gravimetrical analysis after removing the residual **1a** and **1b** with chloroform. Photopolymerization was carried out at 34 °C in vacuo under UV irradiation by using a high-pressure mercury lamp (Fuji Glass Work Type BH-400, 400 W) at a distance of 12 cm. Poly(**1a**): IR (KBr): $\tilde{\nu}$ = 2914 (CH), 1706 (C=O), 1492 (C=C), 1411 (C=C), 1218 (C–O), 811 (CH) cm^{-1}; powder XRD ($Cu_{K\alpha_1}$/40 kV/150 mV, 2θ (relative intensity %): 11.24 (100), 11.62 (23), 13.60 (44), 14.38 (38), 14.78 (39), 16.46 (8), 20.56 (8), 22.06 (18), 23.30 (7), 24.18 (23), 25.80 (17), 29.90 (14), 30.44 (14), 35.94 (8), 40.66 (5), 45.42 (5); elemental analysis calcd (%) for $C_{16}H_{16}O_8$: H 4.80, C 57.14, O 38.06, found: H 4.76, C 56.99, O 38.25.

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[13] Crystal structure data for **1a** (single crystal from chloroform/hexane): formula $C_8H_8O_4$, M_r = 168.15, crystal dimensions 0.50 × 0.30 × 0.30 mm, monoclinic, space group $P2_1/n$ (no. 14), a = 8.6787(7), b = 7.5719(7), c = 12.761(1) Å, β = 105.193(2)°, V = 809.2(1) Å^3, Z = 4, ρ_{calcd} = 1.380 g cm^{-3}, $2\theta_{max}$ = 55.0°, Rigaku RAXIS-RAPID Imaging Plate diffractometer ($Mo_{K\alpha}$, λ = 0.71069 Å, graphite monochromator), ω scans, T = 303 K, 1828 measured reflections, all 1477 independent reflections used in the refinement, Lorenz and polarization factors were applied, μ = 1.12 cm^{-1}. Structure solution and refinement: direct methods (SIR92), full-matrix least-squares refinement of F^2, 109 parameters, all non-hydrogen atoms were refined anisotropically, and hydrogen atoms were located in the ideal positions without further refinement, R_1 = 0.046, R = 0.106, Rw = 0.133, GOF = 1.273, $\Delta\rho_{max}$ = 0.19 e Å^{-3}, $\Delta\rho_{min}$ = −0.25 e Å^{-3}. Crystal structure data for **1b** (single crystal from methanol): formula $C_8H_8O_4$, M = 168.15, crystal dimensions 2.00 × 0.40 × 0.10 mm, triclinic, space group $P\bar{1}$ (no. 2), a = 8.6023(4), b = 8.889(2), c = 5.2870(6) Å, α = 96.305(4), β = 105.636(5), γ = 87.323(8)°, V = 386.87(9) Å^3, Z = 2, ρ_{calcd} = 1.443 g cm^{-3}, $2\theta_{max}$ = 54.9°, Rigaku RAXIS-RAPID Imaging Plate diffractometer ($Mo_{K\alpha}$, λ = 0.71069 Å, graphite monochromator), ω scans, T = 303 K, 1711 measured reflections, all 1360 independent reflections used in the refinement, Lorenz and polarization factors were applied, μ = 1.12 cm^{-1}. Structure solution and refinement: direct methods (SIR92), full-matrix least-squares refinement of F^2, 109 parameters, all non-hydrogen atoms were refined anisotropically, and hydrogen atoms were located in the ideal positions without further refinement, R_1 = 0.062, R = 0.131, Rw = 0.183, GOF = 1.822, $\Delta\rho_{max}$ = 0.30 e Å^{-3}, $\Delta\rho_{min}$ = −0.33 e Å^{-3}. CCDC-182493 (**1a**) and CCDC-182492 (**1b**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

Spherical Homoaromaticity**

Zhongfang Chen, Haijun Jiao, Andreas Hirsch,* and Paul von Ragué Schleyer*

Since aromaticity[1] is not confined only to planar rings but also exists in three-dimensional systems,[2] the same should be true of homoaromaticity.[3–5] Although the $4N+2$ Hückel electron-counting rule is defined for planar systems it has been applied to rationalize the properties of three-dimensional homoaromatic systems.[5] Recently, the $2(N+1)^2$ counterpart of the Hückel rule[6] has been extended successfully[2e,7,8] to the aromaticity of three-dimensional delocalized systems with near spherical geometries: fullerenes, hydrogen and lithium clusters, as well as some well-known *closo*-boranes and Zintl ions. It was found that the highest degree of aromaticity can only be achieved in systems with fully filled valence shells. We now present new conceptual applications of this electron-counting rule to three-dimensional homoaromatic systems with cubane, dodecahedrane, and adamantane frameworks. Families of spherical homoaromatics with both two and eight mobile electrons (including several neutral

