Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for: Triangular graphene nanofragments: open-shell character and doping

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1 Computational details

Table S1: Active space parameter employed in the RAS-SF calculations and spin multiplicity of the Hartree-Fock state employed as a reference configuration (spin reference). RAS1 (RAS3) includes all doubly occupied (virtual) orbitals below (above) the RAS2 space. 1s core orbitals of C, B and N were kept frozen in the construction of RAS-SF wave functions.

molecule	sym.	spin reference	RAS2 electrons	RAS2 orbitals
1	D_{3h}	Doublet	7	$2e''$, $2a_2''$,$1a_1''$, $3e''$,$3a_2''$
1N$_1$	D_{3h}	Triplet	8	$2e''$,$2a_2''$,$1a_1''$, $3e''$,$3a_2''$
1B$_1$	D_{3h}	Triplet	6	$2e''$,$2a_2''$,$1a_1''$, $3a_2''$,$3e''$
1H$_3$	D_{3h}	Quintet	8	$2e''$,$1a_1''$,$4a_2''$, $3e''$,$4e''$
2	D_{3h}	Triplet	10	$3e''$,$1a_1''$,$3a_2''$,$4e''$,$4a_2''$,$5e''$,$2a_1''$
2B$_1$	D_{3h}/C_{2v}	Quartet	3	$3a_2''$,$4e''$,$4a_2''$
2B$_3$	D_{3h}	Quartet	7	$3e''$,$1a_1''$,$3a_2''$,$4e''$,$4a_2''$,$5e''$,$2a_1''$
2N$_1$	D_{3h}/C_{c2v}	Quartet	5	$3a_2''$,$4e''$,$4a_2''$
2N$_3$	D_{3h}	Quartet	13	$3e''$,$1a_1''$, $3a_2''$,$4e''$,$4a_2''$,$5e''$,$2a_1''$
2H$_3a$	D_{3h}	Sextet	9	$3a_2''$,$1a_1'$, $4e''$,$5e''$,$4a_2''$,$2a_1''$,$5a_2''$
2H$_3b$	D_{3h}	Doublet	5	$3e''$,$3a_2''$,$3e''$
2N$_2$	C_{2v}	Singlet	4	$3a''2$,$4e''$,$4a_2''$

2 Pristine compounds

Natural orbitals and occupation numbers for the **1** and **2** ground state (doublet and triplet, respectively) are shown in Figure S1.

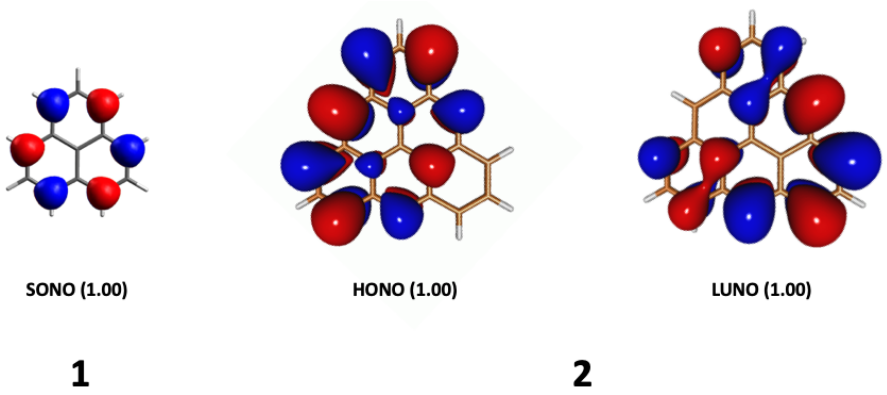

Figure S1: Frontier natural orbitals and occupation numbers of **1** and **2** .

3 B-doped and N-doped TGNF

3.1 Phenalenyl derivatives

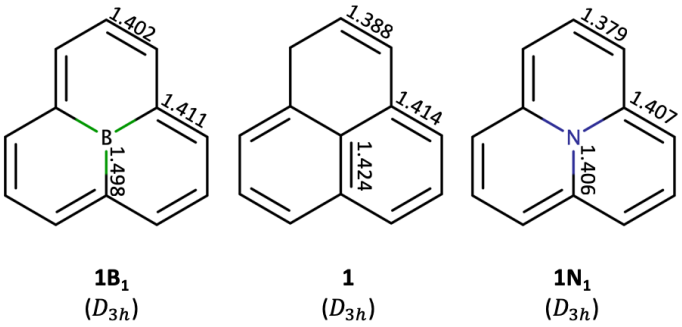

Figure S2: Bond distances on $\mathbf{1B}_1$ (left), **1** (center) and $\mathbf{1N}_1$ (right) systems.

