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

Supplementary Information

Unraveling the flexible aromaticity of $C_{13}H_9^{+/0/-}$: a 2D superatomic-molecule theory

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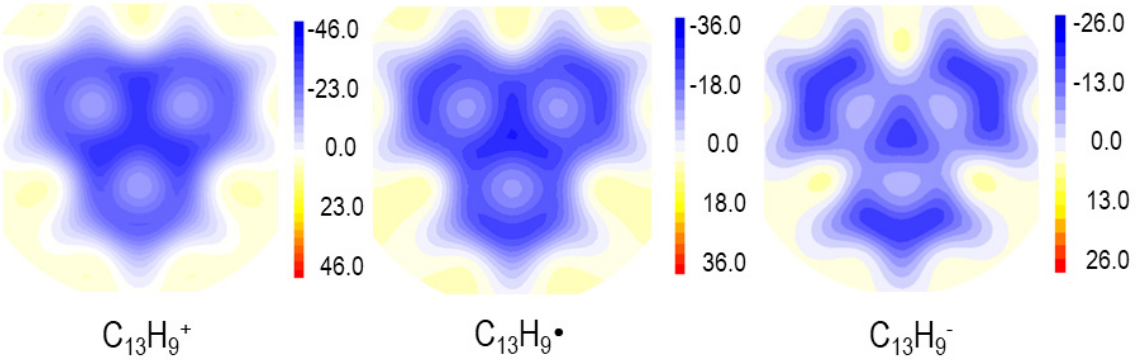

Fig. S1 $NICS_{zz}(1)$ contour planes (ppm) of $C_{13}H_9^+$, $C_{13}H_9$• and $C_{13}H_9^-$.

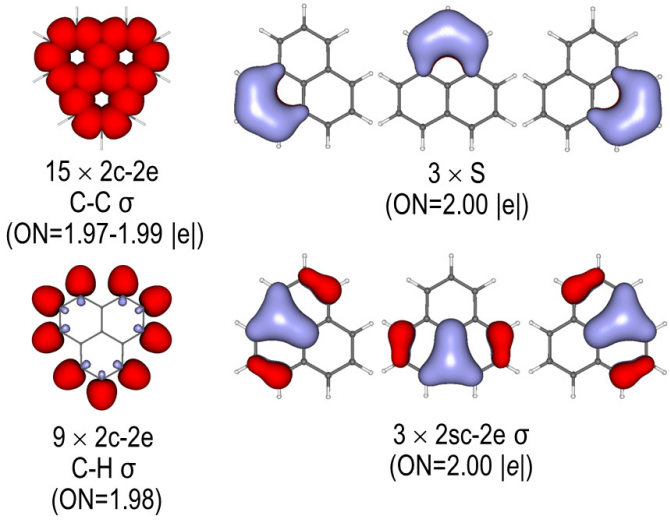

Fig. S2 Chemical bonding picture of $C_{13}H_9^+$.

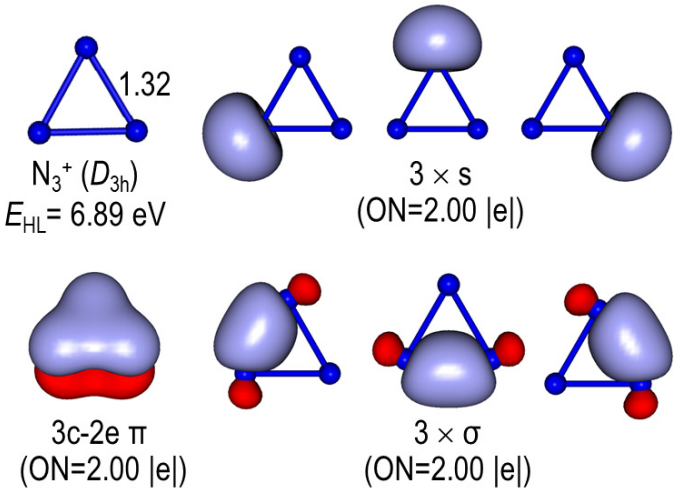

Fig. S3 Chemical bonding picture of N_3^+.