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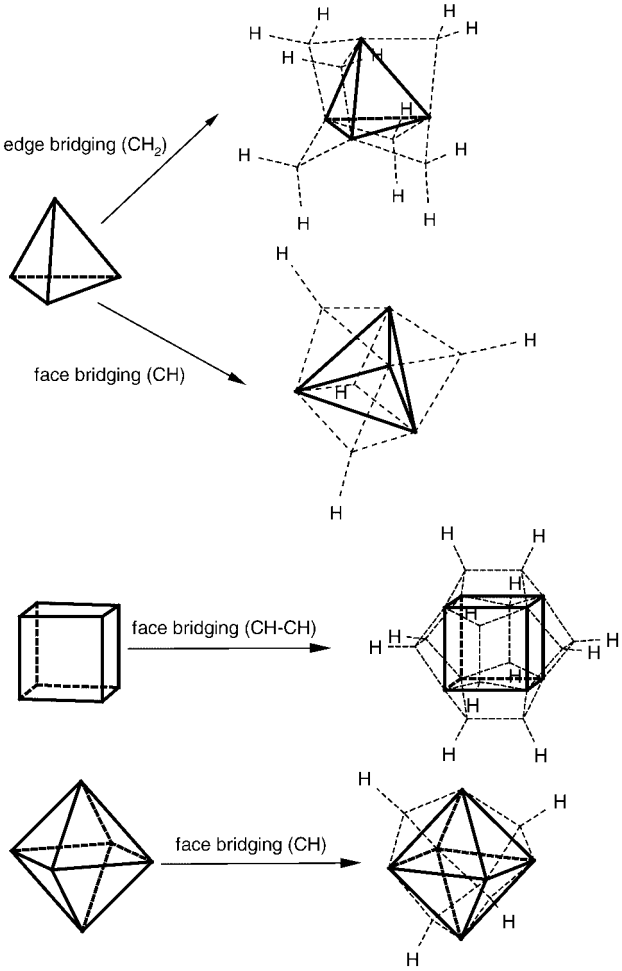
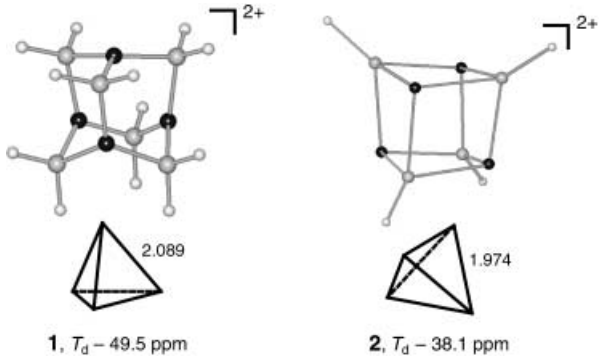
homoaromatic compounds) have been designed and characterized computationally. Each set has complete spherical homoaromaticity, that is, all the sp^2 carbon atoms in the highly symmetrical frameworks are separated by one or two sp^3-hybridized atoms. As shown in Scheme 1, these systems can be constructed by alkyl-bridging of smaller, highly symmetrical carbon cages.



Scheme 1. Construction principles for spherical homoaromatic compounds.

