

Superhalogen and Superacid

Andrey V. Kulsha,¹ Dmitry I. Sharapa^{2,3}

Correspondence to: Andrey V. Kulsha Andrey_601@tut.by; Dmitry I. Sharapa dmitry.sharapa@kit.edu

¹ Andrey V. Kulsha

Lyceum of Belarusian State University, 8 Ulijanuskaja str., Minsk, Belarus, 220030

² Dmitry I. Sharapa

Chair of Theoretical Chemistry and Interdisciplinary Center for Molecular Materials, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

³ Institute of Catalysis Research and Technology (IKFT), Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen, Germany, D-76344

ABSTRACT

A superhalogen $F@C_{20}(CN)_{20}$ and a corresponding Brønsted superacid were designed and investigated on DFT and DLPNO-CCSD(T) levels of theory. Calculated compounds have outstanding electron affinity and deprotonation energy, respectively. We consider superacid $H[F@C_{20}(CN)_{20}]$ to be able to protonate molecular nitrogen. The stability of these structures is discussed, while some of the previous predictions concerning neutral Brønsted superacids of record strength are doubted.

Introduction

Traditionally, a superhalogen is a molecule with high electron affinity, which forms a stable anion. A good example is AuF_6 with electron affinity of about 8.2 eV.¹ Superhalogen anions usually have low proton affinities leading to superacids.^{2,3}

However, few of the known superhalogen neutral molecules are stable in condensed phase. For example, some anions were predicted to have vertical electron detachment energies above 13 eV,^{4,5} but the corresponding neutral molecules are too unstable to be qualified as superhalogens. The goal of this article was to design structures that could behave closer to real halogen atoms and acid molecules, but with extreme properties.

Design

The idea of symmetric cage surrounded with electron-withdrawing groups is barely new.⁶⁻¹³ For example, one of the strongest currently known Brønsted acids is fluorocarborane acid $H[CHB_{11}F_{11}]$.¹⁴ Its anion is formed by a carborane cage surrounded with fluorine atoms and shows superhalogenic behavior. A similar structure with cyano groups, $B_{12}(CN)_{12}^{2-}$, was suggested as a highly stable dianion with second electron bound by 5.3 eV.^{15,16}

Going this way, we designed a dodecahedrane cage with 20 cyano groups. A large noble-gas-like HOMO-LUMO gap should make this structure kinetically more stable than halogenated dodecahedranes like $C_{20}Cl_{20}$ suffering from lone pair crowding and consequent elimination of halogen diatomics.¹⁷ Therefore, the last step to superhalogen was the encapsulation of a single fluorine atom. It is known that atomic fluorine has lower electron affinity than atomic chlorine because of large

density of negative charge in fluoride anion due to its small radius. Encapsulation into $C_{20}(CN)_{20}$ helps to delocalize the excess of negative charge over twenty electron-withdrawing groups and makes $F@C_{20}(CN)_{20}^-$ a very stable anion (Figure 1). Hereinafter we abbreviate $F@C_{20}(CN)_{19}$ structure as **X**, so the short notation for the superhalogenic anion is NCX^- .

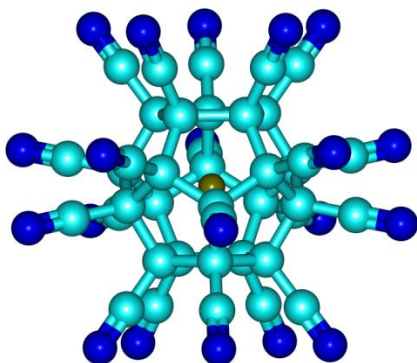


Figure 1. Structure of $F@C_{20}(CN)_{20}^-$.

Color coding: C – cyan, N – dark blue, F – olive.

Computational details

Recently developed DLPNO approach to coupled cluster theory¹⁸⁻²³ induced us to use this level of theory for the single-point computations as implemented in ORCA 4.0 package.²⁴ This method was shown to provide results of canonical coupled-cluster quality.²⁵⁻³¹ All the calculations were performed for gas phase.

The standard cc-pVTZ basis set³² was chosen for all atoms except for nitrogen, where maug-cc-pVTZ³³ was used because nitrogen atoms fill the surface of the anion. The corresponding auxiliary basis sets were cc-pVTZ/C and aug-cc-pVTZ/C,³⁴ respectively. Test calculations (Table 1) were performed with 6-311G* basis set.³⁵

For geometry optimizations we chose a DFT functional PBE0³⁶ as implemented in Gaussian16 package³⁷. This functional is known to produce overall good geometries for organic structures. Usually it underestimates C≡N bond lengths nearly by 0.01Å, and this is the most energy-sensitive deviation for our systems, but

the corresponding shift of energy differences appeared to be negligible for our purposes (about 0.002 eV). Vibrational frequencies were computed on PBE0 level of theory to ensure that the structures being discussed correspond to real minima on their PES. To obtain reaction enthalpies (including electron affinity EA and proton affinity PA) at 0 Kelvins, zero-point vibrational energies (ZPE) were accounted. The corresponding entropies and thermal corrections were used to estimate standard Gibbs energies (including gas-phase basicity GB) at 298.15 Kelvins.

Most of the structures accounted are closed-shell singlets with HOMO-LUMO gap sufficiently large to use NormalPNO cutoffs in ORCA. However, neutral NCX is a doublet with quite small HOMO-LUMO gap; hence we used UHF wavefunction with TightPNO cutoffs for electron affinity determination.^{26,27,38} That choice is confirmed with results of test computations collected in Table 1.

Table 1. Proton affinity of NCX^- and electron affinity of NCX . NormalPNO vs. TightPNO approximations. PBE0 geometry, 6-311G* basis set, no ZPE corrections. (Test calculations)

Method	PA(NCX^-) eV	EA(NCX) eV
Canonic CCSD [a]	9.438	11.131
DLPNO-CCSD / NormalPNO	9.433	10.909
DLPNO-CCSD / TightPNO	9.438	11.157
DLPNO-CCSD(T) / NormalPNO	9.436	10.538
DLPNO-CCSD(T) / TightPNO	9.444	10.649

[a] performed in Gaussian16.

Electron affinity

The ground state of NCX^- anion is a closed-shell singlet of I_h symmetry. According to PBE0 functional, cage C—C bond lengths are 1.586Å, so the distance from the center fluorine to cage carbon is 2.222Å. Outer C—C bond lengths are shortened to 1.460Å, while C≡N bond lengths are 1.148Å.

Neutral NCX radical has an open-shell doublet ground state with lower symmetry D_{3d} due to Jan-Teller effect. However, the stretch along C_3 axis is quite small (only +0.008Å between axial atoms of the cage), so it may be smoothed by

zero-point vibrations. With almost zero spin density on the central fluorine, neutral NCX looks more like fluoride anion inserted in positively charged cage instead of neutral fluorine atom in neutral cage. Table 2 shows the results of electron affinity calculations.

Source	EA(NCX) / eV
PBE0	9.766
PBE0 ZPE correction	-0.161
DLPNO-CCSD	11.428
DLPNO-CCSD(T)	10.913
DLPNO-CCSD(T) + ZPE	10.752

ZPE scaling, basis set enrichment and quadruplets accounting should probably push the final value a bit higher, so we round our result to 10.8 eV. That makes NCX, to our knowledge, a superhalogen with the highest electron affinity ever predicted. However, higher affinities should be possible, and an example will be shown later in section „Possible improvements“.

Superacid

The most favorable protonation site in NCX⁻ is nitrogen atom. The resulting molecule HNCX has singlet ground state of C_{3v} symmetry with dipole moment of 13.96 Debye and NH bond length of 1.008Å according to PBE0 functional. Proton affinity of NCX⁻ was estimated as 9.3 eV (Table 3), corresponding to gas-phase basicity of 208 kcal/mol.

Source	PA(NCX ⁻) / eV
PBE0	9.681
PBE0 ZPE correction	-0.276
DLPNO-CCSD	9.586
DLPNO-CCSD(T)	9.579
DLPNO-CCSD(T) + ZPE	9.303

HNCX superacid also features the strongest single bond known. Indeed, the dissociation energy HNCX = H + NCX could be estimated as PA(NCX⁻) + EA(NCX) – IE(H) = 9.3 eV + 10.8 eV – 13.6 eV = 6.5 eV, or about 150 kcal/mol.

We decided to compare the acidity of HNCX with the acidity of fluorocarborane superacid H[CHB₁₁F₁₁] which is able to protonate CO₂.³⁹ It is known that in highly acidic media proton tends to form bridged structures,⁴⁰ so we compared both HA and AHA⁻ for A = CHB₁₁F₁₁ and A = NCX.

The most favorable protonation site in CHB₁₁F₁₁ appeared to be fluorine atom most distant from carbon, leading to C_s symmetry for neutral H[CHB₁₁F₁₁] and C_{2h} symmetry for H[CHB₁₁F₁₁]₂⁻ anion (Figure 2), while H[NCX]₂⁻ anion features D_{3d} symmetry. Both bridged anions contain short symmetrical hydrogen bonds with N...H distances of 1.259Å in H[NCX]₂⁻ and F...H distances of 1.138Å in H[CHB₁₁F₁₁]₂⁻.

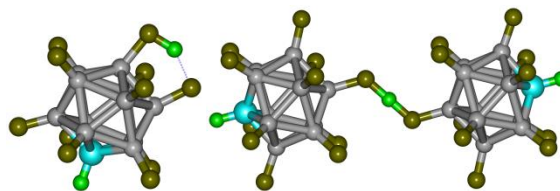


Figure 2. H[CHB₁₁F₁₁] (left) and H[CHB₁₁F₁₁]₂⁻ anion (right). Color coding: C – cyan, B – silver, F – olive, H – green.

Proton binding way	A = NCX	A = CHB ₁₁ F ₁₁ [a]
H ⁺ + A ⁻ = HA	-208.1	-221.0
H ⁺ + 2A ⁻ = AHA ⁻	-229.3	-249.6

[a] maug-cc-pVTZ basis set was used for fluorine atoms.

According to gas-phase protonation Gibbs energies shown in Table 4, HNCX should be much stronger acid than H[CHB₁₁F₁₁], so we wondered the capability of HNCX to protonate molecular nitrogen and to produce a bridged cation [NNHNN]⁺ first observed in 1999.⁴¹

We considered the ion pair [NNHNN]⁺[NCX]⁻ and compared it to similar ion pairs formed by 1,2-dicyanocyclopentadiene and pentacyanotoluene in acetonitrile solution (Table 5). For [NNHNN]⁺[NCX]⁻ we found the ground minimum geometry of C_s symmetry with almost linear NNHNN trapped between three

nearby CN needles. $[(\text{CH}_3\text{CN})_2\text{H}]^+[\text{C}_5\text{H}_3(\text{CN})_2]^-$ appeared to have C_{2v} symmetry with symmetrical cation embowed around two cyano groups of anion, while in $[(\text{CH}_3\text{CN})_2\text{H}]^+[\text{CH}_2\text{C}_6(\text{CN})_5]^-$ methyl groups of cation snuggle to cyano groups in *ortho*- and *para*-positions of benzene ring (Figure 3).

Table 5. Proton solvation comparison in acetonitrile and nitrogen. DLPNO-CCSD(T) + PBE0 thermal correction.	
Gas phase reaction	ΔG (kcal/mol)
$\text{HNCX} + 2\text{N}_2 = [\text{NNHNN}]^+[\text{NCX}]^-$	38.4
$\text{H}[\text{C}_5\text{H}_3(\text{CN})_2] + 2\text{CH}_3\text{CN} = [(\text{CH}_3\text{CN})_2\text{H}]^+[\text{C}_5\text{H}_3(\text{CN})_2]^-$	37.8
$\text{H}[\text{CH}_2\text{C}_6(\text{CN})_5] + 2\text{CH}_3\text{CN} = [(\text{CH}_3\text{CN})_2\text{H}]^+[\text{CH}_2\text{C}_6(\text{CN})_5]^-$	50.0

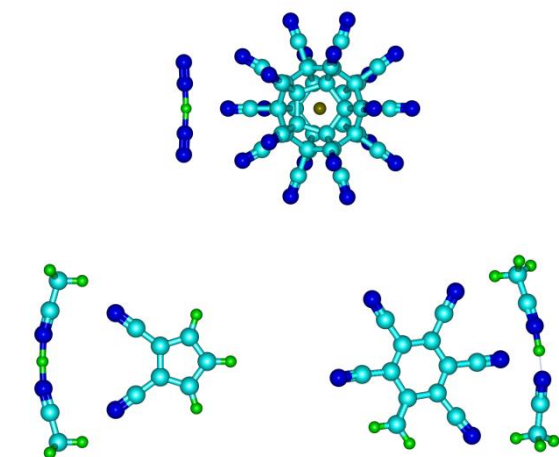


Figure 3. $[\text{NNHNN}]^+[\text{NCX}]^-$ (top), $[(\text{CH}_3\text{CN})_2\text{H}]^+[\text{C}_5\text{H}_3(\text{CN})_2]^-$ (bottom left), $[(\text{CH}_3\text{CN})_2\text{H}]^+[\text{CH}_2\text{C}_6(\text{CN})_5]^-$ (bottom right). Color coding: C – cyan, N – dark blue, H – green.

Experimental pK_a values in CH_3CN are 10.17 for 1,2-dicyanocyclopentadiene⁴² and 20.14 for pentacyanotoluene⁴³; so simple linear interpolation gives us $\text{pK}_a = 10.64$ in nitrogen for HNCX. However, that very rough result should be treated only as qualitative estimation providing some evidence that molecular nitrogen could be indeed protonated by HNCX superacid.

The possibility of auto-ionization of HNCX was also considered. Neutral acid has five possible

protonation sites to form HNCXH^+ tautomers. Their energy depends on the distance between protons (the larger is distance, the lower is energy), so the most favorable tautomer has D_{3d} symmetry. That fact suggests that in condensed phase HNCX will probably form a linear polymer $\cdots\text{H}\cdots[\text{NCX}]\cdots\text{H}\cdots[\text{NCX}]\cdots$ instead of cyclic or zigzag-shaped clusters typical for HF. The calculated gas-phase basicity of neutral HNCX is 164 kcal/mol; accounting earlier results, the Gibbs energy of the autoionization process $3\text{HNCX} = \text{H}[\text{NCX}]_2^- + \text{HNCXH}^+$ appeared to be as small as 23 kcal/mol in gas phase (Table 6), so we expect a high degree of autoionization for HNCX in a solution.

Table 6. Autoionization energy for HNCX. DLPNO-CCSD(T) + PBE0 thermal correction.	
Gas phase reaction	ΔG (kcal/mol)
$\text{HNCX} = \text{NCX}^- + \text{H}^+$	208.1
$\text{HNCX} + \text{H}^+ = \text{HNCXH}^+$	-164.2
$\text{HNCX} + \text{NCX}^- = \text{H}[\text{NCX}]_2^-$	-21.2
$3\text{HNCX} = \text{H}[\text{NCX}]_2^- + \text{HNCXH}^+$	22.7

SbF_5 could be a proper solvent for HNCX because of acidity-enhancing $\text{N}\cdots\text{Sb}$ coordination and quite low basicity of SbF_5 itself.