3.1.1 Excited singlet and triplet states of mono-doped 1

Exchange integral[1] between a_1'' and a_2'' orbitals is approximated as

$$K = \frac{E_S - E_T}{2} \tag{S.1}$$

at CIS/6-31G* level of theory $k = 0.14$ eV and 0.16 for $\mathbf{1B}_1$ and $\mathbf{1N}_1$, respectively. These small values can be understood as the lack of overlap between frontier orbitals, Figure S3 corresponds to $\mathbf{1B}_1$ HOMO and LUMO and the overlap between them, the same ocurres with $\mathbf{1N}_1$.

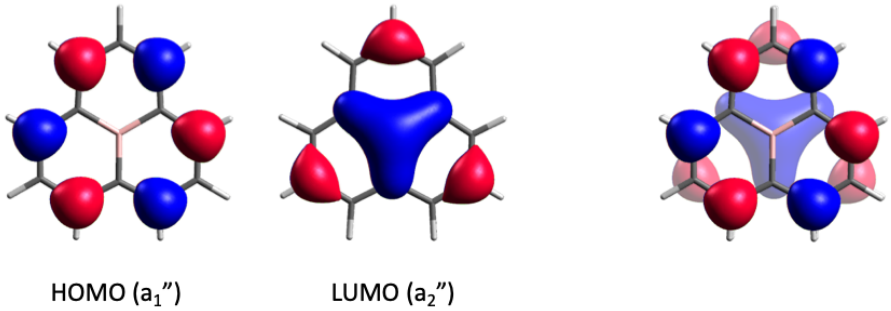

Figure S3: Frontier molecular orbitals (a_1'' and a_2'') of $\mathbf{1B}_1$ (left) and their superposition (right).

The main configuration defining the $1^1A_2'$ and $1^3A_2'$ states of $\mathbf{1B}_1$ and $\mathbf{1N}_1$ ($\approx 80\%$) corresponds to the single electron occupation of a_2'' and a_1'' orbitals. Configurations with four unpaired electrons involving the $3e''$ orbitals contribute to the stabilization of $1^1A_2'$, but not participate significantly to the $1^3A`_2$ wave function.

Table S2: Description of low-lying states of $\mathbf{1B}_1$ and $\mathbf{1N}_1$ energy gaps (in eV). Unpaired electron numbers (N_U) and the main configuration contributions are computed at the RAS-SF/6-311G(d,p) level.

mol.	state	ΔE	N_U	configuration	contributions (%)
$\mathbf{1B}_1$	$1^1A_2'$	0.66	2.40	$(2e'')^4(2a_2'')^1(1a_1'')^1(3e'')^0(3a_2'')^0$	84.13
				$(2e'')^3(2a_2'')^1(1a_1'')^1(3e'')^2(3a_2'')^0$	2.24
				$(2e'')^3(2a_2'')^1(1a_1'')^1(3e'')^2(3a_2'')^0$	2.24
	$1^3A_2'$	0.79	2.36	$(2e'')^4(2a_2'')^1(1a_1'')^1(3e'')^0(3a_2'')^0$	85.46
$\mathbf{1N}_1$	$1^1A_2'$	0.85	2.40	$(2e'')^4(2a_2'')^2(1a_1'')^1(3a_2'')^1(3e'')^0$	84.25
				$(2e'')^4(2a_2'')^1(1a_1'')^1(3a_2'')^1(3e'')^1$	2.10
				$(2e'')^3(2a_2'')^2(1a_1'')^1(3a_2'')^1(3e'')^1$	2.09
	$1^3A_2'$	0.96	2.36	$(2e'')^4(2a_2'')^2(1a_1'')^1(3a_2'')^1(3e'')^0$	85.76

3.2 Triangulene derivatives

Changes in bond length due to the substitution of one or three inner carbon atoms by nitrogen or boron elements shown in Figures S4 and S5.