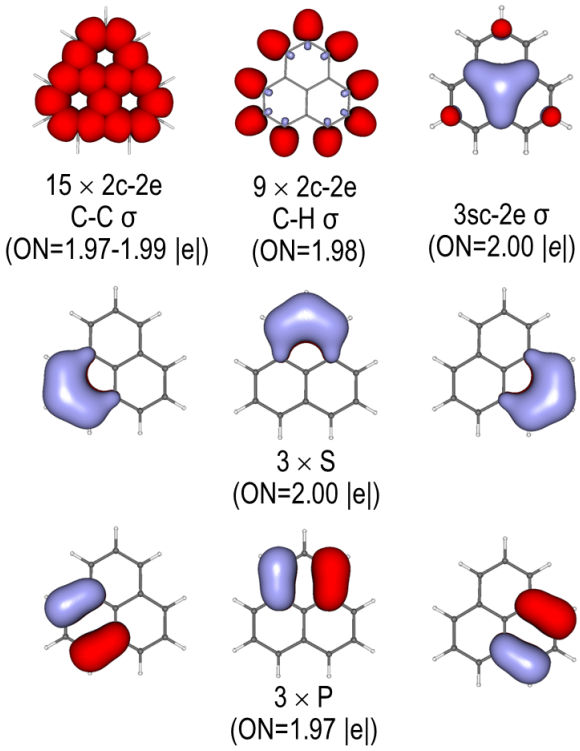

Fig. S4 Chemical bonding picture of $C_{13}H_9^-$.

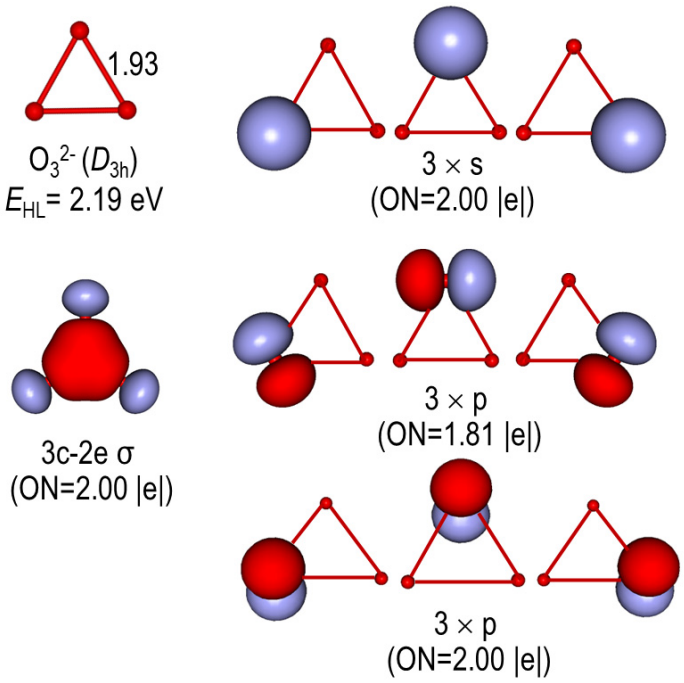

Fig. S5 Chemical bonding picture of O_3^{2-}.