Other simple derivatives

As well as common halogen atoms, neutral NCX readily forms covalent bonds with atoms other than hydrogen and can also exist as a dimer $[\text{NCX}]_2$. Actual bonds are formed by nitrogen atoms of cyano groups.

The $[\text{NCX}]_2$ molecule is analogous to halogen diatomics (Figure 4). It has singlet ground state of D_{3d} symmetry featuring NN bond of length 1.238Å which is close to double bond in N_2H_2 . Another molecule, FNCX, is an analog of interhalogen diatomics. It has C_{3v} singlet ground state with dipole moment of 13.04 Debye that is almost as large as of HNCX, suggesting an outstanding electronegativity of our superhalogen. Quite short FN bond of 1.249Å shows partially double character just like FC bond in FCN.

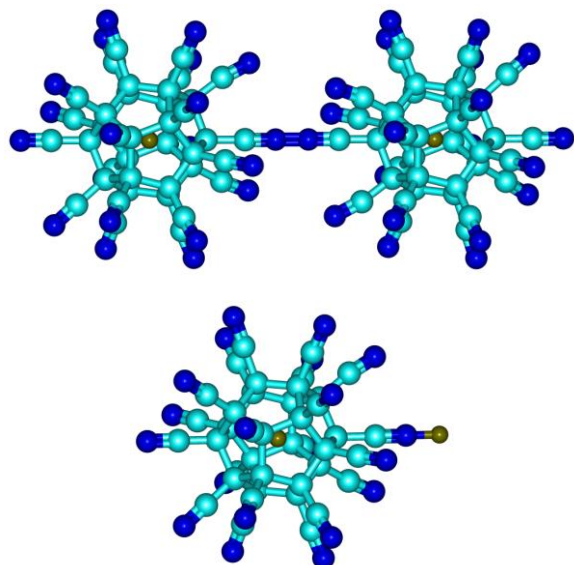


Figure 4. $[\text{NCX}]_2$ (top) and FNCX (bottom). Color coding: C – cyan, N – dark blue, F – olive.

Direct calculation of dissociation energies (DE) for $[\text{NCX}]_2$ and FNCX would need UHF wavefunction with TightPNO cutoffs. In order to avoid heavy calculations, we made sideway estimates using gas phase reactions between closed-shell structures (Table 7).

Table 7. Supplemental calculations for dissociation energy estimations. DLPNO-CCSD(T) + PBE0 ZPE correction.	
Gas phase reaction	Energy / eV
$[\text{NCX}]_2 + 2e^- = 2\text{NCX}^-$	-17.439
$[\text{NCX}]_2 + \text{HF} = \text{HNCX} + \text{FNCX}$ ^[a]	-0.097

^[a] Negative ΔH suggests that $[\text{NCX}]_2$ would oxidize HF.

Thus, $\text{DE}([\text{NCX}]_2)$ was estimated as $2 \cdot \text{EA}(\text{NCX}) - 17.439 \text{ eV} = 4.065 \text{ eV} \approx 4.1 \text{ eV}$, or about 94 kcal/mol, which is much higher than for diatomic halogens. Taking into account previously estimated $\text{DE}(\text{HNCX})$ of 6.5 eV and experimental value of $\text{DE}(\text{HF}) = 5.9 \text{ eV}$ ⁴⁴, we obtain $\text{DE}(\text{FNCX}) = (4.1 + 5.9 + 0.1 - 6.5) \text{ eV} = 3.6 \text{ eV}$, or about 83 kcal/mol.

Stability

It is clear that our predictions have little sense until the stability of our superhalogen and its derivatives is examined. First, the cage C—C bond in NCX^- is predicted to be about 0.05 Å longer than C—C bond in ethane, hinting at some strain. Therefore, we wondered how much energy the encapsulation takes.

The encapsulation of fluorine atom, fluoride anion and neon atom (Table 8) was considered. Again, to avoid heavy calculations, the sideway reaction $\text{C}_{20}(\text{CN})_{20} + \text{HF} = \text{HNCX}$ was used together with known values of $\text{EA}(\text{F}) = 3.401 \text{ eV}$ ⁴⁵ and $\text{PA}(\text{F}^-) = 16.063 \text{ eV}$ ⁴⁴.

Table 8. Encapsulation energies for F^- , F and Ne. DLPNO-CCSD(T) + PBE0 ZPE correction.	
Gas phase reaction	Energy / eV
$\text{C}_{20}(\text{CN})_{20} + \text{Ne} = \text{Ne}@\text{C}_{20}(\text{CN})_{20}$	3.055
$\text{C}_{20}(\text{CN})_{20} + \text{HF} = \text{HNCX}$	1.473
$\text{C}_{20}(\text{CN})_{20} + \text{F}^- = \text{NCX}^-$	-5.287 ^[a]
$\text{C}_{20}(\text{CN})_{20} + \text{F} = \text{NCX}$	2.064 ^[b]

^[a] Calculated as $1.473 \text{ eV} - \text{PA}(\text{F}^-) + \text{PA}(\text{NCX}^-)$.
^[b] Calculated as $-5.287 \text{ eV} - \text{EA}(\text{F}) + \text{EA}(\text{NCX})$.

Exothermic encapsulation of fluoride anion is expectative because of negative charge delocalization noted earlier. However, for isoelectronic process of neon encapsulation we have 8.3 eV larger energy, suggesting some repulsion between the noble electron cloud and the cage. Surprisingly, for fluorine atom the encapsulation is 1 eV less endothermic despite its larger radius compared to neon. That could be explained with proximity of energies, and therefore significant correlation, between fluorine-localized and cage-localized molecular orbitals. In other words, the fluorine atom fits the cage in some sense.

In terms of Gibbs energy, discussed superhalogen is thermodynamically unstable against the loss of fluoride atom by 54 kcal/mol. However, tight pentagonal holes of the cage provide a very high kinetic barrier for this decomposition route. Such a barrier for smaller

helium atom was experimentally proven to be so high that helium endocomplex survive for weeks at room temperature.⁴⁶

The search for a transition state pointed to the fact that another decomposition route is energetically favorable. It is the cleavage of an outer C—C bond despite its partially double character. The key is that fluorine atom may attack one of the cage carbons from inside, pulling it inward and leaving the CN group alone, just like in S_N2. The resulting molecule **X** (structurally related to “in-adamantane”⁴⁷) has a singlet ground state of C_{3v} symmetry with C—F bond length of 1.431 Å (Figure 5). That large bond length is the result of carbon cage strain.

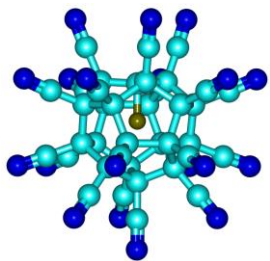


Figure 5. Structure of **X** molecule C₂₀(in-F)(CN)₁₉. Color coding: C – cyan, N – dark blue, F – olive.

The formation of **X** from superhalogen and its derivatives is considered in Table 9. As before, sideway calculations were performed using known values of EA(CN) = 3.862 eV and PA(CN⁻) = 15.199 eV⁴⁸.

Table 9. Stability against the formation of X . DLPNO-CCSD(T) + PBE0 ZPE correction.	
Gas phase reaction	Energy / eV
HNCX = HCN + X	0.810
NCX ⁻ = CN ⁻ + X	6.707 ^[a]
NCX = CN + X	-0.183 ^[b]

^[a] Calculated as 0.810 eV + PA(CN⁻) – PA(NCX⁻).
^[b] Calculated as 6.707 eV + EA(CN) – EA(NCX).

These results show that the superhalogen anion is very stable against the cage concaving, while the superacid is moderately stable. The corresponding gas phase Gibbs energies were

calculated to be +143.1 and +6.8 kcal/mol, respectively.

Considering kinetic stability on PBE0 level of theory, we found that neutral NCX might transform to C₂₀(in-F)(CN)₁₈(C(=N)CN) (Figure 6) through the transition state with distorted cyclobutane unit. The barrier of 23 kcal/mol suggests days of lifetime at 0°C, but we expect that DFT overestimates the kinetic stability of neutral superhalogenic radical, therefore somewhat lower temperatures will be needed to isolate it.

A similar transition state was also found for HNCX, but the calculated barrier of 45 kcal/mol makes the novel superacid stable up to 200°C.

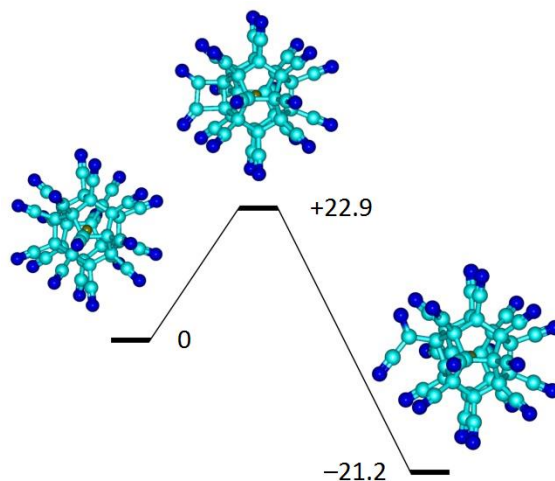


Figure 6. Intramolecular radical substitution reaction of NCX. PBE0 + thermal correction, kcal/mol.

Synthesis

Despite a high amount of papers related to dodecahedrane endocomplexes,⁴⁹⁻⁵⁵ there is only one up to date observed experimentally – He@C₂₀H₂₀, that was obtained by shooting a beam of helium ions at a continuously deposited surface of dodecahedrane.⁴⁶ Encapsulation was detected on the level of 0.01% that definitely cannot be accounted as a “preparative” technique. In our opinion, “molecular surgery” approach that was used for getting different endofullerene complexes,

might be also applied in this case. This methodology involves inserting the “guest”-atom into the cavity of precursor that has reasonably big opening. Being non-experts in “molecular surgery”, authors guess that structures A and B (Figure 7) might be among possible intermediates. These structures are results of F-anion encapsulation into already known precursors of dodecahedrane.⁵⁶⁻⁵⁸

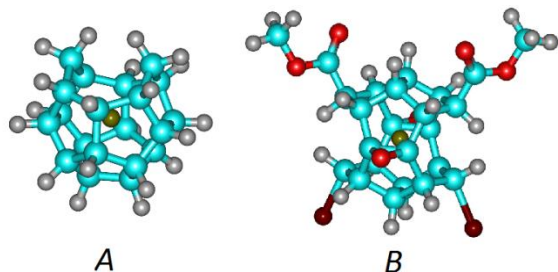


Figure 7. Possible intermediates for encapsulation of fluorine in dodecahedrane cage. Color coding: C – cyan, H – grey, O – red, Br – brown, F – olive.

Structure B seems to be especially attractive because: 1) according to Bertau,⁵⁶ further C—C coupling is performed with a fluoride salt of non-nucleophilic Schwesinger cation; 2) resulted dodecahedrane is highly functionalized that would simplify further transformation to NCX. Nevertheless, authors would like to note that the aim of current paper is mainly the demonstration of the concept, but not the detailed elaboration of synthetic conditions.

Possible improvements

The limits can always be pushed further. We compared our superhalogen to a few other structures, trying to improve either electron affinity or proton affinity value.

First of all, two larger carbon cages were considered: C₂₄ of D_{6d} symmetry and C₂₈ of T_d symmetry, both decorated with cyano groups (Figure 8). However, DFT estimates show that electron affinity does not grow this way (Table 10). Calculated Hartree-Fock HOMO energies for anions support this trend.

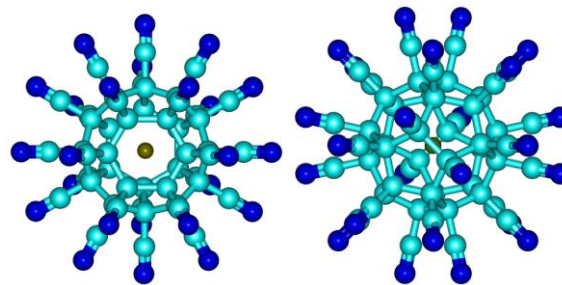


Figure 8. F@D_{6d}-C₂₄(CN)₂₄ (left) and F@T_d-C₂₈(CN)₂₈ (right). Color coding: C – cyan, N – dark blue, F – olive.

Structure	EA / eV (PBE0 without ZPE corrections)	HOMO energy / eV (HF wavefunction for anion)
F@C ₂₀ (CN) ₂₀	9.766	-11.768
F@C ₂₄ (CN) ₂₄	9.502	-11.482
F@C ₂₈ (CN) ₂₈	9.484	-11.455

Thus, dodecahedrane cage seems to be the best fit for fluorine atom. Another try to improve the structure was changing cyano groups to CF₃ ones, but that quickly lead to overcrowding of fluorine atoms, preventing the proper delocalization of negative charge.

Looking at carborane cages, we noticed that the cage CB₁₁ of C_{5v} symmetry, decorated with 12 CF₃ groups (Figure 9), has less crowding and was already proposed in 2000.⁵⁹ As well as B₁₂(CF₃)₁₂ and related structures, it was suggested by Ivo Leito and coworkers^{60,61} as an anion for a Brønsted superacid of record-breaking strength. Unfortunately, we found that claim to be doubtful since CF₃ group is not stable in highly acidic media. To be precise, fluorine atom appears to be the most favorable protonation site, and once it is protonated, HF molecule is eliminated from the structure without any notable barrier. That happens because of larger electronegativity of carbon compared to hydrogen, which makes H—F single bond stronger than C—F single bond. The authors were aware of that issue.⁶²

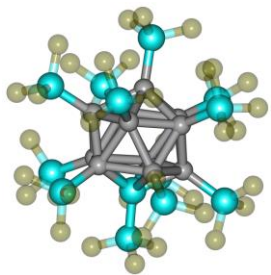


Figure 9. $\text{CB}_{11}(\text{CF}_3)_{12}^-$ anion. Color coding: C – cyan, B – silver, F – transparent olive.

As for electron affinity of $\text{CB}_{11}(\text{CF}_3)_{12}$, the predicted value of 8.8 eV⁵⁹ seems to be too small to compete with NCX , even considering the lower level of theory used for that prediction. Changing CF_3 groups to cyano groups does not rise the electron affinity but provides nitrogen atoms as safe protonation sites. However, PBE0 functional (without ZPE correction) measures the proton affinity of $\text{CB}_{11}(\text{CN})_{12}^-$ as high as 10.366 eV, while for NCX^- the same level of theory gives 9.681 eV, so the novel superacid is again beyond reach.

The last idea was to use our superhalogen itself as an electron-withdrawing group, a concept applied in other form in hyperhalogens. We took boron as a central atom extending the analogy to hydrofluoric (moderately strong) and tetrafluoroboric (very strong) acids. While B–N bonds are strong enough to make boron nitride almost as hard as diamond, we can expect stability of the "tetrasuperhalogenoborate" anion $\text{B}[\text{NCX}]_4^-$ (Figure 10). Its ground state appeared to be a singlet of T symmetry with surprisingly short B–N bonds of 1.517 Å.