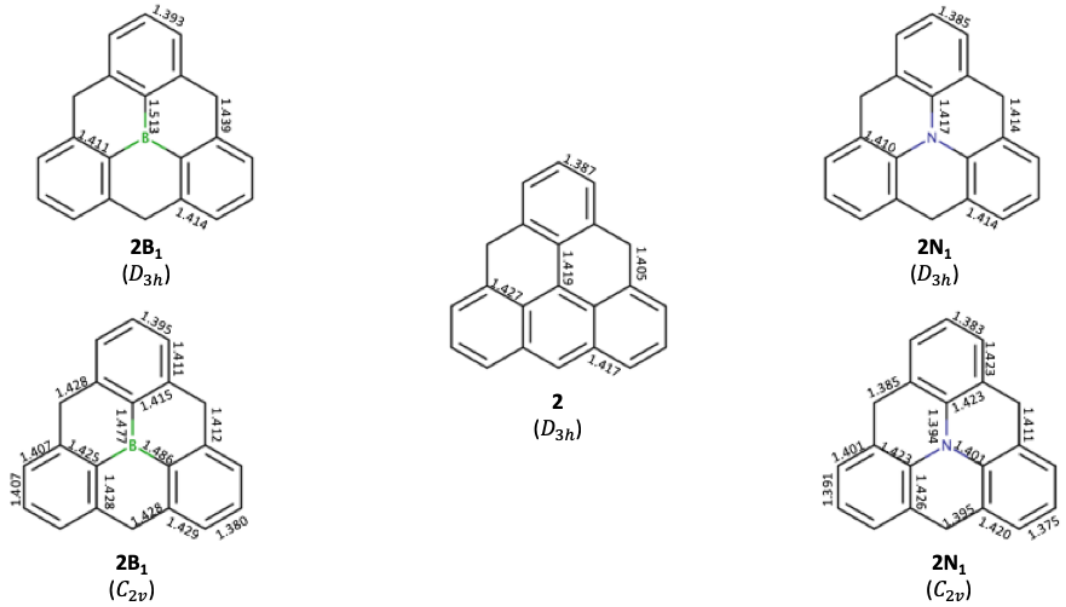

Figure S4: Bond distances of $\mathbf{2B}_1$ (left), **2** (center) and $\mathbf{2N}_1$ (right) systems.

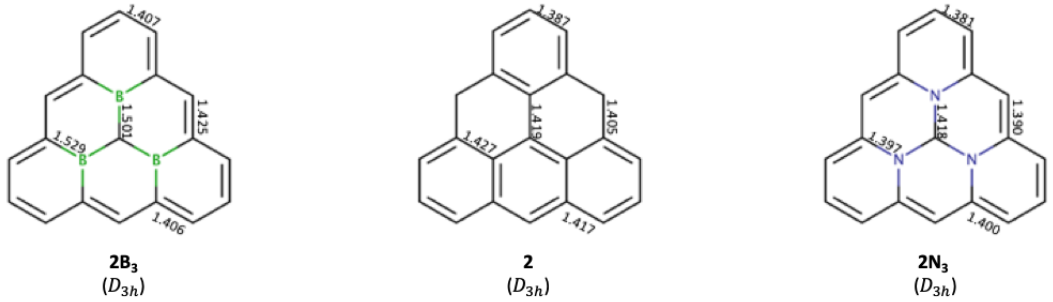

Figure S5: Bond distances of $\mathbf{2B}_3$ (left), **2** (center) and $\mathbf{2N}_3$ (right) systems.

Unpaired electron density is localized over central carbon atom surrounded by doping elements.

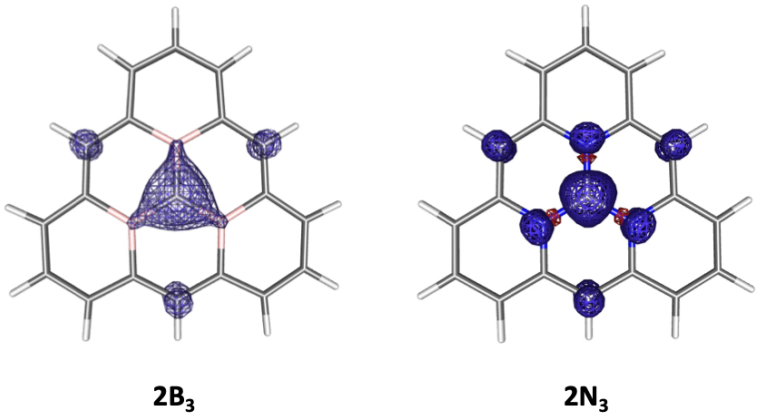

Figure S6: Spin densities of $\mathbf{2B}_3$ and $\mathbf{2N}_3$ doublet ground state computed at M06-2X/6-311G** level.