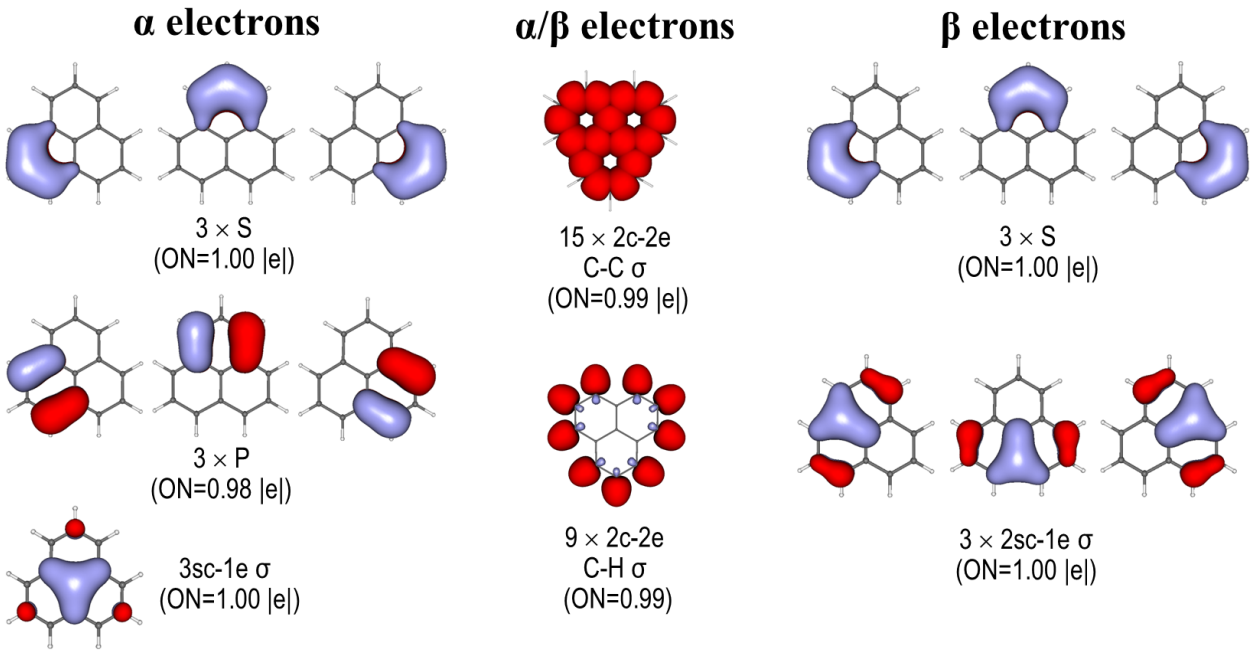

Fig. S6 Chemical bonding picture of $C_{13}H_9^{\bullet}$.

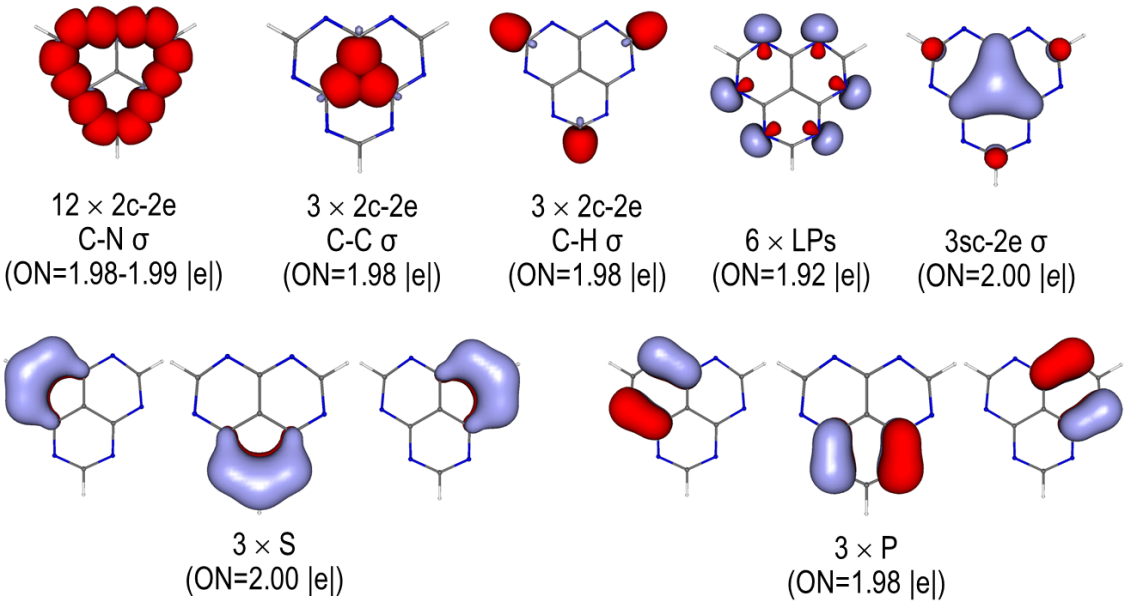

Fig. S7 Chemical bonding picture of $C_7N_6H_3^-$.

