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Supplementary Material

Theoretical Study on Pyramidal C_7N_6–H_3R_3 Molecules

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Table S1. The Atom Coordinates of $C_7N_6H_6$ Optimized at the B3LYP/cc-pVDZ Level of Theory.

atom	X	Y	Z
N	1.390761	-0.028558	0.000000
C	2.008527	-0.028558	1.197310
N	1.360084	-0.028558	2.355734
C	0.032638	-0.028558	2.338091
N	-0.695381	-0.028558	1.204435
C	-2.041165	-0.028558	1.140781
N	-2.720167	-0.028558	0.000000
C	-2.041165	-0.028558	-1.140781
N	-0.695381	-0.028558	-1.204435
C	0.032638	-0.028558	-2.338091
N	1.360084	-0.028558	-2.355734
C	2.008527	-0.028558	-1.197310
C	0.000000	0.637704	0.000000
H	3.087986	-0.266451	1.182922
H	-0.519553	-0.266451	3.265735
H	-2.568433	-0.266451	2.082813
H	-2.568433	-0.266451	-2.082813
H	-0.519553	-0.266451	-3.265735
H	3.087986	-0.266451	-1.182922

Table S2. The Bond Lengths (in Å) of the pyramidal molecules C_7N_6–H_3R_3.

Bond	H	OH	F	CN	N_3	NH_2	NO_2	N=NH	N_2H_3	C≡CH
N1–C2	1.354	1.349	1.346	1.368	1.361	1.359	1.362	1.362	1.366	1.372
N1–C12	1.354	1.361	1.360	1.352	1.357	1.360	1.357	1.357	1.357	1.352
N1–C13	1.515	1.526	1.528	1.515	1.516	1.527	1.545	1.545	1.526	1.514
C2–N3	1.328	1.322	1.307	1.332	1.329	1.331	1.311	1.311	1.325	1.338
N3–C4	1.328	1.330	1.329	1.323	1.325	1.327	1.321	1.321	1.327	1.323
C4–N5	1.354	1.361	1.360	1.352	1.357	1.360	1.357	1.357	1.362	1.352
N5–C6	1.354	1.349	1.346	1.368	1.361	1.359	1.362	1.362	1.362	1.372
N5–C13	1.516	1.526	1.528	1.515	1.516	1.527	1.547	1.547	1.527	1.513
C6–N7	1.328	1.322	1.307	1.332	1.329	1.331	1.311	1.311	1.329	1.338
N7–C8	1.328	1.330	1.329	1.323	1.325	1.327	1.321	1.321	1.324	1.323
C8–N9	1.354	1.361	1.360	1.352	1.357	1.360	1.357	1.357	1.362	1.353
N9–C10	1.354	1.349	1.346	1.368	1.361	1.360	1.361	1.361	1.361	1.372
N9–C13	1.516	1.526	1.528	1.515	1.516	1.527	1.545	1.545	1.530	1.513
C10–N11	1.328	1.322	1.307	1.332	1.329	1.330	1.311	1.311	1.329	1.339
N11–C12	1.328	1.330	1.329	1.323	1.325	1.327	1.321	1.321	1.330	1.322

Table S3. The Lowest Frequencies (in cm^{-1}) of the pyramidal molecules C_7N_6–H_3R_3 at the B3LPY/cc–pVDZ Level.

	H	OH	F	CN	N_3	NH_2	NO_2	N=NH	N_2H_3	C≡CH
Lowest frequencies	150	96	96	58	45	95	33	39	55	57

Table S4. The Bond Lengths (in Å) of Nitrogen–centered Tri–*s*–triazine ($C_6N_7H_3$).

Bond	Length	Bond	Length	Bond	Length
C1–N2	1.338	N4–C5	1.338	N8–C9	1.338
C1–N12	1.338	C5–N6	1.338	C9–N10	1.338
C1–N13	1.407	C5–N13	1.407	C9–N13	1.407
N2–C3	1.335	N6–C7	1.335	N10–C11	1.335
C3–N4	1.335	C7–N8	1.335	C11–N12	1.335
C3–H14	1.096	C7–H15	1.096	C11–H16	1.096

Table S5. The Electron Density Distributions of Orbital #44 of $C_7N_6H_6$.

#44	**AS1**	**AS2**	**AS3**	**AS4**	H atom
1S	0.000	0.000	0.000	0.000	0.000
2S	0.000	0.000	0.000	0.000	0.000
3S	0.000	0.000	0.000	0.000	
4PX	0.000	0.000	0.001	0.000	0.000
4PY	0.000	0.000	0.001	0.000	0.000
4PZ	0.000	0.000	0.075	0.000	0.000
5PX	0.000	0.000	0.001	0.000	
5PY	0.000	0.000	0.001	0.000	
5PZ	0.000	0.000	0.049	0.000	
6D0	0.000	0.000	0.000	0.000	
6D+1	0.000	0.000	0.000	0.000	
6D–1	0.000	0.000	0.000	0.000	
6D+2	0.000	0.000	0.000	0.000	
6D–2	0.000	0.000	0.000	0.000	
Sum	0.000	0.000	0.128	0.000	0.000
Total	0.001	0.001	0.765	0.000	0.000

AS1: Nitrogen atoms N1, N5, and N9;
AS2: Nitrogen atoms N3, N7, and N11;
AS3: Carbon atoms C2, C4, C6, C8, C10, C12;
AS4: Central carbon atom C13;
Sum: The contribution of each atom to orbital #44;
Total: The contribution of each set of atoms to orbital #44.

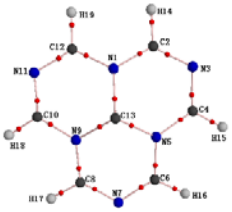

Fig. S1. The BCPs and the bond paths of $C_7N_6H_6$. The unmarked small balls are the BCPs (bonds or intramolecular interactions) and sticks are bond paths.

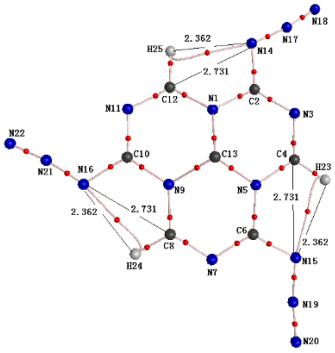

Fig. S2. The BCPs and the bond paths of C_7N_6–$H_3(N_3)_3$. The unmarked small balls are the BCPs (bonds or intramolecular interactions) and the sticks are bond paths.

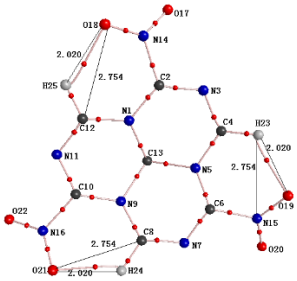

Fig. S3. The BCPs and the bond paths of C_7N_6–$H_3(NO_2)_3$. The unmarked small balls are the BCPs (bonds or intramolecular interactions) and sticksare bond paths**.**