4 Hydrogenated TGNF

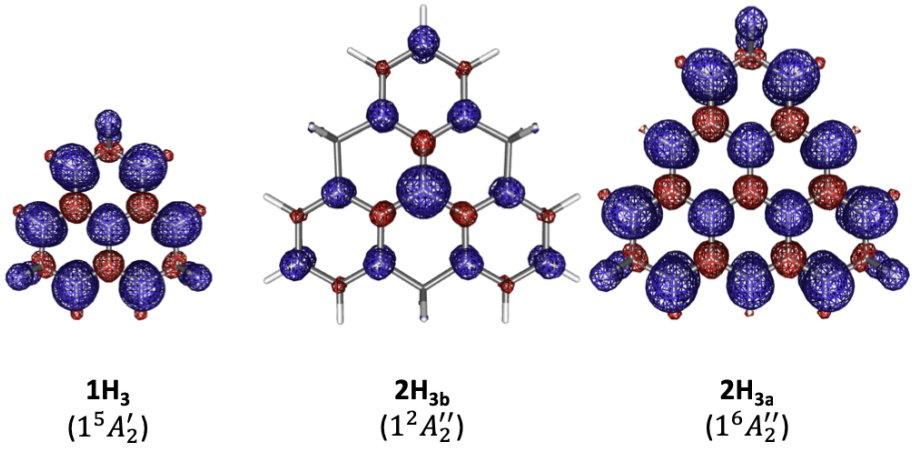

Figure S7: Spin density of hydrogenated derivatives from **1 and 2.**

5 Optimized geometries

1 ($1^2A_1''$)
C 0.00000 0.00000 2.81180
C 1.20613 0.00000 2.12586
C 1.23369 0.00000 0.71233
C 0.00000 0.00000 0.00001
C -1.23369 0.00000 0.71233
C -1.20613 0.00000 2.12586
C 2.44415 0.00000 -0.01844
C 0.00000 0.00000 -1.42433
C 1.23804 0.00000 -2.10735
C 2.43515 0.00000 -1.40585
C -1.23804 0.00000 -2.10735
C -2.43515 0.00000 -1.40585
C -2.44415 0.00000 -0.01844
H -3.38324 0.00000 0.52324
H -3.37364 0.00000 -1.94746
H 3.38324 0.00000 0.52324
H 0.00000 0.00000 3.89575
H 2.14501 0.00000 2.66787
H -2.14501 0.00000 2.66787
H 3.37364 0.00000 -1.94746
H -1.23811 0.00000 -3.19183
H 1.23811 0.00000 -3.19183

2 ($1^3A_2'$)
C -1.20663 0.00000 3.54760
C 1.23650 -0.00000 2.13117
C 1.20663 -0.00000 3.54760
C -0.00000 -0.00000 4.23239
C -0.00000 -0.00000 0.00000
C 2.44236 -0.00000 1.41010
C 2.46390 -0.00000 0.00526
C 2.46899 -0.00000 -2.81877
C 3.66536 -0.00000 -2.11620
C 3.67563 -0.00000 -0.72883
H -2.14526 0.00000 4.09001
H 2.14526 -0.00000 4.09001
H -0.00000 -0.00000 5.31601
H 3.38221 -0.00000 1.95272
H 2.46942 -0.00000 -3.90286
H 4.60380 -0.00000 -2.65800
H 4.61468 -0.00000 -0.18715
C -2.44236 0.00000 1.41010
C -0.00000 -0.00000 1.41868
C -1.23650 0.00000 2.13117
H -3.38221 0.00000 1.95272

C 1.22861 -0.00000 -0.70934
C 1.22739 -0.00000 -2.13643
C 0.00000 0.00000 -2.82020
H 0.00000 0.00000 -3.90543
C -3.67563 0.00000 -0.72883
C -3.66536 0.00000 -2.11620
C -2.46899 0.00000 -2.81877
C -1.22739 0.00000 -2.13643
C -1.22861 0.00000 -0.70934
C -2.46390 0.00000 0.00526
H -4.61468 0.00000 -0.18715
H -4.60380 0.00000 -2.65800
H -2.46942 0.00000 -3.90286