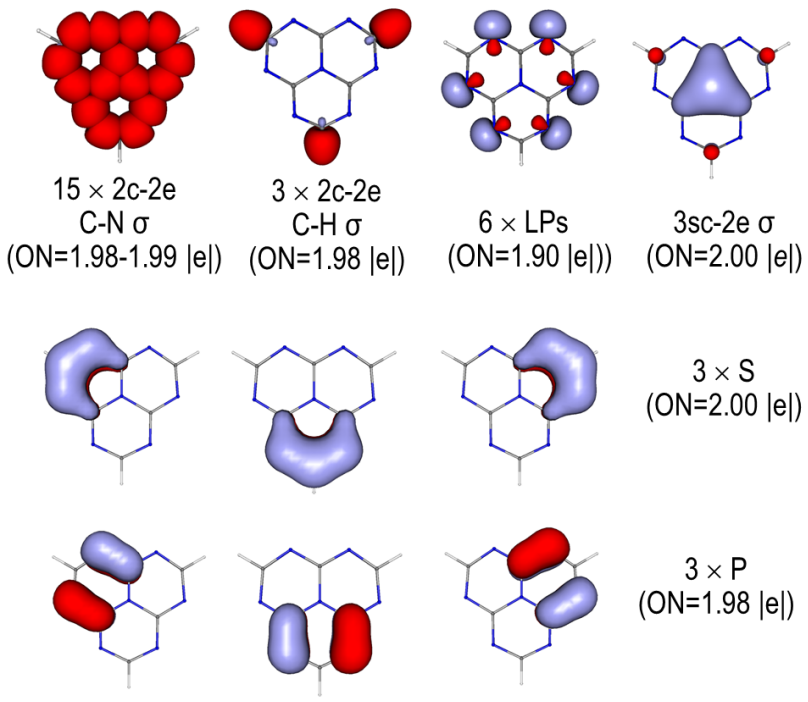

Fig. S8 Chemical bonding picture of $C_6N_7H_3$.