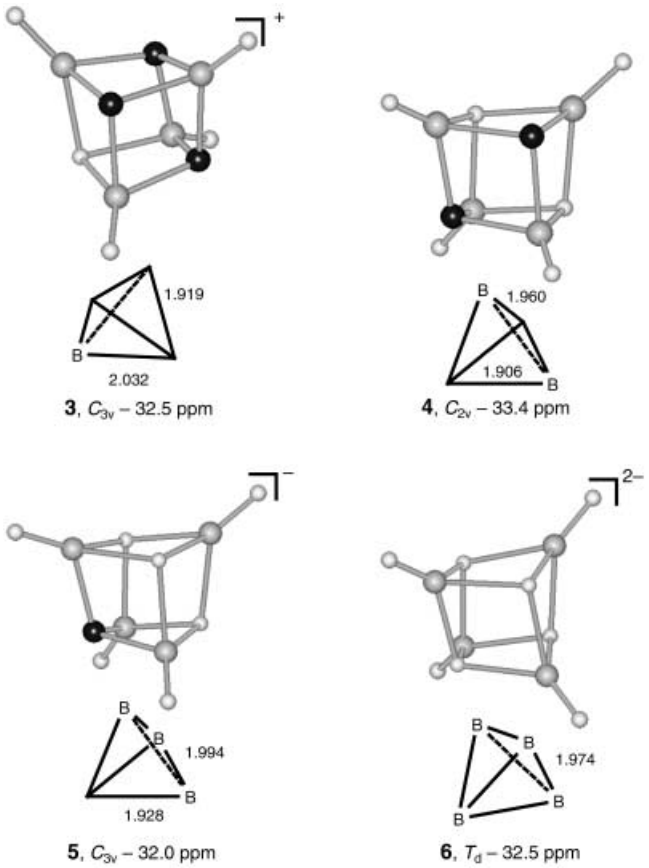
Four-center two-electron systems: Adding six edge-bridging methylene groups to a C_4 tetrahedron gives the adamantane framework. Removal of two electrons leads to the 1,3-dehydro-5,7-adamantanediyl dication ($C_{10}H_{12}^{2+}$, **1**; Figure 1) reported by Schleyer et al.[4] This system represents the three-dimensional four-center two-electron (4c-2e) homoaromatic prototype. A series of isoelectronic charged and neutral 4c-2e species based on this framework also are homoaromatic.[5] Coincidently, both the Hückel rule defined for planar molecules and the $2(N+1)^2$ rule predict the aromaticity of three-dimensional systems with only two π electrons. In addition to the ease of preparation of **1**, its aromaticity was evidenced by magnetic criteria,[4,5] in particular the calculated nucleus-independent chemical shift (NICS)[9] at the cage center: $\delta = -49.5$ ppm in the present work and $\delta = -43.0$ ppm in ref. [5b] determined at a lower level of calculation.



1, T_d – 49.5 ppm **2**, T_d – 38.1 ppm

Figure 1. MP2/6-31G* optimized structures and NICS values of **1** and **2** and schematic representation of the inherent sp^2 framework together with the conjugative distance in Å.

Grafting four face-bridging CH groups onto a C_4 tetrahedron results in a cubane framework with isolated sp^2 C atoms at opposite corners (Scheme 1). Removal of two electrons leads to **2** (Figure 1), which is also highly aromatic: the NICS value is $\delta = -38.1$ ppm at the cage center. The homoconjugative C–C bond lengths of 1.974 Å in **2**, which are shorter than those (2.089 Å) in **1**, facilitate the four-center, two-electron (4c-2e) bonding interactions (Figure 1). Replacing tertiary cations in **2** by boron atoms and adding or removing electrons gives the isoelectronic analogues **3**–**6**, which are also characterized as aromatic by their highly negative NICS values (Figure 2).



3, C_{3v} – 32.5 ppm **4**, C_{2v} – 33.4 ppm

5, C_{3v} – 32.0 ppm **6**, T_d – 32.5 ppm

Figure 2. MP2/6-31G* optimized structures and NICS values of **3**–**6** and schematic representation of the inherent sp^2 framework together with the conjugative distance in Å.

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Eight-center eight-electron systems: The $4N+2$ Hückel and the $2(N+1)^2$ rules differ when the next level of electron occupancy in spherical systems is considered. The Hückel rule is based upon only double degeneracy being possible in the planar ring. The second set of interacting orbitals is triply degenerate in spherical systems, and a total of eight, rather than six, electrons must be accommodated in closed-shell species. More than four interacting orbitals are required for possible delocalization. We consider here eight-electron systems with both six and eight centers.

Complete face bridging a C_8 cube with six $>CH-CH<$ units (Scheme 1) leads to $C_{20}H_{12}$ (T_h) **7**, which has a dodecahedrane framework. Dodecahedrane ($C_{20}H_{20}$)[10] fascinates both theoretical and experimental chemists because of the aesthetic appeal of its unusually high symmetry (I_h). Symmetrical removal of eight noncontiguous hydrogen atoms also gives **7**, in which the eight sp^2 carbon atoms describe a cube (Figure 3). This neutral eight-center, eight-π-electron