1B$_1$ ($1^1A_1'$)
C 0.00264 -1.49803 0.00000
C -1.25116 -2.14554 -0.00000
H -1.31250 -3.23415 -0.00000
C -2.45070 -1.42059 -0.00000
H -3.38793 -1.96365 -0.00000
C -2.48368 -0.01945 -0.00000
H -3.45864 0.46788 -0.00000
C 1.25872 -2.14111 0.00000
H 1.32390 -3.22951 -0.00000
C 2.45569 -1.41194 0.00000
H 3.39483 -1.95169 0.00000
C 2.48373 -0.01070 0.00000
H 3.45697 0.48007 0.00000
C -1.29867 0.74678 -0.00000
C -1.23261 2.15626 -0.00000
H -2.14439 2.75328 -0.00000
C -0.00499 2.83262 0.00000
H -0.00690 3.91619 0.00000
C 1.22500 2.16059 -0.00000
H 2.13467 2.76082 0.00000
C 1.29603 0.75136 -0.00000
B 0.00000 -0.00015 0.00000

1N$_1$ ($1^1A_1'$)
N -0.00000 -0.00030 0.00000
C -0.00073 -1.40582 0.00000
C -1.21715 0.70354 -0.00000
C 1.21788 0.70228 0.00000
C -1.19523 2.11008 -0.00000
H -2.14763 2.61972 -0.00000
C 0.00145 2.79553 -0.00000
H 0.00201 3.87984 -0.00000

C 1.19741 2.10884 0.00000
H 2.15034 2.61750 0.00000
C -2.42526 -0.01740 -0.00000
H -3.34246 0.55313 -0.00000
C -2.42194 -1.39641 -0.00000
H -3.36098 -1.93776 -0.00000
C -1.22999 -2.09007 -0.00000
H -1.19561 -3.17007 -0.00000
C 2.42524 -0.01990 0.00000
H 3.34303 0.54968 0.00000
C 2.42050 -1.39891 0.00000
H 3.35898 -1.94123 0.00000
C 1.22783 -2.09134 0.00000
H 1.19233 -3.17131 0.00000

$\mathbf{2B}_1$ ($1^2E''$)
C -0.00001 -1.47633 0.00000
C -1.24082 -2.15709 -0.00000
C -1.21496 -3.56749 -0.00000
H -2.14474 -4.12923 -0.00000
C -0.00002 -4.25341 0.00000
H -0.00003 -5.33671 -0.00000
C 1.21492 -3.56751 0.00000
H 2.14469 -4.12926 0.00000
C 1.24080 -2.15711 0.00000
C -2.45880 -1.41141 -0.00000
H -3.39681 -1.96132 -0.00000
C -2.50762 -0.00033 -0.00000
C -1.28974 0.73914 -0.00000
C -1.25934 2.16692 -0.00000
C -2.49873 2.83331 -0.00000
H -2.53005 3.91872 -0.00000
C -3.70615 2.11170 -0.00000
H -4.64048 2.66098 -0.00000
C -3.73496 0.73180 -0.00000
H -4.68306 0.20455 -0.00000
C 0.00002 2.84023 0.00000
H 0.00002 3.92669 0.00000
C 1.25936 2.16691 0.00000
C 2.49876 2.83329 0.00000
H 2.53009 3.91869 0.00000
C 3.70617 2.11166 0.00000
H 4.64051 2.66093 0.00000
C 3.73497 0.73176 0.00000
H 4.68306 0.20449 0.00000
C 1.28974 0.73912 0.00000
C 2.50762 -0.00036 0.00000

C 2.45878 -1.41144 0.00000
H 3.39679 -1.96136 0.00000
B -0.00000 0.00056 0.00000

2B$_1$ ($1^4A_2''$)
C 0.00088 -1.51336 0.00000
C -1.23838 -2.18874 0.00000
C 1.24091 -2.18730 0.00000
C 1.22126 -3.60072 0.00000
H 2.15075 -4.15939 0.00000
C 0.00247 -4.27500 -0.00000
H 0.00310 -5.35945 0.00000
C -1.21709 -3.60213 -0.00000
H -2.14594 -4.16187 -0.00000
C -2.45349 -1.41828 -0.00000
H -3.39396 -1.96167 -0.00000
C -2.51477 0.01895 -0.00000
C -1.31103 0.75590 -0.00000
C -1.27632 2.16662 0.00000
C -2.51109 2.85504 -0.00000
H -2.53141 3.93971 -0.00000
C -3.70361 2.13541 -0.00000
H -4.64282 2.67676 -0.00000
C -3.72908 0.74287 -0.00000
H -4.67795 0.21771 -0.00000
C -0.00164 2.83379 0.00000
H -0.00227 3.92033 0.00000
C 1.27381 2.16810 0.00000
C 1.31016 0.75741 -0.00000
C 2.51475 0.02186 0.00000
C 2.50778 2.85794 0.00000
H 2.52685 3.94264 0.00000
C 3.70114 2.13969 0.00000
H 4.63972 2.68213 0.00000
C 3.72822 0.74719 -0.00000
H 4.67770 0.22312 -0.00000
C 2.45513 -1.41544 -0.00000
H 3.39623 -1.95774 -0.00000
B 0.00000 -0.00022 0.00000