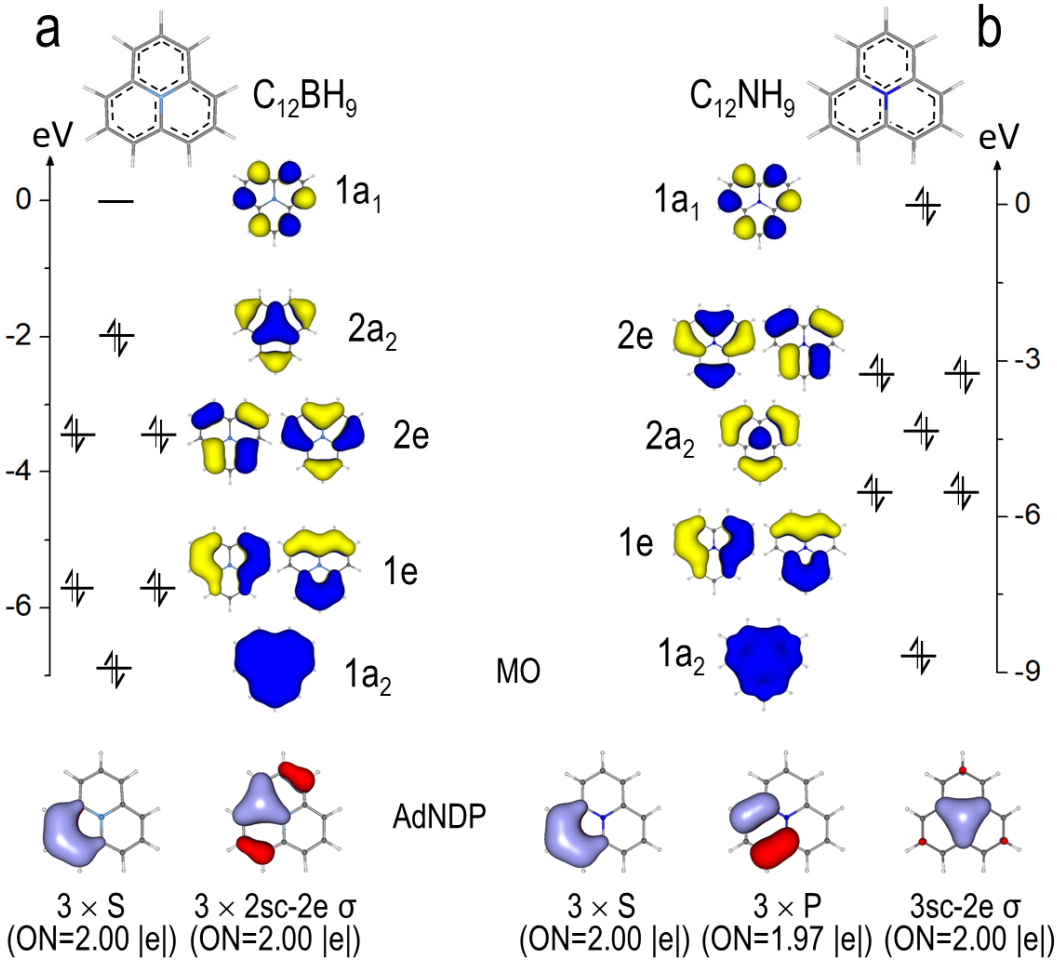

Fig. S9 Canonical MO diagrams and AdNDP bonding patterns of (a) $C_{12}BH_9$ and (b) $C_{12}NH_9$. Only π frameworks are presented.

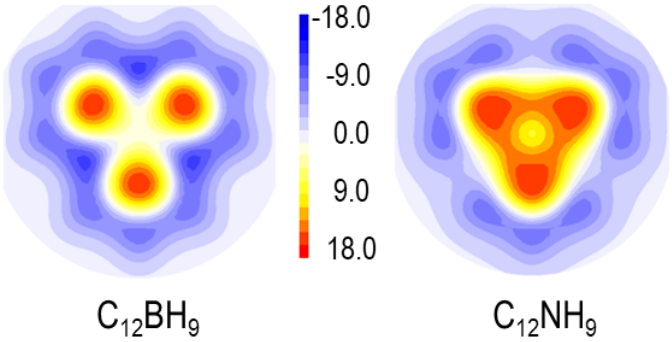

Fig. S10 NICS(1) contour planes (ppm) of $C_{12}BH_9$ (left) and $C_{12}NH_9$ (right).