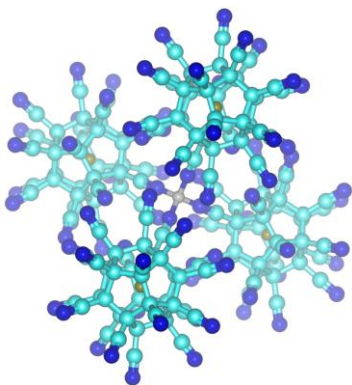


Figure 10. Structure of $\text{B}[\text{NCX}]_4^-$ anion.

Unfortunately, this structure was too big for us to handle it with DLPNO-CCSD(T), say nothing about the possible ways of decomposition. However, Hartree-Fock HOMO energy for $\text{B}[\text{NCX}]_4^-$ is 1.21 eV lower than for NCX^- , providing the hope for record-breaking electron affinity around 12 eV for $\text{B}[\text{NCX}]_4$. The latter molecule in its ground state seems to have D_2 symmetry, although we did not calculate harmonic frequencies for that structure to ensure this. As for proton affinity, there's little chance for $\text{B}[\text{NCX}]_4^-$ to make a new record because of bridge-like protonation: the proton in $\text{HB}[\text{NCX}]_4$ sticks between two CN needles of adjoining cages.

Conclusions

We designed a superhalogen $\text{F}@\text{C}_{20}(\text{CN})_{20}$, named NCX , with electron affinity of 10.8 eV, and considered some of its derivatives: a fluorine superhalogenide FNCX , a superhalogen dimer $[\text{NCX}]_2$, a hyperhalogen $\text{B}[\text{NCX}]_4$ with electron affinity close to 12 eV, and a superacid HNCX with gas-phase deprotonation energy of just 208 kcal/mol.

Being much stronger acid than the current Brønsted champion, fluorocarborane acid, HNCX is expected to have a high degree of autoionization in condensed phase, and to be close to protonation of molecular nitrogen. SbF_5 is suggested as a possible solvent for HNCX to attest its strength.

Both HNCX and NCX^- anion were predicted to be thermodynamically stable, while neutral NCX radical is expected to have only kinetic stability at low temperatures.

Various ways of possible improvements to superhalogenic structures were investigated. The instability of some earlier-claimed superacids of record strength was established.

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Keywords:

Superhalogen, superacid, DLPNO-CCSD(T)

Additional Supporting Information (XYZ coordinates and energies for discussed structures) may be found in the online version of this article.

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Supporting Information

Energy and geometry data is provided for the following structures:

1. Superhalogen NCX
2. Superhalogen anion NCX^-
3. Superacid HNCX
4. Protonated superacid HNCXH^+
5. Superacid bridged anion $\text{H}[\text{NCX}]_2^-$
6. Fluorocarborane acid $\text{HCHB}_{11}\text{F}_{11}$
7. Fluorocarborane anion $\text{CHB}_{11}\text{F}_{11}^-$
8. Fluorocarborane bridged anion $\text{H}[\text{CHB}_{11}\text{F}_{11}]_2^-$
9. Nitrogen NN
10. Ion pair $[\text{NNHNN}]^+[\text{NCX}]^-$
11. Acetonitrile CH_3CN
12. 1,2-dicyanocyclopentadiene $\text{HC}_5\text{H}_3(\text{CN})_2$
13. Pentacyanotoluene $\text{HCH}_2\text{C}_6(\text{CN})_5$
14. Ion pair $[(\text{CH}_3\text{CN})_2\text{H}]^+[\text{C}_5\text{H}_3(\text{CN})_2]^-$
15. Ion pair $[(\text{CH}_3\text{CN})_2\text{H}]^+[\text{CH}_2\text{C}_6(\text{CN})_5]^-$
16. Fluorine superhalogenide FNCX
17. Superhalogen dimer $[\text{NCX}]_2$
18. Empty cage $\text{C}_{20}(\text{CN})_{20}$
19. Neon complex $\text{Ne}@\text{C}_{20}(\text{CN})_{20}$
20. Concaved cage \mathbf{X}
21. Destructed superhalogen
22. Superhalogen transition state
23. Superacid transition state
24. Alternative superhalogen $\text{F}@\text{C}_{24}(\text{CN})_{24}$
25. Alternative superhalogen anion $\text{F}@\text{C}_{24}(\text{CN})_{24}^-$
26. Alternative superhalogen $\text{F}@\text{C}_{28}(\text{CN})_{28}$
27. Alternative superhalogen anion $\text{F}@\text{C}_{28}(\text{CN})_{28}^-$
28. Cyanocarborane acid $\text{HB}_{11}\text{C}(\text{CN})_{12}$
29. Cyanocarborane anion $\text{B}_{11}\text{C}(\text{CN})_{12}^-$
30. Hyperhalogen $\text{B}[\text{NCX}]_4$
31. Hyperhalogen anion $\text{B}[\text{NCX}]_4^-$

1. Superhalogen NCX

Stoichiometry: C₄₀N₂₀F
Charge: 0
Multiplicity: 2
Point group: D_{3d}

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0: -2716.0100217
PBE0 ZPE correction: 0.3092484
PBE0 thermal Gibbs correction: 0.231783
DLPNO-CCSD, UHF/TightPNO: -2713.1960624
DLPNO-CCSD(T), UHF/TightPNO: -2713.7805136

PBE0 entropy (cal/mol-Kelvin): 269.365

Nuclear coordinates (Angströms)

F	0.000000	0.000000	0.000000
C	0.000000	-1.479589	1.656791
C	0.000000	0.000000	2.225960
C	0.000000	0.000000	-2.225960
C	0.000000	1.479589	-1.656791
C	0.790966	-1.934109	-0.739823
C	-0.790966	-1.934109	-0.739823
C	0.790966	1.934109	0.739823
C	-0.790966	1.934109	0.739823
C	2.070471	-0.282058	0.739823
C	-2.070471	-0.282058	0.739823
C	2.070471	0.282058	-0.739823
C	-2.070471	0.282058	-0.739823
C	1.279505	-1.652052	0.739823
C	-1.279505	-1.652052	0.739823
C	1.281362	0.739794	1.656791
C	-1.281362	0.739794	1.656791
C	1.281362	-0.739794	-1.656791
C	-1.281362	-0.739794	-1.656791
C	1.279505	1.652052	-0.739823
C	-1.279505	1.652052	-0.739823
C	3.438821	-0.463624	1.214727
N	4.523769	-0.603011	1.577058
C	0.000000	-2.462170	2.735100
N	0.000000	-3.248551	3.574861
C	0.000000	0.000000	3.683923
N	0.000000	0.000000	4.832469
C	0.000000	0.000000	-3.683923
N	0.000000	0.000000	-4.832469
C	0.000000	2.462170	-2.735100
N	0.000000	3.248551	-3.574861
C	1.317900	-3.209919	-1.214727
N	1.739662	-4.219205	-1.577058
C	-1.317900	-3.209919	-1.214727
N	-1.739662	-4.219205	-1.577058
C	1.317900	3.209919	1.214727
N	1.739662	4.219205	1.577058
C	-1.317900	3.209919	1.214727
N	-1.739662	4.219205	1.577058
C	-3.438821	-0.463624	1.214727
N	-4.523769	-0.603011	1.577058
C	3.438821	0.463624	-1.214727
N	4.523769	0.603011	-1.577058
C	-3.438821	0.463624	-1.214727
N	-4.523769	0.603011	-1.577058
C	2.120921	-2.746294	1.214727
N	2.784107	-3.616194	1.577058
C	-2.120921	-2.746294	1.214727
N	-2.784107	-3.616194	1.577058
C	2.132302	1.231085	2.735100
N	2.813328	1.624276	3.574861
C	-2.132302	1.231085	2.735100
N	-2.813328	1.624276	3.574861
C	2.132302	-1.231085	-2.735100
N	2.813328	-1.624276	-3.574861
C	-2.132302	-1.231085	-2.735100
N	-2.813328	-1.624276	-3.574861
C	2.120921	2.746294	-1.214727
N	2.784107	3.616194	-1.577058
C	-2.120921	2.746294	-1.214727
N	-2.784107	3.616194	-1.577058

2. Superhalogen anion NCX⁻

Stoichiometry: C₄₀N₂₀F
Charge: -1
Multiplicity: 1
Point group: I_h

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0: -2716.3689041
PBE0 ZPE correction: 0.3151805
PBE0 thermal Gibbs correction: 0.242493
DLPNO-CCSD, RHF/NormalPNO: -2713.6443332
DLPNO-CCSD(T), RHF/NormalPNO: -2714.1930136
DLPNO-CCSD, UHF/TightPNO: -2713.6160281
DLPNO-CCSD(T), UHF/TightPNO: -2714.1815628

PBE0 entropy (cal/mol-Kelvin): 255.820

Nuclear coordinates (angströms)

```
F 0.000000 0.000000 0.000000
C -1.282753 -0.416792 1.765558
C -0.792785 1.091175 1.765558
C 0.792785 -1.091175 -1.765558
C 1.282753 0.416792 -1.765558
C 0.000000 -2.182350 0.416792
C -1.282753 -1.765558 -0.416792
C 1.282753 1.765558 0.416792
C 0.000000 2.182350 -0.416792
C 1.282753 -0.416792 1.765558
C -2.075538 0.674383 -0.416792
C 2.075538 -0.674383 0.416792
C -1.282753 0.416792 -1.765558
C 0.000000 -1.348766 1.765558
C -2.075538 -0.674383 0.416792
C 0.792785 1.091175 1.765558
C -1.282753 1.765558 0.416792
C 1.282753 -1.765558 -0.416792
C -0.792785 -1.091175 -1.765558
C 2.075538 0.674383 -0.416792
C 0.000000 1.348766 -1.765558
C 2.125553 -0.690634 2.925573
N 2.788535 -0.906050 3.838089
C -2.125553 -0.690634 2.925573
N -2.788535 -0.906050 3.838089
C -1.313664 1.808103 2.925573
N -1.723409 2.372069 3.838089
C 1.313664 -1.808103 -2.925573
N 1.723409 -2.372069 -3.838089
C 2.125553 0.690634 -2.925573
N 2.788535 0.906050 -3.838089
C 0.000000 -3.616207 0.690634
N 0.000000 -4.744139 0.906050
C -2.125553 -2.925573 -0.690634
N -2.788535 -3.838089 -0.906050
C 2.125553 2.925573 0.690634
N 2.788535 3.838089 0.906050
C 0.000000 3.616207 -0.690634
N 0.000000 4.744139 -0.906050
C -3.439217 1.117469 -0.690634
N -4.511944 1.466020 -0.906050
C 3.439217 -1.117469 0.690634
N 4.511944 -1.466020 0.906050
C -2.125553 0.690634 -2.925573
N -2.788535 0.906050 -3.838089
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N 0.000000 -2.932039 3.838089
C -3.439217 -1.117469 0.690634
N -4.511944 -1.466020 0.906050
C 1.313664 1.808103 2.925573
N 1.723409 2.372069 3.838089
C -2.125553 2.925573 0.690634
N -2.788535 3.838089 0.906050
C 2.125553 -2.925573 -0.690634
N 2.788535 -3.838089 -0.906050
C -1.313664 -1.808103 -2.925573
N -1.723409 -2.372069 -3.838089
C 3.439217 1.117469 -0.690634
N 4.511944 1.466020 -0.906050
C 0.000000 2.234939 -2.925573
N 0.000000 2.932039 -3.838089
```

3. Superacid HNCX

Stoichiometry: HC₄₀N₂₀F
Charge: 0
Multiplicity: 1
Point group: C_{3v}

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N
PBE0: -2716.7246726
PBE0 ZPE correction: 0.3253410
PBE0 thermal Gibbs correction: 0.252933
DLPNO-CCSD, RHF/NormalPNO: -2713.9966111
DLPNO-CCSD(T), RHF/NormalPNO: -2714.5450357

PBE0 entropy (cal/mol-Kelvin): 256.707

Nuclear coordinates (angströms)

H	0.000000	0.000000	-5.757819
F	0.000000	0.000000	0.015827
C	1.289871	0.744707	-1.607853
C	0.793709	1.945020	-0.700487
C	-0.793710	-1.941380	0.779238
C	-1.283504	-0.741031	1.693245
C	0.000000	-1.489415	-1.607853
C	1.287582	-1.659882	-0.700487
C	-1.284430	1.658063	0.779238
C	0.000000	1.482063	1.693245
C	-1.289871	0.744707	-1.607853
C	2.078140	0.283317	0.779238
C	-2.081291	-0.285138	-0.700487
C	1.283504	-0.741031	1.693245
C	0.000000	0.000000	-2.146199
C	2.081291	-0.285138	-0.700487
C	-0.793709	1.945020	-0.700487
C	1.284430	1.658063	0.779238
C	-1.287582	-1.659882	-0.700487
C	0.793710	-1.941380	0.779238
C	-2.078140	0.283317	0.779238
C	0.000000	0.000000	2.257950
C	-2.090363	1.206872	-2.739580
N	-2.629405	1.518088	-3.705526
C	2.090363	1.206872	-2.739580
N	2.629405	1.518088	-3.705526
C	1.318949	3.206667	-1.209988
N	1.735549	4.182983	-1.648778
C	-1.316711	-3.216394	1.255253
N	-1.732392	-4.225169	1.613703
C	-2.127728	-1.228444	2.777239
N	-2.797689	-1.615246	3.625980
C	0.000000	-2.413744	-2.739580
N	0.000000	-3.036176	-3.705526
C	2.117580	-2.745577	-1.209988
N	2.754795	-3.594521	-1.648778
C	-2.127123	2.748502	1.255253
N	-2.792908	3.612880	1.613703
C	0.000000	2.456889	2.777239
N	0.000000	3.230493	3.625980
C	3.443834	0.467892	1.255253
N	4.525300	0.612289	1.613703
C	-3.436529	-0.461090	-1.209988
N	-4.490344	-0.588462	-1.648778
C	2.127728	-1.228444	2.777239
N	2.797689	-1.615246	3.625980
C	0.000000	0.000000	-3.614857
N	0.000000	0.000000	-4.749346
C	3.436529	-0.461090	-1.209988
N	4.490344	-0.588462	-1.648778
C	-1.318949	3.206667	-1.209988
N	-1.735549	4.182983	-1.648778
C	2.127123	2.748502	1.255253
N	2.792908	3.612880	1.613703
C	-2.117580	-2.745577	-1.209988
N	-2.754795	-3.594521	-1.648778
C	1.316711	-3.216394	1.255253
N	1.732392	-4.225169	1.613703
C	-3.443834	0.467892	1.255253
N	-4.525300	0.612289	1.613703
C	0.000000	0.000000	3.715762
N	0.000000	0.000000	4.864140