2N$_1$ ($1^2E''$)
N -0.00000 -0.00309 -0.00000
C 0.00012 1.39080 -0.00000
C -1.21262 -0.70406 0.00000
C 1.21249 -0.70428 -0.00000
C -1.23091 2.10490 -0.00000
C -2.43211 1.41479 0.00000

H -3.36845 1.96017 0.00000
C -2.45499 0.00400 0.00000
C -3.65932 -0.71137 0.00000
H -4.58923 -0.15756 0.00000
C -3.64993 -2.10258 0.00000
H -4.58922 -2.64355 0.00000
C -2.46475 -2.79978 0.00000
H -2.45629 -3.88296 0.00000
C -1.21260 -2.12957 0.00000
C -0.00026 -2.81938 0.00000
H -0.00035 -3.90255 0.00000
C 1.21221 -2.12979 -0.00000
C 2.46424 -2.80022 -0.00000
H 2.45558 -3.88341 -0.00000
C 3.64955 -2.10324 -0.00000
H 4.58874 -2.64438 -0.00000
C 3.65919 -0.71203 -0.00000
H 4.58920 -0.15839 -0.00000
C 2.45499 0.00356 -0.00000
C 2.43237 1.41435 -0.00000
H 3.36881 1.95955 -0.00000
C 1.23130 2.10468 -0.00000
C 1.19880 3.52730 -0.00000
H 2.14467 4.05492 -0.00000
C 0.00038 4.21820 0.00000
H 0.00048 5.30165 0.00000
C -1.19815 3.52752 0.00000
H -2.14393 4.05531 0.00000

2N$_1$ ($1^4A_2''$)
N 0.00000 -0.00035 0.00000
C 0.00084 -1.41737 0.00000
C -1.22160 -2.12068 -0.00000
C 1.22411 -2.11923 0.00000
C -2.44577 -1.41381 -0.00000
H -3.38310 -1.95540 -0.00000
C -2.44753 -0.00047 -0.00000
C -1.22797 0.70795 -0.00000
C -1.22582 2.11802 -0.00000
C -0.00167 2.82471 0.00000
H -0.00231 3.90761 0.00000
C 1.22331 2.11947 0.00000
C 1.22713 0.70940 0.00000
C 2.44752 0.00243 0.00000
C 2.44745 -1.41091 0.00000
H 3.38542 -1.95139 0.00000
C 1.19884 -3.53269 0.00000

H 2.14575 -4.05979 0.00000
C 0.00251 -4.22991 -0.00000
H 0.00315 -5.31321 -0.00000
C -1.19466 -3.53411 -0.00000
H -2.14093 -4.06232 -0.00000
C -3.65907 0.72831 -0.00000
H -4.58925 0.17225 -0.00000
C -3.66464 2.11287 -0.00000
H -4.60285 2.65366 -0.00000
C -2.46346 2.80162 -0.00000
H -2.44787 3.88561 -0.00000
C 3.65821 0.73265 0.00000
H 4.58904 0.17769 0.00000
C 3.66213 2.11721 0.00000
H 4.59970 2.65911 0.00000
C 2.46014 2.80454 0.00000
H 2.44326 3.88851 0.00000