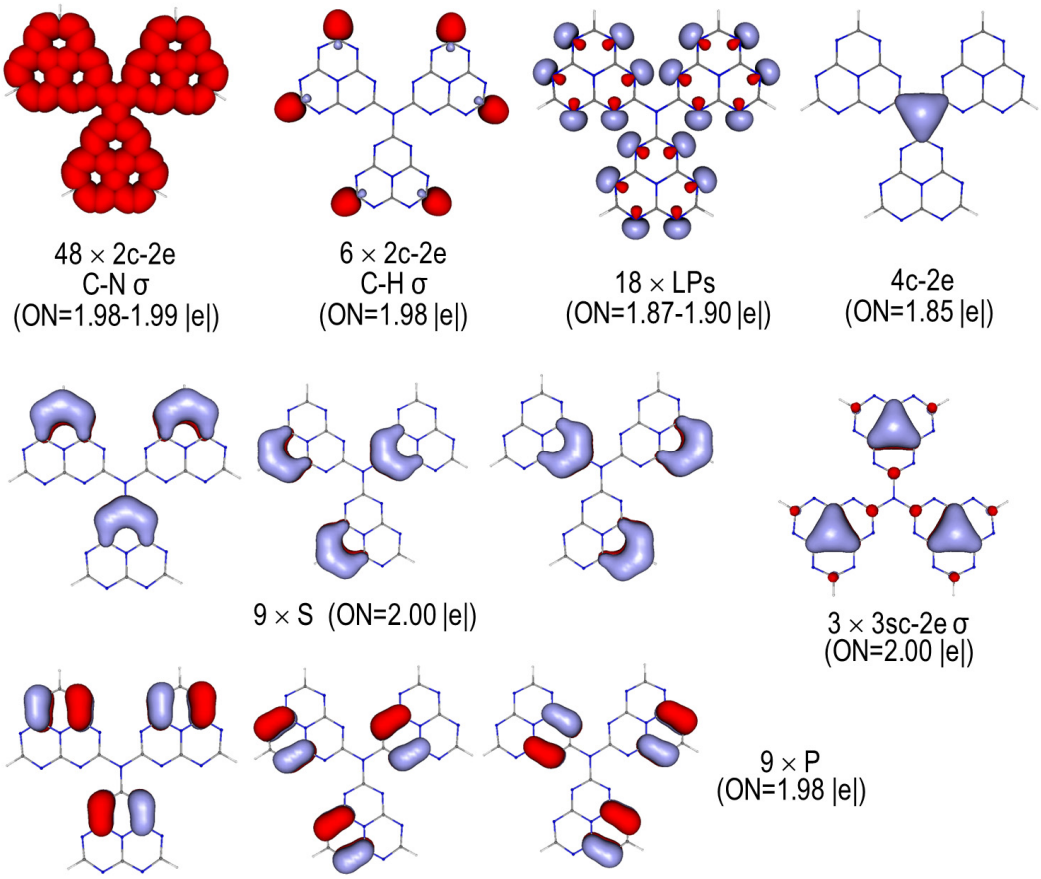

Fig. S11 Chemical bonding picture of $C_{18}H_6N_{22}$.

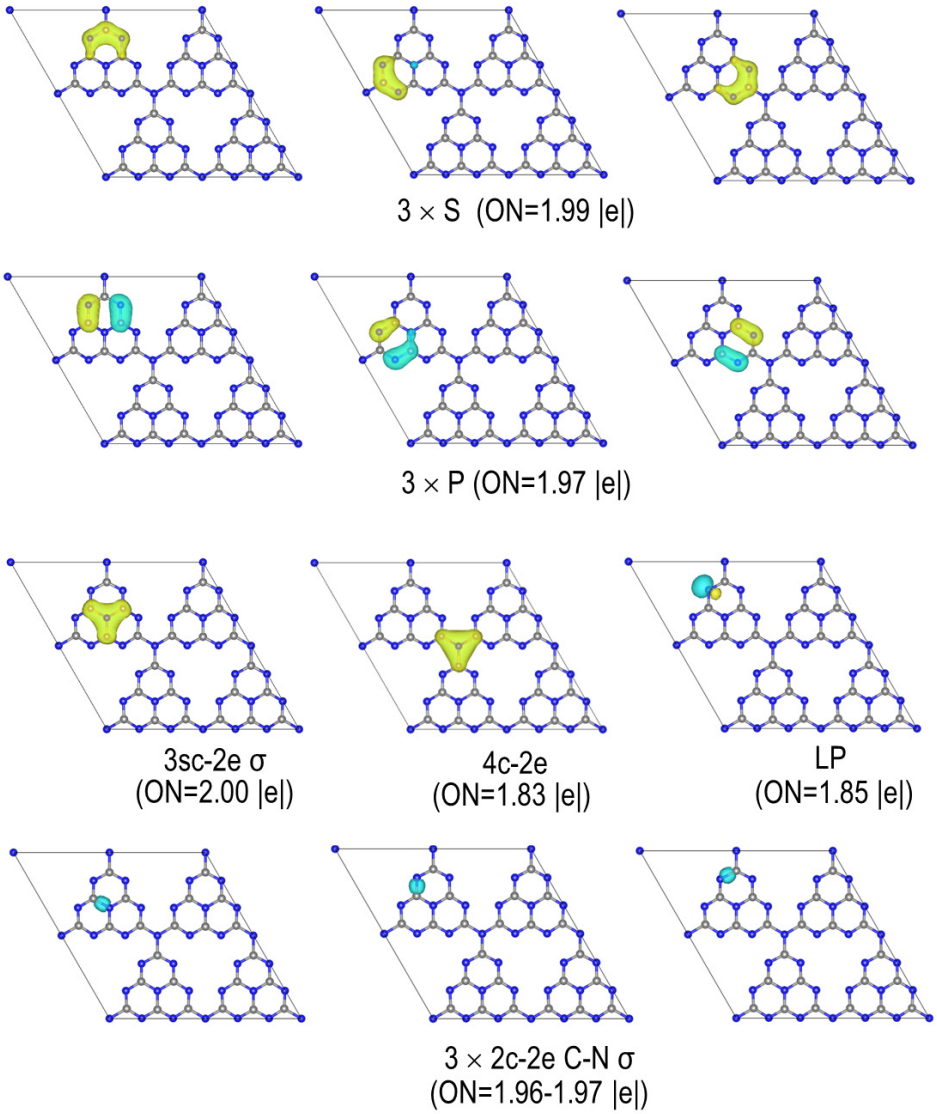

Fig. S12 Chemical bonding picture of g-C_3N_4 crystal (2×2 supercell).