4. Protonated superacid HNCXH⁺

Stoichiometry: H₂C₄₀N₂₀F
Charge: 1
Multiplicity: 1
Point group: D_{3d}

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0: -2717.0090260
PBE0 ZPE correction: 0.3357630
PBE0 thermal Gibbs correction: 0.263424
DLPNO-CCSD, RHF/NormalPNO: -2714.2793178
DLPNO-CCSD(T), RHF/NormalPNO: -2714.8272020

PBE0 entropy (cal/mol-Kelvin): 257.746

Nuclear coordinates (angströms)

H	0.000000	0.000000	5.803343
H	0.000000	0.000000	-5.803343
F	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.186761
C	0.000000	-1.489646	1.646578
C	0.000000	1.489646	-1.646578
C	0.000000	0.000000	-2.186761
C	-0.794340	1.947263	0.739197
C	0.794340	1.947263	0.739197
C	-0.794340	-1.947263	-0.739197
C	0.794340	-1.947263	-0.739197
C	-2.083549	-0.285713	0.739197
C	2.083549	-0.285713	0.739197
C	-2.083549	0.285713	-0.739197
C	2.083549	0.285713	-0.739197
C	-1.290071	0.744823	1.646578
C	1.290071	0.744823	1.646578
C	-1.289209	-1.661550	0.739197
C	1.289209	-1.661550	0.739197
C	-1.289209	1.661550	-0.739197
C	1.289209	1.661550	-0.739197
C	-1.290071	-0.744823	-1.646578
C	1.290071	-0.744823	-1.646578
C	-3.441217	-0.460365	1.237836
N	-4.505161	-0.586036	1.652536
C	0.000000	0.000000	3.657810
N	0.000000	0.000000	4.791736
C	0.000000	-2.417332	2.773077
N	0.000000	-3.050185	3.732310
C	0.000000	2.417332	-2.773077
N	0.000000	3.050185	-3.732310
C	0.000000	0.000000	-3.657810
N	0.000000	0.000000	-4.791736
C	-1.321921	3.210364	1.237836
N	-1.745058	4.194602	1.652536
C	1.321921	3.210364	1.237836
N	1.745058	4.194602	1.652536
C	-1.321921	-3.210364	-1.237836
N	-1.745058	-4.194602	-1.652536
C	1.321921	-3.210364	-1.237836
N	1.745058	-4.194602	-1.652536
C	3.441217	-0.460365	1.237836
N	4.505161	-0.586036	1.652536
C	-3.441217	0.460365	-1.237836
N	-4.505161	0.586036	-1.652536
C	3.441217	0.460365	-1.237836
N	4.505161	0.586036	-1.652536
C	-2.093471	1.208666	2.773077
N	-2.641538	1.525092	3.732310
C	2.093471	1.208666	2.773077
N	2.641538	1.525092	3.732310
C	-2.119296	-2.749999	1.237836
N	-2.760103	-3.608566	1.652536
C	2.119296	-2.749999	1.237836
N	2.760103	-3.608566	1.652536
C	-2.119296	2.749999	-1.237836
N	-2.760103	3.608566	-1.652536
C	2.119296	2.749999	-1.237836
N	2.760103	3.608566	-1.652536
C	-2.093471	-1.208666	-2.773077
N	-2.641538	-1.525092	-3.732310
C	2.093471	-1.208666	-2.773077
N	2.641538	-1.525092	-3.732310

5. Superacid bridged anion $H[NCX]_2^-$

Stoichiometry: $HC_{80}N_{40}F_2$
Charge: -1
Multiplicity: 1
Point group: D_{3d}

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N
PBE0: -5433.1409233
PBE0 ZPE correction: 0.6376640
PBE0 thermal Gibbs correction: 0.509806
DLPNO-CCSD, RHF/NormalPNO: -5427.6881324
DLPNO-CCSD(T), RHF/NormalPNO: -5428.7861835

PBE0 entropy (cal/mol-Kelvin): 478.922

Nuclear coordinates (angströms)

H	0.000000	0.000000	0.000000	F	0.000000	0.000000	-6.054358
F	0.000000	0.000000	6.054358	C	-1.286592	0.742814	-4.415022
C	1.286592	-0.742814	4.415022	C	-2.078537	-0.284230	-5.326475
C	2.078537	0.284230	5.326475	C	2.076770	0.283107	-6.806804
C	-2.076770	-0.283107	6.806804	C	1.283055	-0.740772	-7.721468
C	-1.283055	0.740772	7.721468	C	1.286592	0.742814	-4.415022
C	-1.286592	-0.742814	4.415022	C	0.793119	1.942181	-5.326475
C	-0.793119	-1.942181	5.326475	C	-0.793207	-1.940090	-6.806804
C	0.793207	1.940090	6.806804	C	-1.283055	-0.740772	-7.721468
C	1.283055	0.740772	7.721468	C	0.000000	-1.485629	-4.415022
C	0.000000	1.485629	4.415022	C	-1.283563	1.656982	-6.806804
C	1.283563	-1.656982	6.806804	C	1.285419	-1.657951	-5.326475
C	-1.285419	1.657951	5.326475	C	0.000000	1.481545	-7.721468
C	0.000000	-1.481545	7.721468	C	0.000000	0.000000	-3.864532
C	0.000000	0.000000	3.864532	C	-0.793119	1.942181	-5.326475
C	0.793119	-1.942181	5.326475	C	-1.285419	-1.657951	-5.326475
C	1.285419	1.657951	5.326475	C	-2.076770	0.283107	-6.806804
C	2.076770	-0.283107	6.806804	C	2.078537	-0.284230	-5.326475
C	-2.078537	0.284230	5.326475	C	1.283563	1.656982	-6.806804
C	-1.283563	-1.656982	6.806804	C	0.793207	-1.940090	-6.806804
C	-0.793207	1.940090	6.806804	C	0.000000	0.000000	-8.286656
C	0.000000	0.000000	8.286656	C	0.000000	-2.434056	-3.304779
C	0.000000	2.434056	3.304779	N	0.000000	-3.122650	-2.385355
N	0.000000	3.122650	2.385355	C	-2.107954	1.217028	-3.304779
C	2.107954	-1.217028	3.304779	N	-2.704294	1.561325	-2.385355
N	2.704294	-1.561325	2.385355	C	-3.438312	-0.464689	-4.829396
C	3.438312	0.464689	4.829396	N	-4.503310	-0.600390	-4.421591
N	4.503310	0.600390	4.421591	C	3.441144	0.468240	-7.289033
C	-3.441144	-0.468240	7.289033	N	4.517319	0.613439	-7.662485
N	-4.517319	-0.613439	7.662485	C	2.126156	-1.227537	-8.807946
C	-2.126156	1.227537	8.807946	N	2.791486	-1.611665	-9.661431
N	-2.791486	1.611665	9.661431	C	2.107954	1.217028	-3.304779
C	-2.107954	-1.217028	3.304779	N	2.704294	1.561325	-2.385355
N	-2.704294	-1.561325	2.385355	C	1.316723	3.210011	-4.829396
C	-1.316723	3.210011	4.829396	N	1.731702	4.200176	-4.421591
N	-1.731702	-4.200176	4.421591	C	-1.315064	-3.214238	-7.289033
C	1.315064	3.214238	7.289033	N	-1.727405	-4.218833	-7.662485
N	1.727405	4.218833	7.662485	C	-2.126156	-1.227537	-8.807946
C	2.126156	1.227537	8.807946	N	-2.791486	-1.611665	-9.661431
N	2.791486	-1.611665	9.661431	C	-2.126080	2.745998	-7.289033
C	-2.126080	2.745998	7.289033	N	-2.789914	3.605393	-7.662485
N	-2.789914	3.605393	7.662485	C	2.121589	-2.745321	-4.829396
C	2.121589	-2.745321	4.829396	N	2.771608	-3.599786	-4.421591
N	2.771608	-3.599786	4.421591	C	0.000000	2.455073	-8.807946
C	0.000000	2.455073	8.807946	N	0.000000	3.223331	-9.661431
N	0.000000	3.223331	9.661431	C	0.000000	0.000000	-2.397544
C	0.000000	0.000000	2.397544	N	0.000000	0.000000	-1.258871
N	0.000000	0.000000	1.258871	C	-1.316723	3.210011	-4.829396
C	1.316723	-3.210011	4.829396	N	-1.731702	4.200176	-4.421591
N	-1.731702	4.200176	4.421591	C	-2.121589	-2.745321	-4.829396
C	2.121589	-2.745321	4.829396	N	-2.771608	-3.599786	-4.421591
N	2.771608	-3.599786	4.421591	C	-3.441144	0.468240	-7.289033
C	3.441144	-0.468240	7.289033	N	-4.517319	0.613439	-7.662485
N	-4.517319	0.613439	7.662485	C	3.438312	-0.464689	-4.829396
C	-3.438312	0.464689	4.829396	N	4.503310	-0.600390	-4.421591
N	4.503310	-0.600390	4.421591	C	2.126080	2.745998	-7.289033
C	-2.126080	2.745998	7.289033	N	2.789914	3.605393	-7.662485
N	-2.789914	3.605393	7.662485	C	1.315064	-3.214238	-7.289033
C	-1.315064	3.214238	7.289033	N	1.727405	-4.218833	-7.662485
N	-1.727405	4.218833	7.662485	C	0.000000	0.000000	-9.745492
C	0.000000	0.000000	9.745492	N	0.000000	0.000000	-10.893811
N	0.000000	0.000000	10.893811				

6. Fluorocarborane acid $\text{HCHB}_{11}\text{F}_{11}$

Stoichiometry: $\text{H}_2\text{B}_{11}\text{CF}_{11}$
Charge: 0
Multiplicity: 1
Point group: C_s

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on F

PBE0:	-1410.6951684
PBE0 ZPE correction:	0.1106439
PBE0 thermal Gibbs correction:	0.066542
DLPNO-CCSD, RHF/NormalPNO:	-1409.5302555
DLPNO-CCSD(T), RHF/NormalPNO:	-1409.6822524

PBE0 entropy (cal/mol-Kelvin): 135.538

Nuclear coordinates (angströms)

H	-1.771157	-2.441476	0.000000
C	1.494173	0.696174	0.000000
B	0.156073	1.778411	0.000000
B	0.105912	-1.574608	0.000000
B	-1.304056	-0.555874	0.000000
B	1.347159	-0.742543	0.919036
B	1.347159	-0.742543	-0.919036
B	-1.106679	0.922362	0.931275
B	-1.106679	0.922362	-0.931275
B	0.614810	0.829675	1.469159
B	0.614810	0.829675	-1.469159
B	-0.339218	-0.644568	1.492639
B	-0.339218	-0.644568	-1.492639
H	2.478822	1.153180	0.000000
F	0.377443	3.099747	0.000000
F	-0.414300	-2.896730	0.000000
F	-2.386885	-1.621471	0.000000
F	2.404057	-1.241853	1.570174
F	2.404057	-1.241853	-1.570174
F	-2.068073	1.540663	1.638691
F	-2.068073	1.540663	-1.638691
F	1.156319	1.476001	2.509462
F	1.156319	1.476001	-2.509462
F	-0.815047	-1.331009	2.555005
F	-0.815047	-1.331009	-2.555005

7. Fluorocarborane anion $\text{CHB}_{11}\text{F}_{11}^-$

Stoichiometry: $\text{HB}_{11}\text{CF}_{11}$
Charge: -1
Multiplicity: 1
Point group: C_{5v}

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on F

PBE0: -1410.3229740
PBE0 ZPE correction: 0.1006824
PBE0 thermal Gibbs correction: 0.058132
DLPNO-CCSD, RHF/NormalPNO: -1409.1611665
DLPNO-CCSD(T), RHF/NormalPNO: -1409.3117029

PBE0 entropy (cal/mol-Kelvin): 131.956

Nuclear coordinates (angströms)

C	0.000000	0.000000	-1.630282
B	0.000000	-1.525572	-0.861773
B	0.000000	1.544443	0.644395
B	0.000000	0.000000	1.573708
B	0.896709	1.234214	-0.861773
B	-0.896709	1.234214	-0.861773
B	0.907801	-1.249481	0.644395
B	-0.907801	-1.249481	0.644395
B	1.450906	-0.471428	-0.861773
B	-1.450906	-0.471428	-0.861773
B	1.468853	0.477259	0.644395
B	-1.468853	0.477259	0.644395
H	0.000000	0.000000	-2.713547
F	0.000000	-2.650450	-1.617509
F	0.000000	2.761999	1.253980
F	0.000000	0.000000	2.935554
F	1.557896	2.144259	-1.617509
F	-1.557896	2.144259	-1.617509
F	1.623462	-2.234504	1.253980
F	-1.623462	-2.234504	1.253980
F	2.520728	-0.819034	-1.617509
F	-2.520728	-0.819034	-1.617509
F	2.626817	0.853505	1.253980
F	-2.626817	0.853505	1.253980

8. Fluorocarborane bridged anion $\text{H}[\text{CHB}_{11}\text{F}_{11}]_2^-$

Stoichiometry: $\text{H}_3\text{B}_{22}\text{C}_2\text{F}_{22}$
Charge: -1
Multiplicity: 1
Point group: C_{2h}

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on F

PBE0: -2821.0733864
PBE0 ZPE correction: 0.2110411
PBE0 thermal Gibbs correction: 0.138006
DLPNO-CCSD, RHF/NormalPNO: -2818.7512231
DLPNO-CCSD(T), RHF/NormalPNO: -2819.0529438

PBE0 entropy (cal/mol-Kelvin): 241.572

Nuclear coordinates (angströms)

H	0.000000	0.000000	0.000000
C	0.453478	5.267456	0.000000
B	1.732273	4.133357	0.000000
B	-1.644274	3.492397	0.000000
B	-0.369432	2.251544	0.000000
B	-0.942313	4.860413	0.900244
B	-0.942313	4.860413	-0.900244
B	1.069534	2.758861	0.914579
B	1.069534	2.758861	-0.914579
B	0.709983	4.413023	1.457942
B	0.709983	4.413023	-1.457942
B	-0.606538	3.213804	1.481752
B	-0.606538	3.213804	-1.481752
H	0.738074	6.313464	0.000000
F	3.008523	4.567049	0.000000
F	-2.964518	3.195503	0.000000
F	-0.754817	0.851262	0.000000
F	-1.617637	5.826875	1.554512
F	-1.617637	5.826875	-1.554512
F	1.823899	1.868065	1.604065
F	1.823899	1.868065	-1.604065
F	1.241651	5.051153	2.519736
F	1.241651	5.051153	-2.519736
F	-1.127221	2.693107	2.616944
F	-1.127221	2.693107	-2.616944
C	-0.453478	-5.267456	0.000000
B	-1.732273	-4.133357	0.000000
B	1.644274	-3.492397	0.000000
B	0.369432	-2.251544	0.000000
B	0.942313	-4.860413	-0.900244
B	0.942313	-4.860413	0.900244
B	-1.069534	-2.758861	-0.914579
B	-1.069534	-2.758861	0.914579
B	-0.709983	-4.413023	-1.457942
B	-0.709983	-4.413023	1.457942
B	0.606538	-3.213804	-1.481752
B	0.606538	-3.213804	1.481752
H	-0.738074	-6.313464	0.000000
F	-3.008523	-4.567049	0.000000
F	2.964518	-3.195503	0.000000
F	0.754817	-0.851262	0.000000
F	1.617637	-5.826875	-1.554512
F	1.617637	-5.826875	1.554512
F	-1.823899	-1.868065	-1.604065
F	-1.823899	-1.868065	1.604065
F	-1.241651	-5.051153	-2.519736
F	-1.241651	-5.051153	2.519736
F	1.127221	-2.693107	-2.616944
F	1.127221	-2.693107	2.616944

