	-0.0046376	5.1422183	0.0000000
H	0.0010194	0.4393389	0.0000000