Cartesian coordinates (in Å) of the optimized geometries.

		x	*y*	*z*
$C_{13}H_9^-$	C	0.000000	0.000000	0.000000
	C	1.247239	2.122915	0.000000
	C	2.462118	0.018683	0.000000
	C	-2.462118	0.018683	0.000000
	C	-1.247239	2.122915	0.000000
	C	1.214879	-2.141598	0.000000
	C	-1.214879	-2.141598	0.000000
	C	0.000000	1.441795	0.000000
	C	1.248631	-0.720898	0.000000
	C	2.441253	1.409458	0.000000
	C	-1.248631	-0.720898	0.000000
	C	-2.441253	1.409458	0.000000
	C	0.000000	-2.818916	0.000000
	H	1.254204	3.209172	0.000000
	H	3.406326	-0.518413	0.000000
	H	3.383832	1.953656	0.000000
	H	-3.406326	-0.518413	0.000000
	H	-3.383832	1.953656	0.000000
	H	-1.254204	3.209172	0.000000
	H	2.152122	-2.690759	0.000000
	H	0.000000	-3.907312	0.000000
	H	-2.152122	-2.690759	0.000000
$C_{13}H_9^+$	C	0.000000	0.000000	0.000000
	C	1.238068	2.105669	0.000000
	C	2.442597	0.019364	0.000000
	C	-2.442597	0.019364	0.000000
	C	-1.238068	2.105669	0.000000
	C	1.204529	-2.125033	0.000000
	C	-1.204529	-2.125033	0.000000
	C	0.000000	1.420136	0.000000
	C	1.229874	-0.710068	0.000000
	C	2.443471	1.410739	0.000000
	C	-1.229874	-0.710068	0.000000
	C	-2.443471	1.410739	0.000000
	C	0.000000	-2.821478	0.000000

	H	1.240911	3.190497	0.000000
	H	3.383507	-0.520588	0.000000
	H	3.380922	1.951976	0.000000
	H	-3.383507	-0.520588	0.000000
	H	-3.380922	1.951976	0.000000
	H	-1.240911	3.190497	0.000000
	H	2.142596	-2.669909	0.000000
	H	0.000000	-3.903953	0.000000
	H	-2.142596	-2.669909	0.000000
$C_{13}H_9$•	C	0.000000	0.000000	0.000000
	C	1.241573	2.112776	0.000000
	C	2.450504	0.018845	0.000000
	C	-2.450504	0.018845	0.000000
	C	-1.241573	2.112776	0.000000
	C	1.208932	-2.131622	0.000000
	C	-1.208932	-2.131622	0.000000
	C	0.000000	1.429531	0.000000
	C	1.23801	-0.714766	0.000000
	C	2.441359	1.409519	0.000000
	C	-1.23801	-0.714766	0.000000
	C	-2.441359	1.409519	0.000000
	C	0.000000	-2.819039	0.000000
	H	1.244694	3.197434	0.000000
	H	3.391406	-0.520781	0.000000
	H	3.380365	1.951655	0.000000
	H	-3.391406	-0.520781	0.000000
	H	-3.380365	1.951655	0.000000
	H	-1.244694	3.197434	0.000000
	H	2.146712	-2.676654	0.000000
	H	0.000000	-3.903309	0.000000
	H	-2.146712	-2.676654	0.000000
$C_7N_6H_3^-$	C	0.000000	0.000000	0.000000
	N	1.180623	2.082909	0.000000
	N	2.394164	-0.019005	0.000000
	N	-2.394164	-0.019005	0.000000
	N	-1.180623	2.082909	0.000000
	N	1.213541	-2.063904	0.000000