9. Nitrogen NN

Stoichiometry: N₂
Charge: 0
Multiplicity: 1
Point group: D_{∞h}

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0:	-109.4430008
PBE0 ZPE correction:	0.0056515
PBE0 thermal Gibbs correction:	-0.012772
DLPNO-CCSD, RHF/NormalPNO:	-109.3571109
DLPNO-CCSD(T), RHF/NormalPNO:	-109.3744331

PBE0 entropy (cal/mol-Kelvin): 45.730

Nuclear coordinates (angströms)

N	0.000000	0.000000	-0.545063
N	0.000000	0.000000	0.545063

10. Ion pair [NNHNN]⁺[NCX]⁻

Stoichiometry: HC₄₀N₂₄F
Charge: 0
Multiplicity: 1
Point group: C_s

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0: -2935.5713822
PBE0 ZPE correction: 0.3371506
PBE0 thermal Gibbs correction: 0.253243
DLPNO-CCSD, RHF/NormalPNO: -2932.6731340
DLPNO-CCSD(T), RHF/NormalPNO: -2933.2585654

PBE0 entropy (cal/mol-Kelvin): 293.710

Nuclear coordinates (angströms)

N	-0.011528	6.466656	-2.359380
N	0.017090	6.417199	-1.274424
H	0.050537	6.351215	0.000000
N	0.017090	6.417199	1.274424
N	-0.011528	6.466656	2.359380
F	0.000742	-0.487443	0.000000
C	-0.337806	1.276567	1.283273
C	-1.716444	0.668351	0.792919
C	1.715740	-1.669007	-0.793332
C	0.337050	-2.281136	-1.283376
C	1.827228	0.764140	0.000000
C	1.784484	-0.163418	1.284636
C	-1.783763	-0.836482	-1.283879
C	-1.825319	-1.766924	0.000000
C	-0.337806	1.276567	-1.283273
C	-0.447036	-1.154024	2.077155
C	0.447440	0.154852	-2.077408
C	0.337050	-2.281136	1.283376
C	0.516061	1.647723	0.000000
C	0.447440	0.154852	2.077408
C	-1.716444	0.668351	-0.792919
C	-1.783763	-0.836482	1.283879
C	1.784484	-0.163418	-1.284636
C	1.715740	-1.669007	0.793332
C	-0.447036	-1.154024	-2.077155
C	-0.514551	-2.659697	0.000000
C	-0.549808	2.472344	-2.097851
N	-0.690077	3.461712	-2.663039
C	-0.549808	2.472344	2.097851
N	-0.690077	3.461712	2.663039
C	-2.831010	1.454638	1.313170
N	-3.682793	2.109575	1.718779
C	2.844363	-2.431049	-1.315736
N	3.738224	-3.020852	-1.730393
C	0.558312	-3.449095	-2.128390
N	0.733529	-4.364932	-2.798693
C	3.007140	1.624732	0.000000
N	3.896320	2.351767	0.000000
C	2.954226	0.071746	2.124246
N	3.872506	0.282169	2.781072
C	-2.956141	-1.045513	-2.126369
N	-3.881749	-1.190201	-2.790584
C	-3.025866	-2.595116	0.000000
N	-3.976305	-3.239671	0.000000
C	-0.738398	-1.574603	3.443118
N	-0.965864	-1.889975	4.523692
C	0.733942	0.608763	-3.434540
N	0.949771	1.005913	-4.490354
C	0.558312	-3.449095	2.128390
N	0.733529	-4.364932	2.798693
C	0.839549	3.074518	0.000000
N	1.034281	4.204376	0.000000
C	0.733942	0.608763	3.434540
N	0.949771	1.005913	4.490354
C	-2.831010	1.454638	-1.313170
N	-3.682793	2.109575	-1.718779
C	-2.956141	-1.045513	2.126369
N	-3.881749	-1.190201	2.790584
C	2.954226	0.071746	-2.124246
N	3.872506	0.282169	-2.781072
C	2.844363	-2.431049	1.315736
N	3.738224	-3.020852	1.730393
C	-0.738398	-1.574603	-3.443118
N	-0.965864	-1.889975	-4.523692
C	-0.853264	-4.078227	0.000000
N	-1.121788	-5.194756	0.000000

11. Acetonitrile CH₃CN

Stoichiometry: H₃C₂N
Charge: 0
Multiplicity: 1
Point group: C_{3v}

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0:	-132.6387035
PBE0 ZPE correction:	0.0453593
PBE0 thermal Gibbs correction:	0.022397
DLPNO-CCSD, RHF/NormalPNO:	-132.5036745
DLPNO-CCSD(T), RHF/NormalPNO:	-132.5272271

PBE0 entropy (cal/mol-Kelvin): 57.893

Nuclear coordinates (angströms)

H	0.000000	1.024009	-1.545714
H	0.886818	-0.512005	-1.545714
H	-0.886818	-0.512005	-1.545714
C	0.000000	0.000000	-1.171141
C	0.000000	0.000000	0.278299
N	0.000000	0.000000	1.427741

12. 1,2-dicyanocyclopentadiene $\text{HC}_5\text{H}_3(\text{CN})_2$

Stoichiometry: $\text{H}_4\text{C}_7\text{N}_2$
Charge: 0
Multiplicity: 1
Point group: C_s

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0: -378.2663159
PBE0 ZPE correction: 0.0905533
PBE0 thermal Gibbs correction: 0.058225
DLPNO-CCSD, RHF/NormalPNO: -377.8430334
DLPNO-CCSD(T), RHF/NormalPNO: -377.9188934

PBE0 entropy (cal/mol-Kelvin): 85.846

Nuclear coordinates (angströms)

C	0.000000	0.667813	0.000000
C	-0.128641	-0.685326	0.000000
C	-1.543365	-1.035711	0.000000
C	-1.365368	1.275839	0.000000
C	-2.266914	0.093129	0.000000
H	-1.909812	-2.051531	0.000000
H	-3.344846	0.162428	0.000000
H	-1.516875	1.918997	0.875085
H	-1.516875	1.918997	-0.875085
C	1.194541	1.414573	0.000000
N	2.149566	2.061712	0.000000
C	0.927963	-1.630789	0.000000
N	1.761734	-2.425434	0.000000

13. Pentacyanotoluene $\text{HCH}_2\text{C}_6(\text{CN})_5$

Stoichiometry: $\text{H}_3\text{C}_{12}\text{N}_5$
Charge: 0
Multiplicity: 1
Point group: C_s

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0: -732.1203514
PBE0 ZPE correction: 0.1202144
PBE0 thermal Gibbs correction: 0.076745
DLPNO-CCSD, RHF/NormalPNO: -731.3270836
DLPNO-CCSD(T), RHF/NormalPNO: -731.4760134

PBE0 entropy (cal/mol-Kelvin): 125.852

Nuclear coordinates (angströms)

C	0.000000	1.254790	0.000000
C	1.206315	0.547978	0.000000
C	-1.207828	0.547175	0.000000
C	1.199705	-0.855560	0.000000
C	-1.196140	-0.852813	0.000000
C	0.002364	-1.578956	0.000000
C	-0.023233	-3.068860	0.000000
H	-0.560853	-3.438303	0.876363
H	0.979182	-3.490116	0.000000
H	-0.560853	-3.438303	-0.876363
C	-0.000656	2.677829	0.000000
N	-0.002196	3.828454	0.000000
C	-2.445242	1.250754	0.000000
N	-3.448371	1.814605	0.000000
C	-2.427986	-1.569395	0.000000
N	-3.402566	-2.181945	0.000000
C	2.442776	-1.554293	0.000000
N	3.437314	-2.133760	0.000000
C	2.442077	1.254421	0.000000
N	3.442908	1.822404	0.000000

14. Ion pair $[(\text{CH}_3\text{CN})_2\text{H}]^+[\text{C}_5\text{H}_3(\text{CN})_2]^-$

Stoichiometry: $\text{H}_{10}\text{C}_{11}\text{N}_4$
Charge: 0
Multiplicity: 1
Point group: C_{2v}

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0: -643.5261260
PBE0 ZPE correction: 0.1796041
PBE0 thermal Gibbs correction: 0.129331
DLPNO-CCSD, RHF/NormalPNO: -642.8128879
DLPNO-CCSD(T), RHF/NormalPNO: -642.9393882

PBE0 entropy (cal/mol-Kelvin): 144.967

Nuclear coordinates (angströms)

C	0.000000	0.716832	2.232570
C	0.000000	-0.716832	2.232570
C	0.000000	-1.135499	3.572028
C	0.000000	1.135499	3.572028
C	0.000000	0.000000	4.384732
H	0.000000	-2.165526	3.897099
H	0.000000	0.000000	5.465199
H	0.000000	2.165526	3.897099
C	0.000000	1.545661	1.110557
N	0.000000	2.238885	0.179113
C	0.000000	-1.545661	1.110557
N	0.000000	-2.238885	0.179113
H	0.000000	3.729756	-1.365208
H	-0.893640	4.228243	-2.849853
H	0.893640	4.228243	-2.849853
C	0.000000	3.737855	-2.462803
C	0.000000	2.355823	-2.846119
N	0.000000	1.252815	-3.144718
H	0.000000	0.000000	-3.194294
N	0.000000	-1.252815	-3.144718
C	0.000000	-2.355823	-2.846119
C	0.000000	-3.737855	-2.462803
H	0.000000	-3.729756	-1.365208
H	-0.893640	-4.228243	-2.849853
H	0.893640	-4.228243	-2.849853

15. Ion pair $[(\text{CH}_3\text{CN})_2\text{H}]^+[\text{CH}_2\text{C}_6(\text{CN})_5]^-$

Stoichiometry: $\text{H}_9\text{C}_{16}\text{N}_7$
Charge: 0
Multiplicity: 1
Point group: C_1

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0: -997.3624651
PBE0 ZPE correction: 0.2100321
PBE0 thermal Gibbs correction: 0.152355
DLPNO-CCSD, RHF/NormalPNO: -996.2828796
DLPNO-CCSD(T), RHF/NormalPNO: -996.4816113

PBE0 entropy (cal/mol-Kelvin): 175.350

Nuclear coordinates (angströms)

H	-2.821717	-3.613097	-0.057776
H	-3.952367	-3.986442	-1.394375
H	-4.575517	-3.761021	0.260866
C	-3.826946	-3.434616	-0.462088
C	-3.981575	-2.026663	-0.707387
N	-4.091130	-0.903169	-0.895193
H	-3.962089	0.451597	-0.851117
N	-3.774086	1.603154	-0.752585
C	-3.443169	2.669848	-0.517464
C	-3.006564	3.999811	-0.216395
H	-1.953941	3.943110	0.110783
H	-3.090163	4.623993	-1.107062
H	-3.622765	4.408732	0.585667
C	1.053560	0.985309	0.443523
C	2.404100	0.819148	0.020058
C	0.295957	-0.187256	0.654622
C	2.954196	-0.424890	-0.168450
C	0.811663	-1.450495	0.446071
C	2.198690	-1.664969	0.035908
C	2.731483	-2.886419	-0.147170
H	3.760475	-3.004150	-0.455861
H	2.143913	-3.779735	0.014445
C	0.449152	2.243051	0.572780
N	-0.106912	3.254729	0.668030
C	-1.060465	-0.050752	1.072797
N	-2.157111	0.074493	1.402707
C	-0.049162	-2.560720	0.581298
N	-0.769778	-3.461704	0.654979
C	4.302321	-0.540281	-0.591103
N	5.393669	-0.684065	-0.936258
C	3.184794	1.988613	-0.219739
N	3.786198	2.951520	-0.411556

16. Fluorine superhalogenide FNCX

Stoichiometry: C₄₀N₂₀F₂
Charge: 0
Multiplicity: 1
Point group: C_{3v}

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0: -2815.7842193
PBE0 ZPE correction: 0.3178725
PBE0 thermal Gibbs correction: 0.243539
DLPNO-CCSD, RHF/NormalPNO: -2812.9885468
DLPNO-CCSD(T), RHF/NormalPNO: -2813.5453373

PBE0 entropy (cal/mol-Kelvin): 262.977

Nuclear coordinates (angströms)

F	0.000000	0.000000	5.878777
F	0.000000	0.000000	-0.137753
C	0.000000	-1.488381	1.483640
C	0.000000	0.000000	2.018594
C	0.000000	0.000000	-2.380964
C	0.000000	1.482132	-1.816341
C	0.793815	-1.941588	-0.902470
C	-0.793815	-1.941588	-0.902470
C	0.794048	1.945193	0.577241
C	-0.794048	1.945193	0.577241
C	2.081610	-0.284930	0.577241
C	-2.081610	-0.284930	0.577241
C	2.078372	0.283330	-0.902470
C	-2.078372	0.283330	-0.902470
C	1.287562	-1.660262	0.577241
C	-1.287562	-1.660262	0.577241
C	1.288976	0.744190	1.483640
C	-1.288976	0.744190	1.483640
C	1.283564	-0.741066	-1.816341
C	-1.283564	-0.741066	-1.816341
C	1.284557	1.658258	-0.902470
C	-1.284557	1.658258	-0.902470
C	3.436267	-0.459744	1.088374
N	4.489016	-0.585121	1.530342
C	0.000000	-2.405031	2.621843
N	0.000000	-3.010423	3.598779
C	0.000000	0.000000	3.496455
N	0.000000	0.000000	4.629906
C	0.000000	0.000000	-3.838714
N	0.000000	0.000000	-4.987096
C	0.000000	2.456900	-2.900310
N	0.000000	3.230602	-3.748964
C	1.316868	-3.216566	-1.378313
N	1.732837	-4.225479	-1.736060
C	-1.316868	-3.216566	-1.378313
N	-1.732837	-4.225479	-1.736060
C	1.319983	3.205766	1.088374
N	1.737779	4.180162	1.530342
C	-1.319983	3.205766	1.088374
N	-1.737779	4.180162	1.530342
C	-3.436267	-0.459744	1.088374
N	-4.489016	-0.585121	1.530342
C	3.444062	0.467841	-1.378313
N	4.525790	0.612058	-1.736060
C	-3.444062	0.467841	-1.378313
N	-4.525790	0.612058	-1.736060
C	2.116283	-2.746022	1.088374
N	2.751238	-3.595042	1.530342
C	-2.116283	-2.746022	1.088374
N	-2.751238	-3.595042	1.530342
C	2.082818	1.202515	2.621843
N	2.607102	1.505211	3.598779
C	-2.082818	1.202515	2.621843
N	-2.607102	1.505211	3.598779
C	2.127738	-1.228450	-2.900310
N	2.797783	-1.615301	-3.748964
C	-2.127738	-1.228450	-2.900310
N	-2.797783	-1.615301	-3.748964
C	2.127193	2.748724	-1.378313
N	2.792953	3.613420	-1.736060
C	-2.127193	2.748724	-1.378313
N	-2.792953	3.613420	-1.736060