$\mathbf{2B}_3$ ($1^2A_2''$)
C 1.24818 0.00000 3.63183
C -1.34415 -0.00000 2.22905
C -1.24818 -0.00000 3.63183
C 0.00000 -0.00000 4.28100
C 0.00000 -0.00000 0.00007
C -2.55215 -0.00000 1.47336
C -2.60257 -0.00000 0.04959
C -2.52138 -0.00000 -2.89678
C -3.70762 -0.00000 -2.14041
C -3.76955 -0.00000 -0.73498
H 2.14100 0.00000 4.25599
H -2.14100 -0.00000 4.25599
H 0.00000 -0.00000 5.36560
H -3.50026 -0.00000 2.02039
H -2.61590 -0.00000 -3.98256
H -4.64667 -0.00000 -2.68236
H -4.75684 -0.00000 -0.27411
C 2.55215 0.00000 1.47336
B 0.00000 -0.00000 1.50083
C 1.34415 0.00000 2.22905
H 3.50026 0.00000 2.02039
B -1.29997 -0.00000 -0.75061
C -1.25841 -0.00000 -2.27856
C -0.00000 0.00000 -2.94677
H -0.00000 0.00000 -4.04177
C 3.76955 0.00000 -0.73498
C 3.70762 0.00000 -2.14041
C 2.52138 0.00000 -2.89678

C 1.25841 0.00000 -2.27856
B 1.29997 0.00000 -0.75061
C 2.60257 0.00000 0.04959
H 4.75684 0.00000 -0.27411
H 4.64667 0.00000 -2.68236
H 2.61590 0.00000 -3.98256

2N$_3$ ($1^2A_2''$)
N 0.00106 -1.41819 0.00000
C -1.21192 -2.11096 0.00000
C -2.39828 -1.38695 0.00000
H -3.33214 -1.92673 0.00000
C -2.43437 0.00220 0.00000
C 1.21506 -2.10915 0.00000
C 2.40034 -1.38337 0.00000
H 3.33501 -1.92176 0.00000
C 2.43437 0.00583 0.00000
N -1.22916 0.70853 0.00000
C -1.22235 2.10500 0.00000
C -0.00206 2.77018 0.00000
H -0.00287 3.84918 0.00000
C 1.21922 2.10682 -0.00000
N 1.22810 0.71037 -0.00000
C 1.19862 -3.50954 -0.00000
H 2.15327 -4.01550 -0.00000
C 0.00313 -4.20088 -0.00000
H 0.00394 -5.28471 -0.00000
C -1.19339 -3.51132 -0.00000
H -2.14728 -4.01871 0.00000
C -2.44457 2.78909 0.00000
H -2.40746 3.86926 0.00000
C -3.63998 2.09760 0.00000
H -4.57872 2.63850 0.00000
C -3.63909 0.71666 0.00000
H -4.55482 0.14332 -0.00000
C 2.44041 2.79273 -0.00000
H 2.40169 3.87285 0.00000
C 3.63685 2.10302 -0.00000
H 4.57478 2.64532 -0.00000
C 3.63802 0.72208 -0.00000
H 4.55460 0.15011 -0.00000
C 0.00000 -0.00006 0.00000

2N$_2$ ($1^2A_1'$)
N 1.20549 -0.69449 0.00000
C -0.00000 0.00388 0.00000
N -1.20544 -0.69458 -0.00000

C -0.00005 1.40207 0.00000
C -2.43111 0.01595 -0.00000
C -2.42722 1.39206 -0.00000
H -3.38345 1.89800 -0.00000
C -1.23995 2.12939 0.00000
C -1.21091 3.53038 0.00000
H -2.14883 4.07128 0.00000
C -0.00015 4.20615 0.00000
H -0.00019 5.29068 0.00000
C 1.21066 3.53046 0.00000
H 2.14854 4.07144 0.00000
C 1.23980 2.12948 0.00000
C 2.42712 1.39223 0.00000
H 3.38331 1.89824 0.00000
C 2.43110 0.01612 -0.00000
C -3.64613 -0.71361 -0.00000
H -4.56025 -0.13795 -0.00000
C -3.64438 -2.08054 -0.00000
H -4.58099 -2.62483 -0.00000
C -2.44018 -2.77963 -0.00000
H -2.41147 -3.85996 -0.00000
C -1.22002 -2.11467 -0.00000
C 0.00010 -2.77347 -0.00000
H 0.00014 -3.85294 -0.00000
C 1.22017 -2.11459 -0.00000
C 2.44038 -2.77946 -0.00000
H 2.41174 -3.85979 -0.00000
C 3.64453 -2.08028 0.00000
H 4.58118 -2.62451 0.00000
C 3.64618 -0.71335 0.00000
H 4.56026 -0.13762 0.00000