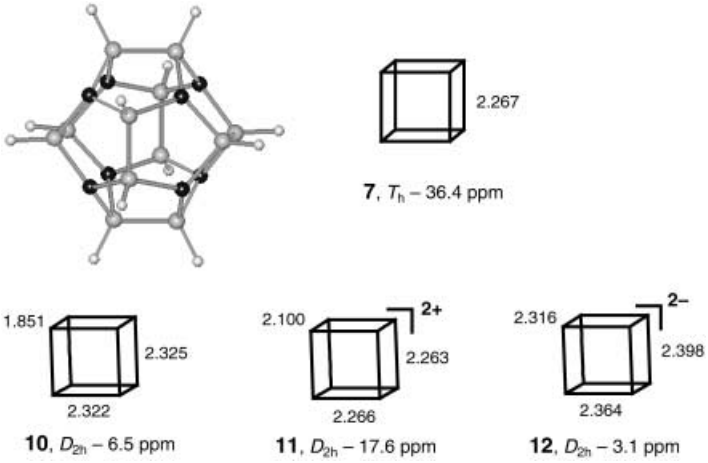

Figure 3. MP2/6-31G* optimized structures and NICS values of $C_{20}H_{12}$ (**7**) and its charged singlet analogues (**9**–**10**) and schematic representation of the inherent sp^2 framework together with the conjugative distance in Å. (For simplicity, only cuboid frameworks of **10**–**12** are given).

(8c-8e) species is highly aromatic as indicated by the NICS value of $\delta = -36.4$ ppm. The homoconjugative distance (2.267 Å) is similar to the partial bond distances computed in typical electrocyclic transition states.[11]

The stabilization energy (SE) of **7** is very large, and can be estimated in various ways. The simplest (and perhaps the best when the number of centers equal the number of mobile electrons) is to compare the energy of the singlet with its much less stable (84.9 kcal mol^{-1}) high-spin nonet state. As expected, **7** is much higher in energy than the classical $C_{20}H_{12}$ dodecahedratetraenes (131.9 and 131.0 kcal mol^{-1} for the two isomers **8** (D_{2h}) and **9** (C_2), respectively;[12] Figure 4), as a result of the bond energy of the four C=C bonds. However, taking 65–70 kcal mol^{-1} to be the π-bond energy range of ethene,[13] the total π-bond energy of **7** would be in the 260–280 kcal mol^{-1} energy range. The energy difference between **7** and **8** or **9** (without the π-bond energy) would be about 128–149 kcal mol^{-1}, thus providing a very rough, but confirming, SE estimate for **7**. This estimate is consistent with its large

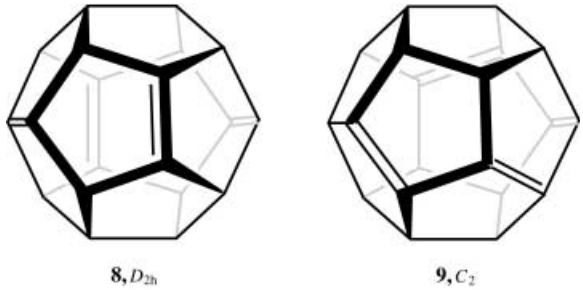

Figure 4. Structures of classical $C_{20}H_{12}$ dodecahedratetraenes **8** and **9**.

NICS value (the NICS(π) value at the center of benzene is −20.7 ppm).[14]

An important point is that direct overlap may not be required for such spherical homoaromaticity. The symmetry of the wavefunction is the key and this does not depend on the separation among the component orbitals. Hoffmann anticipated this long ago with his "through bond coupling."[15]

As a demonstration, the NICS value was computed on $C_{20}H_{12}$ (T_h) using the B3LYP-6-31G* optimized $C_{20}H_{20}$ (I_h) geometry (by just removing the eight hydrogen atoms). The GIAO NICS in the center is −30.1 ppm (not much different from the value of −36.4 ppm found with the optimized geometry) despite the larger C···C separations (2.518 Å), which are too large for effective overlap. Thus, the symmetry is more important than the separations.

Isomer **7** is also 32.3 kcal mol^{-1} more stable than its nonhomoconjugative analogue **10** with a distorted sp^2 carbon framework (D_{2h} symmetry). Thus, **7** is a beautiful example of a neutral spherical homoaromatic system. Removing or adding two electrons to **7** leads to the Jahn–Teller-distorted six- or ten-electron systems, **11** ($C_{20}H_{12}^{2+}$) and **12** ($C_{20}H_{12}^{2-}$), respectively, that conform formally to the $4N+2$ rule. However, according to the NICS criterion **11** and especially **12** are less aromatic than their 8c-8e analogue **7**.