17. Superhalogen dimer [NCX]₂

Stoichiometry: C₈₀N₄₀F₂
Charge: 0
Multiplicity: 1
Point group: D_{3d}

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0: -5432.1160581
PBE0 ZPE correction: 0.6296862
PBE0 thermal Gibbs correction: 0.502865
DLPNO-CCSD, RHF/NormalPNO: -5426.6430985
DLPNO-CCSD(T), RHF/NormalPNO: -5427.7444875
PBE0 entropy (cal/mol-Kelvin): 476.653

Nuclear coordinates (angströms)

F	0.000000	0.000000	5.375430	C	0.000000	1.482544	-7.058701
C	1.292319	-0.746121	3.763837	C	0.000000	0.000000	-3.237075
C	2.084285	0.285726	4.665487	C	-0.794696	1.947907	-4.665487
C	-2.079434	-0.283412	6.145329	C	-1.289589	-1.662180	-4.665487
C	-1.283921	0.741272	7.058701	C	-2.079434	0.283412	-6.145329
C	-1.292319	-0.746121	3.763837	C	2.084285	-0.285726	-4.665487
C	-0.794696	-1.947907	4.665487	C	1.285159	1.659137	-6.145329
C	0.794275	1.942548	6.145329	C	0.794275	-1.942548	-6.145329
C	1.283921	0.741272	7.058701	C	0.000000	0.000000	-7.622991
C	0.000000	1.492242	3.763837	C	0.000000	-2.381286	-2.601472
C	1.285159	-1.659137	6.145329	N	0.000000	-2.923115	-1.587126
C	-1.289589	1.662180	4.665487	C	-2.062254	1.190643	-2.601472
C	0.000000	-1.482544	7.058701	N	-2.531492	1.461557	-1.587126
C	0.000000	0.000000	3.237075	C	-3.436192	-0.455058	-4.147348
C	0.794696	-1.947907	4.665487	N	-4.484442	-0.571160	-3.691790
C	1.289589	1.662180	4.665487	C	3.445438	0.467470	-6.618814
C	2.079434	-0.283412	6.145329	N	4.528817	0.611089	-6.971989
C	-2.084285	0.285726	4.665487	C	2.128062	-1.228637	-8.142062
C	-1.285159	-1.659137	6.145329	N	2.799109	-1.616066	-8.989724
C	-0.794275	1.942548	6.145329	C	2.062254	1.190643	-2.601472
C	0.000000	0.000000	7.622991	N	2.531492	1.461557	-1.587126
C	0.000000	2.381286	2.601472	C	1.324004	3.203359	-4.147348
N	0.000000	2.923115	1.587126	N	1.747582	4.169220	-3.691790
C	2.062254	-1.190643	2.601472	C	-1.317878	-3.217572	-6.618814
N	2.531492	-1.461557	1.587126	N	-1.735190	-4.227615	-6.971989
C	3.436192	0.455058	4.147348	C	-2.128062	-1.228637	-8.142062
N	4.484442	0.571160	3.691790	N	-2.799109	-1.616066	-8.989724
C	-3.445438	-0.467470	6.618814	C	-2.127559	2.750102	-6.618814
N	-4.528817	-0.611089	6.971989	N	-2.793628	3.616526	-6.971989
C	-2.128062	1.228637	8.142062	C	2.112188	-2.748301	-4.147348
N	-2.799109	1.616066	8.989724	N	2.736860	-3.598061	-3.691790
C	-2.062254	-1.190643	2.601472	C	0.000000	2.457275	-8.142062
N	-2.531492	-1.461557	1.587126	N	0.000000	3.232132	-8.989724
C	-1.324004	-3.203359	4.147348	C	0.000000	0.000000	-1.770098
N	-1.747582	-4.169220	3.691790	N	0.000000	0.000000	-0.619073
C	1.317878	3.217572	6.618814	C	-1.324004	3.203359	-4.147348
N	1.735190	4.227615	6.971989	N	-1.747582	4.169220	-3.691790
C	2.128062	1.228637	8.142062	C	-2.112188	-2.748301	-4.147348
N	2.799109	1.616066	8.989724	N	-2.736860	-3.598061	-3.691790
C	2.127559	-2.750102	6.618814	C	-3.445438	0.467470	-6.618814
N	2.793628	-3.616526	6.971989	N	-4.528817	0.611089	-6.971989
C	-2.112188	2.748301	4.147348	C	3.436192	-0.455058	-4.147348
N	-2.736860	3.598061	3.691790	N	4.484442	-0.571160	-3.691790
C	0.000000	-2.457275	8.142062	C	2.127559	2.750102	-6.618814
N	0.000000	-3.232132	8.989724	N	2.793628	3.616526	-6.971989
C	0.000000	0.000000	1.770098	C	1.317878	-3.217572	-6.618814
N	0.000000	0.000000	0.619073	N	1.735190	-4.227615	-6.971989
C	1.324004	-3.203359	4.147348	C	0.000000	0.000000	-9.080302
N	1.747582	-4.169220	3.691790	N	0.000000	0.000000	-10.228713
C	2.112188	2.748301	4.147348				
N	2.736860	3.598061	3.691790				
C	3.445438	-0.467470	6.618814				
N	4.528817	-0.611089	6.971989				
C	-3.436192	0.455058	4.147348				
N	-4.484442	0.571160	3.691790				
C	-2.127559	-2.750102	6.618814				
N	-2.793628	-3.616526	6.971989				
C	-1.317878	3.217572	6.618814				
N	-1.735190	4.227615	6.971989				
C	0.000000	0.000000	9.080302				
N	0.000000	0.000000	10.228713				
F	0.000000	0.000000	-5.375430				
C	-1.292319	0.746121	-3.763837				
C	-2.084285	-0.285726	-4.665487				
C	2.079434	0.283412	-6.145329				
C	1.283921	-0.741272	-7.058701				
C	1.292319	0.746121	-3.763837				
C	0.794696	1.947907	-4.665487				
C	-0.794275	-1.942548	-6.145329				
C	-1.283921	-0.741272	-7.058701				
C	0.000000	-1.492242	-3.763837				
C	-1.285159	1.659137	-6.145329				
C	1.289589	-1.662180	-4.665487				

18. Empty cage C₂₀(CN)₂₀

Stoichiometry: C₄₀N₂₀
Charge: 0
Multiplicity: 1
Point group: I_h

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0: -2616.3993929
PBE0 ZPE correction: 0.3119728
PBE0 thermal Gibbs correction: 0.239099
DLPNO-CCSD, RHF/NormalPNO: -2613.7167422
DLPNO-CCSD(T), RHF/NormalPNO: -2614.2570040

PBE0 entropy (cal/mol-Kelvin): 255.826

Nuclear coordinates (angströms)

C	-1.275327	-0.414379	1.755337
C	-0.788195	1.084858	1.755337
C	0.788195	-1.084858	-1.755337
C	1.275327	0.414379	-1.755337
C	0.000000	-2.169716	0.414379
C	-1.275327	-1.755337	-0.414379
C	1.275327	1.755337	0.414379
C	0.000000	2.169716	-0.414379
C	1.275327	-0.414379	1.755337
C	-2.063523	0.670479	-0.414379
C	2.063523	-0.670479	0.414379
C	-1.275327	0.414379	-1.755337
C	0.000000	-1.340958	1.755337
C	-2.063523	-0.670479	0.414379
C	0.788195	1.084858	1.755337
C	-1.275327	1.755337	0.414379
C	1.275327	-1.755337	-0.414379
C	-0.788195	-1.084858	-1.755337
C	2.063523	0.670479	-0.414379
C	0.000000	1.340958	-1.755337
C	2.114711	-0.687111	2.910650
N	2.777694	-0.902527	3.823167
C	-2.114711	-0.687111	2.910650
N	-2.777694	-0.902527	3.823167
C	-1.306963	1.798881	2.910650
N	-1.716709	2.362847	3.823167
C	1.306963	-1.798881	-2.910650
N	1.716709	-2.362847	-3.823167
C	2.114711	0.687111	-2.910650
N	2.777694	0.902527	-3.823167
C	0.000000	-3.597762	0.687111
N	0.000000	-4.725695	0.902527
C	-2.114711	-2.910650	-0.687111
N	-2.777694	-3.823167	-0.902527
C	2.114711	2.910650	0.687111
N	2.777694	3.823167	0.902527
C	0.000000	3.597762	-0.687111
N	0.000000	4.725695	-0.902527
C	-3.421675	1.111770	-0.687111
N	-4.494403	1.460320	-0.902527
C	3.421675	-1.111770	0.687111
N	4.494403	-1.460320	0.902527
C	-2.114711	0.687111	-2.910650
N	-2.777694	0.902527	-3.823167
C	0.000000	-2.223539	2.910650
N	0.000000	-2.920640	3.823167
C	-3.421675	-1.111770	0.687111
N	-4.494403	-1.460320	0.902527
C	1.306963	1.798881	2.910650
N	1.716709	2.362847	3.823167
C	-2.114711	2.910650	0.687111
N	-2.777694	3.823167	0.902527
C	2.114711	-2.910650	-0.687111
N	2.777694	-3.823167	-0.902527
C	-1.306963	-1.798881	-2.910650
N	-1.716709	-2.362847	-3.823167
C	3.421675	1.111770	-0.687111
N	4.494403	1.460320	-0.902527
C	0.000000	2.223539	-2.910650
N	0.000000	2.920640	-3.823167

19. Neon complex Ne@C₂₀(CN)₂₀

Stoichiometry: C₄₀N₂₀Ne
Charge: 0
Multiplicity: 1
Point group: I_h

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0: -2745.1260811
PBE0 ZPE correction: 0.3131669
PBE0 thermal Gibbs correction: 0.239660
DLPNO-CCSD, RHF/NormalPNO: -2742.4011332
DLPNO-CCSD(T), RHF/NormalPNO: -2742.9484224

PBE0 entropy (cal/mol-Kelvin): 259.005

Nuclear coordinates (angströms)

Ne	0.000000	0.000000	0.000000
C	-1.293541	-0.420297	1.780407
C	-0.799452	1.100352	1.780407
C	0.799452	-1.100352	-1.780407
C	1.293541	0.420297	-1.780407
C	0.000000	-2.200704	0.420297
C	-1.293541	-1.780407	-0.420297
C	1.293541	1.780407	0.420297
C	0.000000	2.200704	-0.420297
C	1.293541	-0.420297	1.780407
C	-2.092994	0.680055	-0.420297
C	2.092994	-0.680055	0.420297
C	-1.293541	0.420297	-1.780407
C	0.000000	-1.360110	1.780407
C	-2.092994	-0.680055	0.420297
C	0.799452	1.100352	1.780407
C	-1.293541	1.780407	0.420297
C	1.293541	-1.780407	-0.420297
C	-0.799452	-1.100352	-1.780407
C	2.092994	0.680055	-0.420297
C	0.000000	1.360110	-1.780407
C	2.130879	-0.692365	2.932903
N	2.793928	-0.907802	3.845512
C	-2.130879	-0.692365	2.932903
N	-2.793928	-0.907802	3.845512
C	-1.316956	1.812634	2.932903
N	-1.726742	2.376657	3.845512
C	1.316956	-1.812634	-2.932903
N	1.726742	-2.376657	-3.845512
C	2.130879	0.692365	-2.932903
N	2.793928	0.907802	-3.845512
C	0.000000	-3.625268	0.692365
N	0.000000	-4.753314	0.907802
C	-2.130879	-2.932903	-0.692365
N	-2.793928	-3.845512	-0.907802
C	2.130879	2.932903	0.692365
N	2.793928	3.845512	0.907802
C	0.000000	3.625268	-0.692365
N	0.000000	4.753314	-0.907802
C	-3.447835	1.120269	-0.692365
N	-4.520670	1.468855	-0.907802
C	3.447835	-1.120269	0.692365
N	4.520670	-1.468855	0.907802
C	-2.130879	0.692365	-2.932903
N	-2.793928	0.907802	-3.845512
C	0.000000	-2.240539	2.932903
N	0.000000	-2.937710	3.845512
C	-3.447835	-1.120269	0.692365
N	-4.520670	-1.468855	0.907802
C	1.316956	1.812634	2.932903
N	1.726742	2.376657	3.845512
C	-2.130879	2.932903	0.692365
N	-2.793928	3.845512	0.907802
C	2.130879	-2.932903	-0.692365
N	2.793928	-3.845512	-0.907802
C	-1.316956	-1.812634	-2.932903
N	-1.726742	-2.376657	-3.845512
C	3.447835	1.120269	-0.692365
N	4.520670	1.468855	-0.907802
C	0.000000	2.240539	-2.932903
N	0.000000	2.937710	-3.845512

20. Concaved cage **x**

Stoichiometry: C₃₉N₁₉F
Charge: 0
Multiplicity: 1
Point group: C_{3v}

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0: -2623.3494927
PBE0 ZPE correction: 0.3048446
PBE0 thermal Gibbs correction: 0.232803
DLPNO-CCSD, RHF/NormalPNO: -2620.7071718
DLPNO-CCSD(T), RHF/NormalPNO: -2621.2365236

PBE0 entropy (cal/mol-Kelvin): 252.365

Nuclear coordinates (angströms)