	N	-1.213541	-2.063904	0.000000
	C	0.000000	1.415722	0.000000
	C	1.226051	-0.707861	0.000000
	C	2.270658	1.310965	0.000000
	C	-1.226051	-0.707861	0.000000
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	C	0.000000	-2.62193	0.000000
	H	3.214831	1.856083	0.000000
	H	-3.214831	1.856083	0.000000
	H	0.000000	-3.712167	0.000000
$C_6N_7H_3$	N	0.000000	0.000000	0.000000
	N	1.164564	2.055911	0.000000
	N	2.362753	-0.019414	0.000000
	N	-2.362753	-0.019414	0.000000
	N	-1.164564	2.055911	0.000000
	N	1.19819	-2.036497	0.000000
	N	-1.19819	-2.036497	0.000000
	C	0.000000	1.407911	0.000000
	C	1.219286	-0.703955	0.000000
	C	2.264521	1.307422	0.000000
	C	-1.219286	-0.703955	0.000000
	C	-2.264521	1.307422	0.000000
	C	0.000000	-2.614844	0.000000
	H	3.205329	1.850598	0.000000
	H	-3.205329	1.850598	0.000000
	H	0.000000	-3.701195	0.000000
$C_{18}N_{22}H_6$	N	0.000000	0.000000	0.000000
	N	1.16815	-6.175955	0.000000
	C	0.000000	-5.534219	0.000000
	C	1.202716	-3.411443	0.000000
	N	2.354625	-4.088356	0.000000
	C	2.262423	-5.415393	0.000000
	C	-1.202716	-3.411443	0.000000
	N	-2.354625	-4.088356	0.000000
	C	-2.262423	-5.415393	0.000000
	N	-1.16815	-6.175955	0.000000
	N	1.172139	-2.089635	0.000000

	C	0.000000	-1.471101	0.000000
	N	-1.172139	-2.089635	0.000000
	N	-3.576923	2.065137	0.000000
	N	-2.363308	4.083344	0.000000
	C	-2.353038	2.747304	0.000000
	C	-4.792774	2.767109	0.000000
	N	-4.764459	4.099625	0.000000
	C	-3.558656	4.667012	0.000000
	C	-3.555754	0.664139	0.000000
	N	-2.395747	0.029715	0.000000
	C	-1.27401	0.73555	0.000000
	N	-1.223607	2.05992	0.000000
	N	-5.932609	2.07633	0.000000
	C	-5.821079	0.748381	0.000000
	N	-4.717933	0.005013	0.000000
	N	0.000000	-4.130275	0.000000
	N	3.576923	2.065137	0.000000
	N	4.717933	0.005013	0.000000
	C	3.555754	0.664139	0.000000
	C	4.792774	2.767109	0.000000
	N	5.932609	2.07633	0.000000
	C	5.821079	0.748381	0.000000
	C	2.353038	2.747304	0.000000
	N	1.223607	2.05992	0.000000
	C	1.27401	0.73555	0.000000
	N	2.395747	0.029715	0.000000
	N	4.764459	4.099625	0.000000
	C	3.558656	4.667012	0.000000
	N	2.363308	4.083344	0.000000
	H	3.207024	-5.952257	0.000000
	H	-3.551294	5.753492	0.000000
	H	-6.758318	0.198764	0.000000
	H	6.758318	0.198764	0.000000
	H	-3.207024	-5.952257	0.000000
	H	3.551294	5.753492	0.000000

Structural information of g-C_3N_4 monolayer.

lattice parameters (Å, °)

a = b = 7.13205 c = 20

α = β = 90 γ= 120

fractional coordinates

	x	*y*	*z*
C	0.1194100009999985	0.0597100000000026	0.5000000000000000
C	0.4402900039999977	0.0597100000000026	0.5000000000000000
C	0.4402900039999977	0.3805800080000026	0.5000000000000000
C	0.2769599849999977	0.0539299989999975	0.5000000000000000
C	0.4460699859999977	0.2230399999999975	0.5000000000000000
C	0.2769599849999977	0.2230300009999979	0.5000000000000000
C	0.6194099780000002	0.0597100000000026	0.5000000000000000
C	0.9402899740000024	0.0597100000000026	0.5000000000000000
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C	0.1194100009999985	0.5597100259999976	0.5000000000000000
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C	0.4402900039999977	0.8805800080000026	0.5000000000000000
C	0.2769599849999977	0.5539299850000035	0.5000000000000000
C	0.4460699859999977	0.7230399849999998	0.5000000000000000
C	0.2769599849999977	0.7230299710000025	0.5000000000000000
C	0.6194099780000002	0.5597100259999976	0.5000000000000000
C	0.9402899740000024	0.5597100259999976	0.5000000000000000
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C	0.7769600150000002	0.5539299850000035	0.5000000000000000
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N	0.5000000000000000	0.5000000000000000	0.5000000000000000