Six-center eight-electron systems: Bridging four non-adjacent delta faces of a carbon octahedron by CH groups (Scheme 1) and removing four electrons leads to the 6c-8e system **13** ($C_{10}H_4^{4+}$; Figure 5). This electron count may not be obvious, but can be understood easily by considering this system in another way. Removal of all twelve methylene hydrogen atoms from adamantane ($C_{10}H_{16}$) leaves six carbene

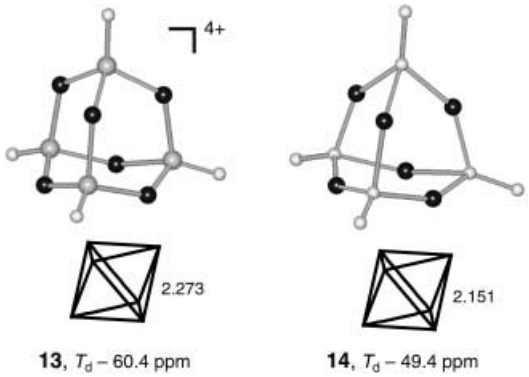

Figure 5. MP2/6-31G* optimized structures and NICS values of **13** and **14** and schematic representation of the inherent sp^2 framework together with the conjugative distance in Å.

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centers with twelve electrons; further removal of four electrons leads to tetracation **13** ($C_{10}H_4^{4+}$), which is a 6c-8e system. The eight electrons are delocalized over six centers in overall T_d symmetry. The separation among the six homoconjugating carbon atoms is 2.273 Å, nearly the same as in **7**. The NICS value of −60.4 ppm for **13** is very large, which indicates there is a high degree of electron delocalization (spherical aromaticity). The neutral isoelectronic T_d analogue ($C_6H_4B_4$, **14**) is a more realistic synthetic target than the tetracation **13**. The homoconjugative separation is only 2.151 Å in **14** and the NICS value of $\delta = -49.4$ ppm (Figure 5) illustrates its strong aromaticity.

The homoaromatic character of three-dimensional species arises from their closed π-electron-shell structures. As an example, the closed π shell of **7** is shown in the molecular orbital scheme in Figure 6. Incomplete filling of the shells reduces the aromatic character as in the doubly charged analogues, **11** and **12** (with 6 and 10 electrons, respectively).

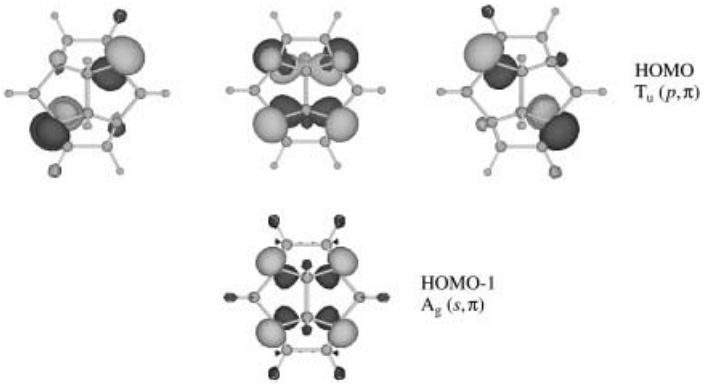

Figure 6. Representation of cluster s and π and p and π orbitals of of $C_{20}H_{12}$ (T_h).

In summary, guided by the $2(N+1)^2$ rule for spherical aromaticity, three-dimensional homoaromatics were designed by bridging sp^2 carbon atoms in highly symmetrical carbon polyhedrane units. After adjusting the number of electrons to two or to eight, the aromaticity is manifested by their highly negative NICS values and reasonable separations among the homoconjugative centers. In particular, the neutral, **4**, **7,** and **14** homoaromatic compounds challenge the synthetic ingenuity of experimental chemists.

Calculations

The geometries reported were optimized at the MP2/6-31G* and B3LYP/6-31G* levels. Vibrational frequencies, computed at the B3LYP/6-31G* level, were all real, and characterized all the stationary points as minima. Nucleus independent chemical shifts (NICS, in ppm),[9] calculated at the centers of the cages by using the GIAO-SCF/6-31G* method on the optimized geometries, were employed to evaluate the mobility of electrons on the cage surfaces. NICS is a well-evaluated criterion of aromaticity.[9] All the calculations were carried out with the Gaussian 98 program.[16]

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