F	0.000000	0.000000	0.218647
C	1.281839	-0.740070	1.728891
C	0.822480	-1.993196	0.850068
C	-0.803414	1.962863	-0.632133
C	-1.289735	0.744629	-1.537491
C	0.000000	1.480141	1.728891
C	1.314918	1.708886	0.850068
C	-1.298182	-1.677208	-0.632133
C	0.000000	-1.489257	-1.537491
C	-1.281839	-0.740070	1.728891
C	2.101596	-0.285655	-0.632133
C	-2.137398	0.284310	0.850068
C	1.289735	0.744629	-1.537491
C	0.000000	0.000000	1.650010
C	2.137398	0.284310	0.850068
C	-0.822480	-1.993196	0.850068
C	1.298182	-1.677208	-0.632133
C	-1.314918	1.708886	0.850068
C	0.803414	1.962863	-0.632133
C	-2.101596	-0.285655	-0.632133
C	0.000000	0.000000	-2.097035
C	-1.783354	-1.029620	3.049909
N	-2.165079	-1.250009	4.110340
C	1.783354	-1.029620	3.049909
N	2.165079	-1.250009	4.110340
C	1.358233	-3.229214	1.377142
N	1.785738	-4.194087	1.830497
C	-1.318470	3.227872	-1.128771
N	-1.731214	4.233429	-1.499595
C	-2.122975	1.225700	-2.627293
N	-2.786356	1.608704	-3.482909
C	0.000000	2.059240	3.049909
N	0.000000	2.500018	4.110340
C	2.117465	2.790872	1.377142
N	2.739317	3.643537	1.830497
C	-2.136184	-2.755765	-1.128771
N	-2.800650	-3.615990	-1.499595
C	0.000000	-2.451400	-2.627293
N	0.000000	-3.217407	-3.482909
C	3.454654	-0.472107	-1.128771
N	4.531864	-0.617439	-1.499595
C	-3.475698	0.438342	1.377142
N	-4.525054	0.550549	1.830497
C	2.122975	1.225700	-2.627293
N	2.786356	1.608704	-3.482909
C	3.475698	0.438342	1.377142
N	4.525054	0.550549	1.830497
C	-1.358233	-3.229214	1.377142
N	-1.785738	-4.194087	1.830497
C	2.136184	-2.755765	-1.128771
N	2.800650	-3.615990	-1.499595
C	-2.117465	2.790872	1.377142
N	-2.739317	3.643537	1.830497
C	1.318470	3.227872	-1.128771
N	1.731214	4.233429	-1.499595
C	-3.454654	-0.472107	-1.128771
N	-4.531864	-0.617439	-1.499595
C	0.000000	0.000000	-3.550774
N	0.000000	0.000000	-4.699172

21. Destructed superhalogen

Stoichiometry: C₄₀N₂₀F
Charge: 0
Multiplicity: 2
Point group: C_s

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0: -2716.0496002

PBE0 ZPE correction: 0.3135234

PBE0 thermal Gibbs correction: 0.237584

PBE0 entropy (cal/mol-Kelvin): 264.614

Nuclear coordinates (angströms)

F	-0.092377	0.058076	0.000000
C	-0.880155	1.265816	0.000000
C	-1.538158	0.899650	1.284598
C	1.498024	-1.019814	-1.288821
C	1.182487	-1.895287	0.000000
C	-0.195939	0.723452	-2.134629
C	0.997742	1.505868	-1.313696
C	-1.021328	-1.589454	1.296894
C	0.140736	-0.827128	2.099642
C	-2.097179	-0.524130	-0.819877
C	0.997742	1.505868	1.313696
C	-1.021328	-1.589454	-1.296894
C	2.020934	0.403362	0.801896
C	-1.538158	0.899650	-1.284598
C	0.327453	2.136201	0.000000
C	-2.097179	-0.524130	0.819877
C	-0.195939	0.723452	2.134629
C	0.140736	-0.827128	-2.099642
C	2.020934	0.403362	-0.801896
C	-0.368251	-2.243227	0.000000
C	1.498024	-1.019814	1.288821
C	-3.419851	-0.768694	-1.353767
N	-4.474442	-0.930092	-1.779175
C	-1.125609	4.251885	0.000000
N	-2.173327	4.727738	0.000000
C	-2.518763	1.803546	1.833356
N	-3.302607	2.511374	2.284079
C	2.497178	-1.668205	-2.122556
N	3.285742	-2.174701	-2.786220
C	1.979735	-3.111142	0.000000
N	2.609683	-4.071331	0.000000
C	-0.357082	1.244493	-3.475002
N	-0.515424	1.680889	-4.525607
C	1.623359	2.504057	-2.153435
N	2.091884	3.301268	-2.835122
C	-1.650173	-2.596732	2.135129
N	-2.163740	-3.379702	2.800096
C	0.257429	-1.344571	3.452962
N	0.339988	-1.734372	4.530098
C	1.623359	2.504057	2.153435
N	2.091884	3.301268	2.835122
C	-1.650173	-2.596732	-2.135129
N	-2.163740	-3.379702	-2.800096
C	3.353021	0.677938	1.315215
N	4.399294	0.914238	1.725648
C	-2.518763	1.803546	-1.833356
N	-3.302607	2.511374	-2.284079
C	0.175428	3.648332	0.000000
N	1.196914	4.379727	0.000000
C	-3.419851	-0.768694	1.353767
N	-4.474442	-0.930092	1.779175
C	-0.357082	1.244493	3.475002
N	-0.515424	1.680889	4.525607
C	0.257429	-1.344571	-3.452962
N	0.339988	-1.734372	-4.530098
C	3.353021	0.677938	-1.315215
N	4.399294	0.914238	-1.725648
C	-0.575406	-3.682322	0.000000
N	-0.746393	-4.817920	0.000000
C	2.497178	-1.668205	2.122556
N	3.285742	-2.174701	2.786220

22. Superhalogen transition state

Stoichiometry: C₄₀N₂₀F
Charge: 0
Multiplicity: 2
Point group: C_s

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0: -2715.9777681
PBE0 ZPE correction: 0.3101156
PBE0 thermal Gibbs correction: 0.236039

PBE0 entropy (cal/mol-Kelvin): 259.901

Nuclear coordinates (angströms)

F	-0.011757	0.021374	0.000000
C	-0.553031	1.924230	0.000000
C	-1.168795	1.363262	1.299457
C	1.161059	-1.418917	-1.285901
C	0.596826	-2.159227	0.000000
C	0.083078	0.767967	-2.096738
C	1.421783	1.131080	-1.287302
C	-1.398853	-1.182883	1.289456
C	-0.070448	-0.810471	2.084989
C	-2.085915	0.159606	-0.800859
C	1.421783	1.131080	1.287302
C	-1.398853	-1.182883	-1.289456
C	2.082623	-0.224429	0.796735
C	-1.168795	1.363262	-1.299457
C	0.969299	1.891829	0.000000
C	-2.085915	0.159606	0.800859
C	0.083078	0.767967	2.096738
C	-0.070448	-0.810471	-2.084989
C	2.082623	-0.224429	-0.796735
C	-0.982135	-2.012190	0.000000
C	1.161059	-1.418917	1.285901
C	-3.435910	0.302149	-1.324751
N	-4.497310	0.441325	-1.741032
C	-0.465964	3.655586	0.000000
N	-1.312129	4.481562	0.000000
C	-1.908451	2.350145	2.065106
N	-2.475415	3.161189	2.648579
C	1.917120	-2.336066	-2.128241
N	2.518718	-3.050262	-2.796734
C	0.988269	-3.562374	0.000000
N	1.298338	-4.668120	0.000000
C	0.137799	1.310838	-3.445306
N	0.185473	1.776242	-4.494337
C	2.334847	1.956525	-2.062090
N	3.035252	2.676076	-2.620497
C	-2.310114	-1.943789	2.133675
N	-3.034915	-2.531503	2.803188
C	-0.117868	-1.319955	3.448870
N	-0.155300	-1.701516	4.531485
C	2.334847	1.956525	2.062090
N	3.035252	2.676076	2.620497
C	-2.310114	-1.943789	-2.133675
N	-3.034915	-2.531503	-2.803188
C	3.435807	-0.342052	1.321708
N	4.503110	-0.405892	1.741097
C	-1.908451	2.350145	-2.065106
N	-2.475415	3.161189	-2.648579
C	1.083673	3.400977	0.000000
N	1.869845	4.333044	0.000000
C	-3.435910	0.302149	1.324751
N	-4.497310	0.441325	1.741032
C	0.137799	1.310838	3.445306
N	0.185473	1.776242	4.494337
C	-0.117868	-1.319955	-3.448870
N	-0.155300	-1.701516	-4.531485
C	3.435807	-0.342052	-1.321708
N	4.503110	-0.405892	-1.741097
C	-1.628052	-3.318002	0.000000
N	-2.141089	-4.345439	0.000000
C	1.917120	-2.336066	2.128241
N	2.518718	-3.050262	2.796734

23. Superacid transition state

Stoichiometry: HC₄₀N₂₀F
Charge: 0
Multiplicity: 1
Point group: C_s

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N

PBE0: -2716.6500940

PBE0 ZPE correction: 0.3234939

PBE0 thermal Gibbs correction: 0.250084

PBE0 entropy (cal/mol-Kelvin): 258.084

Nuclear coordinates (angströms)

F	-0.026744	0.017533	0.000000
C	-0.866682	1.764838	0.000000
C	-1.390017	1.129854	1.299925
C	1.384155	-1.204883	-1.285283
C	0.956165	-2.031548	0.000000
C	-0.054704	0.760705	-2.097306
C	1.203355	1.353396	-1.286457
C	-1.178534	-1.416689	1.289759
C	0.066440	-0.819940	2.084809
C	-2.088304	-0.213772	-0.801971
C	1.203355	1.353396	1.286457
C	-1.178534	-1.416689	-1.289759
C	2.085496	0.131274	0.796180
C	-1.390017	1.129854	-1.299925
C	0.629941	2.040907	0.000000
C	-2.088304	-0.213772	0.801971
C	-0.054704	0.760705	2.097306
C	0.066440	-0.819940	-2.084809
C	2.085496	0.131274	-0.796180
C	-0.624397	-2.160446	0.000000
C	1.384155	-1.204883	1.285283
C	-3.442352	-0.306823	-1.325751
N	-4.511888	-0.355240	-1.741524
C	-1.117000	3.543168	0.000000
N	-2.111309	4.163585	0.000000
C	-2.286645	1.975633	2.066061
N	-2.983900	2.662837	2.666547
C	2.287427	-1.978192	-2.126888
N	3.003329	-2.578579	-2.794604
C	1.584007	-3.345950	0.000000
N	2.080103	-4.381650	0.000000
C	-0.097731	1.301294	-3.447062
N	-0.136172	1.761995	-4.498479
C	1.958470	2.308435	-2.082994
N	2.517586	3.115132	-2.679392
C	-1.943446	-2.324710	2.133763
N	-2.555097	-3.029733	2.802917
C	0.108481	-1.332104	3.447874
N	0.137854	-1.717390	4.529389
C	1.958470	2.308435	2.082994
N	2.517586	3.115132	2.679392
C	-1.943446	-2.324710	-2.133763
N	-2.555097	-3.029733	-2.802917
C	3.439392	0.246129	1.320303
N	4.502308	0.364402	1.738896
C	-2.286645	1.975633	-2.066061
N	-2.983900	2.662837	-2.666547
C	0.485487	3.530697	0.000000
N	1.243611	4.484026	0.000000
C	-3.442352	-0.306823	1.325751
N	-4.511888	-0.355240	1.741524
C	-0.097731	1.301294	3.447062
N	-0.136172	1.761995	4.498479
C	0.108481	-1.332104	-3.447874
N	0.137854	-1.717390	-4.529389
C	3.439392	0.246129	-1.320303
N	4.502308	0.364402	-1.738896
C	-1.033780	-3.558518	0.000000
N	-1.360860	-4.659344	0.000000
C	2.287427	-1.978192	2.126888
N	3.003329	-2.578579	2.794604
H	0.943346	5.453781	0.000000

24. Alternative superhalogen F@C₂₄(CN)₂₄

Stoichiometry: C₄₈N₂₄F
Charge: 0
Multiplicity: 2
Point group: D_{6d}

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N
PBE0: -3239.2337414

Nuclear coordinates (angströms)

F	0.000000	0.000000	0.000000
C	0.000000	2.508671	0.432323
C	1.254335	2.172573	-0.432323
C	-1.254335	2.172573	-0.432323
C	0.795635	1.378081	-1.734587
C	-0.795635	1.378081	-1.734587
C	-2.172573	1.254335	0.432323
C	-2.508671	0.000000	-0.432323
C	-1.591270	0.000000	-1.734587
C	-1.378081	0.795635	1.734587
C	0.000000	1.591270	1.734587
C	1.378081	0.795635	1.734587
C	-1.378081	-0.795635	1.734587
C	0.000000	-1.591270	1.734587
C	1.378081	-0.795635	1.734587
C	-2.172573	-1.254335	0.432323
C	2.508671	0.000000	-0.432323
C	2.172573	1.254335	0.432323
C	2.172573	-1.254335	0.432323
C	1.254335	-2.172573	-0.432323
C	0.000000	-2.508671	0.432323
C	-1.254335	-2.172573	-0.432323
C	1.591270	0.000000	-1.734587
C	0.795635	-1.378081	-1.734587
C	-0.795635	-1.378081	-1.734587
C	-1.229438	2.129448	-2.920264
N	-1.565878	2.712180	-3.856727
C	2.458875	0.000000	-2.920264
N	3.131756	0.000000	-3.856727
C	1.229438	2.129448	-2.920264
N	1.565878	2.712180	-3.856727
C	-2.458875	0.000000	-2.920264
N	-3.131756	0.000000	-3.856727
C	-1.229438	-2.129448	-2.920264
N	-1.565878	-2.712180	-3.856727
C	1.229438	-2.129448	-2.920264
N	1.565878	-2.712180	-3.856727
C	2.129448	-1.229438	2.920264
N	2.712180	-1.565878	3.856727
C	2.129448	1.229438	2.920264
N	2.712180	1.565878	3.856727
C	0.000000	-2.458875	2.920264
N	0.000000	-3.131756	3.856727
C	0.000000	2.458875	2.920264
N	0.000000	3.131756	3.856727
C	-2.129448	-1.229438	2.920264
N	-2.712180	-1.565878	3.856727
C	-2.129448	1.229438	2.920264
N	-2.712180	1.565878	3.856727
C	-3.915868	0.000000	-0.817188
N	-5.023282	0.000000	-1.122098
C	-1.957934	-3.391241	-0.817188
N	-2.511641	-4.350290	-1.122098
C	0.000000	3.915868	0.817188
N	0.000000	5.023282	1.122098
C	-1.957934	3.391241	-0.817188
N	-2.511641	4.350290	-1.122098
C	-3.391241	1.957934	0.817188
N	-4.350290	2.511641	1.122098
C	-3.391241	-1.957934	0.817188
N	-4.350290	-2.511641	1.122098
C	0.000000	-3.915868	0.817188
N	0.000000	-5.023282	1.122098
C	1.957934	-3.391241	-0.817188
N	2.511641	-4.350290	-1.122098
C	3.391241	-1.957934	0.817188
N	4.350290	-2.511641	1.122098
C	3.915868	0.000000	-0.817188
N	5.023282	0.000000	-1.122098
C	3.391241	1.957934	0.817188
N	4.350290	2.511641	1.122098
C	1.957934	3.391241	-0.817188
N	2.511641	4.350290	-1.122098

25. Alternative superhalogen anion $F@C_{24}(CN)_{24}^-$

Stoichiometry: $C_{48}N_{24}F$
Charge: -1
Multiplicity: 1
Point group: D_{6d}

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N
PBE0: -3239.5829212

Nuclear coordinates (angströms)