$\mathbf{1H}_{3a}$ ($1^5A_2'$)
C 0.00000 -0.00001 -0.00000
C 0.00047 -1.44407 -0.00000
C 1.21495 -2.13943 0.00000
H 1.19129 -3.22379 0.00000
C -1.21356 -2.14022 -0.00000
H -1.18919 -3.22456 -0.00000
C 1.25061 0.72263 0.00000
C 1.24545 2.12190 0.00000
H 2.19606 2.64344 0.00000
C 2.46034 0.01906 0.00000
H 3.38728 0.58156 0.00000
C -1.25108 0.72182 -0.00000
C -1.24682 2.12109 -0.00000
H -2.19778 2.64201 -0.00000

C -2.46036 0.01746 -0.00000
H -3.38766 0.57936 -0.00000
C 2.54759 -1.46978 0.00000
H 3.13665 -1.80916 0.86779
H 3.13665 -1.80916 -0.86779
C -2.54663 -1.47144 -0.00000
H -3.13547 -1.81120 0.86779
H -3.13547 -1.81120 -0.86779
C -0.00096 2.94107 0.00000
H -0.00118 3.62109 0.86758
H -0.00118 3.62109 -0.86758

2H$_{3a}$ ($1^6A_2''$)
C 0.00000 -0.00015 0.00000
C 0.00093 -1.42002 0.00000
C -1.23031 0.70923 0.00000
C 1.22938 0.71084 0.00000
C -1.23898 2.15076 0.00000
C -2.44121 2.84551 0.00000
H -2.41901 3.93012 0.00000
C -0.00185 2.83241 -0.00000
H -0.00256 3.91754 -0.00000
C 1.23617 2.15238 -0.00000
C 2.43749 2.84870 -0.00000
H 2.41387 3.93328 -0.00000
C -2.48235 -0.00585 0.00000
C -3.68584 0.68666 0.00000
H -4.61335 0.12469 0.00000
C -2.45231 -1.41783 0.00000
H -3.39157 -1.96053 -0.00000
C -1.24341 -2.14849 0.00000
C -1.24379 -3.53683 -0.00000
H -2.19388 -4.05978 -0.00000
C 2.48235 -0.00261 -0.00000
C 3.68494 0.69147 -0.00000
H 4.61319 0.13072 -0.00000
C 2.45416 -1.41462 -0.00000
H 3.39413 -1.95609 -0.00000
C 1.24622 -2.14686 -0.00000
C 1.24841 -3.53520 0.00000
H 2.19918 -4.05690 0.00000
C -3.77400 2.17566 -0.00000
H -4.36340 2.51495 0.86748
H -4.36340 2.51495 -0.86748
C 3.77115 2.18060 0.00000
H 4.36011 2.52065 0.86748
H 4.36011 2.52065 -0.86748

C 0.00285 -4.35604 0.00000
H 0.00329 -5.03631 0.86726
H 0.00329 -5.03631 -0.86726

2H$_{3b}$ ($1^2A_2''$)
C -0.00000 -0.00009 0.00000
C 0.00039 -1.44624 -0.00000
C -1.21233 -2.17049 -0.00000
C -1.19682 -3.55848 0.00000
H -2.14109 -4.09389 -0.00000
C 0.00114 -4.26131 0.00000
H 0.00143 -5.34487 0.00000
C 1.19873 -3.55784 0.00000
H 2.14329 -4.09274 0.00000
C 1.21350 -2.16984 0.00000
C -1.25291 0.72292 0.00000
C -1.27365 2.13499 0.00000
C -2.48351 2.81567 0.00000
H -2.47532 3.90152 0.00000
C -3.69113 2.12962 0.00000
H -4.62943 2.67078 0.00000
C -3.68070 0.74086 0.00000
H -4.61646 0.19070 0.00000
C -2.48597 0.03401 0.00000
C 1.25252 0.72359 -0.00000
C 1.27251 2.13567 0.00000
C 2.48200 2.81700 -0.00000
H 2.47323 3.90285 0.00000
C 3.68999 2.13160 -0.00000
H 4.62800 2.67326 -0.00000
C 3.68030 0.74283 -0.00000
H 4.61635 0.19318 -0.00000
C 2.48595 0.03535 -0.00000
C -2.54320 -1.46915 0.00000
H -3.11716 -1.80021 0.87393
H -3.11716 -1.80021 -0.87393
C 2.54399 -1.46778 -0.00000
H 3.11813 -1.79854 0.87393
H 3.11813 -1.79854 -0.87393
C -0.00079 2.93678 -0.00000
H -0.00096 3.59928 0.87319
H -0.00096 3.59928 -0.87319

References

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