F	0.000000	0.000000	0.000000
C	0.000000	2.506807	0.432897
C	1.253403	2.170958	-0.432897
C	-1.253403	2.170958	-0.432897
C	0.798093	1.382337	-1.742645
C	-0.798093	1.382337	-1.742645
C	-2.170958	1.253403	0.432897
C	-2.506807	0.000000	-0.432897
C	-1.596185	0.000000	-1.742645
C	-1.382337	0.798093	1.742645
C	0.000000	1.596185	1.742645
C	1.382337	0.798093	1.742645
C	-1.382337	-0.798093	1.742645
C	0.000000	-1.596185	1.742645
C	1.382337	-0.798093	1.742645
C	-2.170958	-1.253403	0.432897
C	2.506807	0.000000	-0.432897
C	2.170958	1.253403	0.432897
C	2.170958	-1.253403	0.432897
C	1.253403	-2.170958	-0.432897
C	0.000000	-2.506807	0.432897
C	-1.253403	-2.170958	-0.432897
C	1.596185	0.000000	-1.742645
C	0.798093	-1.382337	-1.742645
C	-0.798093	-1.382337	-1.742645
C	-1.241983	2.151178	-2.912651
N	-1.596710	2.765583	-3.815532
C	2.483966	0.000000	-2.912651
N	3.193420	0.000000	-3.815532
C	1.241983	2.151178	-2.912651
N	1.596710	2.765583	-3.815532
C	-2.483966	0.000000	-2.912651
N	-3.193420	0.000000	-3.815532
C	-1.241983	-2.151178	-2.912651
N	-1.596710	-2.765583	-3.815532
C	1.241983	-2.151178	-2.912651
N	1.596710	-2.765583	-3.815532
C	2.151178	-1.241983	2.912651
N	2.765583	-1.596710	3.815532
C	2.151178	1.241983	2.912651
N	2.765583	1.596710	3.815532
C	0.000000	-2.483966	2.912651
N	0.000000	-3.193420	3.815532
C	0.000000	2.483966	2.912651
N	0.000000	3.193420	3.815532
C	-2.151178	-1.241983	2.912651
N	-2.765583	-1.596710	3.815532
C	-2.151178	1.241983	2.912651
N	-2.765583	1.596710	3.815532
C	-3.918598	0.000000	-0.806772
N	-5.031937	0.000000	-1.087285
C	-1.959299	-3.393605	-0.806772
N	-2.515968	-4.357785	-1.087285
C	0.000000	3.918598	0.806772
N	0.000000	5.031937	1.087285
C	-1.959299	3.393605	-0.806772
N	-2.515968	4.357785	-1.087285
C	-3.393605	1.959299	0.806772
N	-4.357785	2.515968	1.087285
C	-3.393605	-1.959299	0.806772
N	-4.357785	-2.515968	1.087285
C	0.000000	-3.918598	0.806772
N	0.000000	-5.031937	1.087285
C	1.959299	-3.393605	-0.806772
N	2.515968	-4.357785	-1.087285
C	3.393605	-1.959299	0.806772
N	4.357785	-2.515968	1.087285
C	3.918598	0.000000	-0.806772
N	5.031937	0.000000	-1.087285
C	3.393605	1.959299	0.806772
N	4.357785	2.515968	1.087285
C	1.959299	3.393605	-0.806772
N	2.515968	4.357785	-1.087285

26. Alternative superhalogen $F@C_{28}(CN)_{28}$

Stoichiometry: $C_{56}N_{28}F$
Charge: 0
Multiplicity: 2
Point group: T_d

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N
PBE0: -3762.3782380

Nuclear coordinates (angströms)

F	0.000000	0.000000	0.000000
C	1.882025	-0.056479	1.882025
C	0.564343	2.507059	0.564343
C	-0.056479	1.882025	1.882025
C	0.564343	0.564343	2.507059
C	1.576960	-1.576960	1.576960
C	-0.564343	-0.564343	2.507059
C	0.056479	-1.882025	1.882025
C	-1.576960	1.576960	1.576960
C	1.882025	-1.882025	0.056479
C	2.507059	-0.564343	-0.564343
C	1.882025	0.056479	-1.882025
C	0.564343	-2.507059	-0.564343
C	-0.056479	-1.882025	-1.882025
C	0.564343	-0.564343	-2.507059
C	-0.564343	-2.507059	0.564343
C	0.056479	1.882025	-1.882025
C	1.576960	1.576960	-1.576960
C	-0.564343	2.507059	-0.564343
C	-0.564343	0.564343	-2.507059
C	1.882025	1.882025	-0.056479
C	2.507059	0.564343	0.564343
C	-1.882025	-0.056479	-1.882025
C	-1.576960	-1.576960	-1.576960
C	-1.882025	0.056479	1.882025
C	-2.507059	-0.564343	0.564343
C	-1.882025	-1.882025	-0.056479
C	-2.507059	0.564343	-0.564343
C	-1.882025	1.882025	0.056479
C	2.919852	0.008481	2.919852
C	0.876296	3.909842	0.876296
C	0.008481	2.919852	2.919852
C	0.876296	0.876296	3.909842
C	2.420315	-2.420315	2.420315
C	-0.876296	-0.876296	3.909842
C	-0.008481	-2.919852	2.919852
C	-2.420315	2.420315	2.420315
C	2.919852	-2.919852	-0.008481
C	3.909842	-0.876296	-0.876296
C	2.919852	-0.008481	-2.919852
C	0.876296	-3.909842	-0.876296
C	0.008481	-2.919852	-2.919852
C	0.876296	-0.876296	-3.909842
C	-0.876296	-3.909842	0.876296
C	-0.008481	2.919852	-2.919852
C	2.420315	2.420315	-2.420315
C	-0.876296	3.909842	-0.876296
C	-0.876296	0.876296	-3.909842
C	2.919852	2.919852	0.008481
C	3.909842	0.876296	0.876296
C	-2.919852	0.008481	-2.919852
C	-2.420315	-2.420315	-2.420315
C	-2.919852	-0.008481	2.919852
C	-3.909842	-0.876296	0.876296
C	-2.919852	-2.919852	0.008481
C	-3.909842	0.876296	-0.876296
C	-2.919852	2.919852	-0.008481
N	3.732922	0.050669	3.732922
N	1.114257	5.010591	1.114257
N	0.050669	3.732922	3.732922
N	1.114257	1.114257	5.010591
N	3.083439	-3.083439	3.083439
N	-1.114257	-1.114257	5.010591
N	-0.050669	-3.732922	3.732922
N	-3.083439	3.083439	3.083439
N	3.732922	-3.732922	-0.050669
N	5.010591	-1.114257	-1.114257
N	3.732922	-0.050669	-3.732922
N	1.114257	-5.010591	-1.114257
N	0.050669	-3.732922	-3.732922
N	1.114257	-1.114257	-5.010591
N	-1.114257	-5.010591	1.114257
N	-0.050669	3.732922	-3.732922
N	3.083439	3.083439	-3.083439
N	-1.114257	5.010591	-1.114257
N	-1.114257	1.114257	-5.010591
N	3.732922	3.732922	0.050669
N	5.010591	1.114257	1.114257
N	-3.732922	0.050669	-3.732922
N	-3.083439	-3.083439	-3.083439
N	-3.732922	-0.050669	3.732922
N	-5.010591	-1.114257	1.114257
N	-3.732922	-3.732922	0.050669
N	-5.010591	1.114257	-1.114257
N	-3.732922	3.732922	-0.050669

27. Alternative superhalogen anion $F@C_{28}(CN)_{28}^-$

Stoichiometry: $C_{56}N_{28}F$
Charge: -1
Multiplicity: 1
Point group: T_d

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N
PBE0: -3762.7267553

Nuclear coordinates (angströms)

F	0.000000	0.000000	0.000000
C	0.056499	1.884861	1.884861
C	-2.512119	0.565416	0.565416
C	-1.884861	-0.056499	1.884861
C	-0.565416	0.565416	2.512119
C	1.576809	1.576809	1.576809
C	0.565416	-0.565416	2.512119
C	1.884861	0.056499	1.884861
C	-1.576809	-1.576809	1.576809
C	1.884861	1.884861	0.056499
C	0.565416	2.512119	-0.565416
C	-0.056499	1.884861	-1.884861
C	2.512119	0.565416	-0.565416
C	1.884861	-0.056499	-1.884861
C	0.565416	0.565416	-2.512119
C	2.512119	-0.565416	0.565416
C	-1.884861	0.056499	-1.884861
C	-1.576809	1.576809	-1.576809
C	-2.512119	-0.565416	-0.565416
C	-0.565416	-0.565416	-2.512119
C	-1.884861	1.884861	-0.056499
C	-0.565416	2.512119	0.565416
C	0.056499	-1.884861	-1.884861
C	1.576809	-1.576809	-1.576809
C	-0.056499	-1.884861	1.884861
C	0.565416	-2.512119	0.565416
C	1.884861	-1.884861	-0.056499
C	-0.565416	-2.512119	-0.565416
C	-1.884861	-1.884861	0.056499
C	0.003120	2.923437	2.923437
C	-3.916221	0.874944	0.874944
C	-2.923437	-0.003120	2.923437
C	-0.874944	0.874944	3.916221
C	2.420983	2.420983	2.420983
C	0.874944	-0.874944	3.916221
C	2.923437	0.003120	2.923437
C	-2.420983	-2.420983	2.420983
C	2.923437	2.923437	0.003120
C	0.874944	3.916221	-0.874944
C	-0.003120	2.923437	-2.923437
C	3.916221	0.874944	-0.874944
C	2.923437	-0.003120	-2.923437
C	0.874944	0.874944	-3.916221
C	3.916221	-0.874944	0.874944
C	-2.923437	0.003120	-2.923437
C	-2.420983	2.420983	-2.420983
C	-3.916221	-0.874944	-0.874944
C	-0.874944	-0.874944	-3.916221
C	-2.923437	2.923437	-0.003120
C	-0.874944	3.916221	0.874944
C	0.003120	-2.923437	-2.923437
C	2.420983	-2.420983	-2.420983
C	-0.003120	-2.923437	2.923437
C	0.874944	-3.916221	0.874944
C	2.923437	-2.923437	-0.003120
C	-0.874944	-3.916221	-0.874944
C	-2.923437	-2.923437	0.003120
N	-0.017859	3.735123	3.735123
N	-5.016088	1.108056	1.108056
N	-3.735123	0.017859	3.735123
N	-1.108056	1.108056	5.016088
N	3.083909	3.083909	3.083909
N	1.108056	-1.108056	5.016088
N	3.735123	-0.017859	3.735123
N	-3.083909	-3.083909	3.083909
N	3.735123	3.735123	-0.017859
N	1.108056	5.016088	-1.108056
N	0.017859	3.735123	-3.735123
N	5.016088	1.108056	-1.108056
N	3.735123	0.017859	-3.735123
N	1.108056	1.108056	-5.016088
N	5.016088	-1.108056	1.108056
N	-3.735123	-0.017859	-3.735123
N	-3.083909	3.083909	-3.083909
N	-5.016088	-1.108056	-1.108056
N	-1.108056	-1.108056	-5.016088
N	-3.735123	3.735123	0.017859
N	-1.108056	5.016088	1.108056
N	-0.017859	-3.735123	-3.735123
N	3.083909	-3.083909	-3.083909
N	0.017859	-3.735123	3.735123
N	1.108056	-5.016088	1.108056
N	3.735123	-3.735123	0.017859
N	-1.108056	-5.016088	-1.108056
N	-3.735123	-3.735123	-0.017859

28. Cyanocarborane acid $\text{HB}_{11}\text{C}(\text{CN})_{12}$

Stoichiometry: $\text{HB}_{11}\text{C}_{13}\text{N}_{12}$
Charge: 0
Multiplicity: 1
Point group: C_{5v}

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N
PBE0: -1425.2286610

Nuclear coordinates (angströms)

H	0.000000	0.000000	5.300376
C	0.000000	0.000000	-1.579757
B	0.000000	1.532087	-0.773574
B	0.000000	-1.536770	0.730568
B	0.000000	0.000000	1.614400
B	-0.900538	-1.239484	-0.773574
B	0.900538	-1.239484	-0.773574
B	-0.903291	1.243273	0.730568
B	0.903291	1.243273	0.730568
B	-1.457101	0.473441	-0.773574
B	1.457101	0.473441	-0.773574
B	-1.461555	-0.474888	0.730568
B	1.461555	-0.474888	0.730568
C	-2.689450	0.873855	-1.567111
C	0.000000	0.000000	-3.011634
C	0.000000	2.827855	-1.567111
C	0.000000	-2.868951	1.472944
C	0.000000	0.000000	3.156360
C	-1.662172	-2.287783	-1.567111
C	1.662172	-2.287783	-1.567111
C	-1.686327	2.321031	1.472944
C	1.686327	2.321031	1.472944
C	2.689450	0.873855	-1.567111
C	-2.728535	-0.886555	1.472944
C	2.728535	-0.886555	1.472944
N	-3.631290	1.179878	-2.152062
N	0.000000	0.000000	-4.160106
N	0.000000	3.818165	-2.152062
N	0.000000	-3.833133	2.100596
N	0.000000	0.000000	4.294289
N	-2.244261	-3.088960	-2.152062
N	2.244261	-3.088960	-2.152062
N	-2.253059	3.101069	2.100596
N	2.253059	3.101069	2.100596
N	3.631290	1.179878	-2.152062
N	-3.645526	-1.184503	2.100596
N	3.645526	-1.184503	2.100596

29. Cyanocarborane anion $B_{11}C(CN)_{12}^-$

Stoichiometry: $B_{11}C_{13}N_{12}$
Charge: -1
Multiplicity: 1
Point group: C_{5v}

Energy calculations (Hartree), cc-pVTZ, maug-cc-pVTZ on N
PBE0: -1424.8477151

Nuclear coordinates (angströms)

C	0.000000	0.000000	-1.512330
B	0.000000	1.523426	-0.698224
B	0.000000	-1.525522	0.811819
B	0.000000	0.000000	1.750360
B	-0.895448	-1.232478	-0.698224
B	0.895448	-1.232478	-0.698224
B	-0.896679	1.234173	0.811819
B	0.896679	1.234173	0.811819
B	-1.448865	0.470765	-0.698224
B	1.448865	0.470765	-0.698224
B	-1.450858	-0.471412	0.811819
B	1.450858	-0.471412	0.811819
C	-2.679436	0.870602	-1.504557
C	0.000000	0.000000	-2.944468
C	0.000000	2.817326	-1.504557
C	0.000000	-2.908659	1.462142
C	0.000000	0.000000	3.279386
C	-1.655983	-2.279265	-1.504557
C	1.655983	-2.279265	-1.504557
C	-1.709667	2.353154	1.462142
C	1.709667	2.353154	1.462142
C	2.679436	0.870602	-1.504557
C	-2.766299	-0.898825	1.462142
C	2.766299	-0.898825	1.462142
N	-3.610929	1.173262	-2.107262
N	0.000000	0.000000	-4.092812
N	0.000000	3.796755	-2.107262
N	0.000000	-3.951759	1.946892
N	0.000000	0.000000	4.429696
N	-2.231677	-3.071639	-2.107262
N	2.231677	-3.071639	-2.107262
N	-2.322786	3.197040	1.946892
N	2.322786	3.197040	1.946892
N	3.610929	1.173262	-2.107262
N	-3.758346	-1.221161	1.946892
N	3.758346	-1.221161	1.946892

