The only possible evidence to date for the low-lying $^{3}A_{2u}$ state in quadruple metal–metal bonds is the work of Clark and Franks,[35] who observed a weak absorption at 6250 cm^{-1} (0.8 eV) in certain $Mo_2Cl_8^{4-}$ salts that they ascribed to $^{1}A_{1g} \rightarrow {}^{3}A_{2u}$ absorption. In $Re_2Cl_8^{2-}$ itself, the $^{3}A_{2u}$ state (calculated to lie at 4000 cm^{-1}) has apparently remained totally elusive.

Summary

A comprehensive theoretical study of the electronic states of the quadruply bonded $Re_2Cl_8^{2-}$ species has revealed a rich spectrum of states below 6 eV (50 000 cm^{-1}). The nature of these states is discussed in terms of the orbitals involved in the excitations. The weak coupling between the metal orbitals of the δ bond in particular necessitates a multiconfiguration description in terms of MO's, and a valence bond interpretation can often yield insights into the nature of the states. Of the states arising from δ–δ^* excitations, the $^{1}A_{2u}$ state (calculated 2.8 eV; observed 1.8 eV) has been well characterized experimentally, while the $^{3}A_{2u}$ (calculated 0.40 eV) and $2^{1}A_{1g}$ (calculated 3.22 eV) apparently have oscillator strengths too weak to be observed (cf. Tables II and VII). All three δ–δ^* excited states should undergo torsional distortions toward D_{4d} geometries. A large number of other weakly absorbing and forbidden states are found to lie between the strong $^{1}A_{2u}$ absorption and the LMCT states at 3.8 eV—a region that has been the subject of detailed spectroscopy studies.[4,25]

Acknowledgment. We thank Professor Harry Gray for the hospitality of his group and for useful discussions on the nature of the absorption and emission spectra of $Re_2Cl_8^{2-}$. We also thank Professor F. A. Cotton and Dr. Bruce Bursten for helpful discussions and for results of their unpublished absorption spectra and theoretical calculations prior to publication. This work was carried out under the auspices of the U.S. Department of Energy.

Registry No. $Re_2Cl_8^{2-}$, 19584-24-8.

Supplementary Material Available: Gaussian basis sets and effective core potentials used in these calculations (Tables VIII and IX) (2 pages). Ordering information is given on any current masthead page.

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Overlap Control and Stability of Polyhedral Molecules. *closo*-Carboranes

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Abstract: *closo*-Carboranes that can be formally divided into rings and caps follow a six-electron rule. The relative stability of various isomers within a given carborane depends on the size of the ring on which the polyhedral structure is based. With three- and four-membered rings the CH group fits in as the best cap; the overlap of the orbitals of CH with the orbitals of three- and four-membered borocycles is favorable. Thus 1,5-$C_2B_3H_5$ is more stable than 1,2-$C_2B_3H_5$. The BH group with more diffuse orbitals overlaps better with the orbitals of a five-membered ring; 1,7-$C_2B_5H_7$ is less stable than 1,2-$C_2B_5H_7$, which, in turn, is less stable than 2,4-$C_2B_5H_7$. The orbitals of BH are not diffuse enough to overlap favorably with the orbitals of a six-membered ring; $C_2B_6H_8$ prefers a dodecahedron to a hexagonal bipyramid. Caps with more diffuse orbitals such as BeH, Li, and transition-metal fragments should stabilize polyhedra based on six-membered rings.

The *closo*-carboranes represent one of the most studied sets of polyhedral molecules.[1] Despite the various electron-counting rules[2] and theoretical studies[3] available, the factors controlling the isomer stabilities of carboranes are not yet understood. Consider the series of *closo*-carboranes given in Figure 1. **1a**, the trans isomer (1,5-$C_2B_3H_5$), is more stable than the 1,2- and 2,3-isomers.[1a,3] Similarly **2a** (1,6-$C_2B_4H_6$) is more stable than **2b**. But **3a** is the least stable of the four $C_2B_5H_7$ isomers.[3] Carboranes based on six-membered rings as in **4** are unknown; $C_2B_6H_8$ prefers the dodecahedron, **5**, compared to the hexagonal bipyramid, **4**.[4] In contrast to the propensity of polyhedra based on four- (**6**) and five- (**7**) membered rings (Figure 2), those based on six-membered rings (**8**) are absent among carboranes.[1] There is no consistent set of explanations for these observations. The suggestion that the more electronegative atoms prefer to be farthest apart in the most stable isomer works in **1**, **2**, **6**, and **7** but fails in **3**.[1a] The postulate that the position isomer having the largest number of B–C bonds will be most stable within a given set of isomers also does not work uniformly.[1b] The empirical observation that carbon prefers a site of less coordination seems to explain most of them, but a theoretical explanation for this preference is lacking.[2a] The absence of carboranes of the types **4** and **8** also remains a puzzle. We present here a criterion based on overlap of orbitals to determine relative isomer stabilities of polyhedral carboranes.

Carboranes considered in this paper can be formally constructed from caps and rings. The electronic structure of carboranes can be then understood by a six-electron rule. Let us consider **2a**, which has a four-membered borocycle, B_4H_4, with two CH caps attached from either side. With the assumption of two-center

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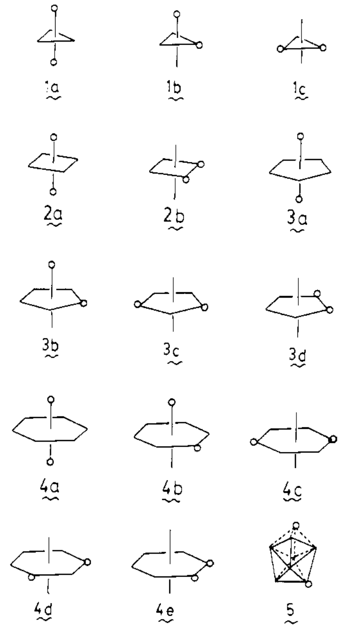


Figure 1. Structural isomers **1–4** of *closo*-carboranes based on the interaction of one ring and two caps. **5** is the preferred structure of $C_2B_6H_8$. The open circles indicate CH groups while unmarked vertices stand for BH groups throughout the paper.

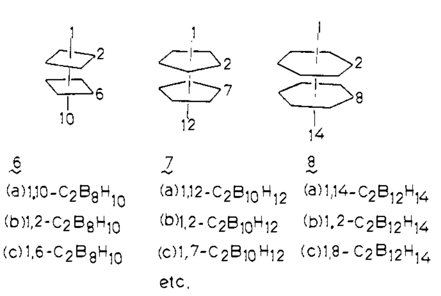


Figure 2. Structure and numbering in polyhedral systems with two caps and a stack of two rings.

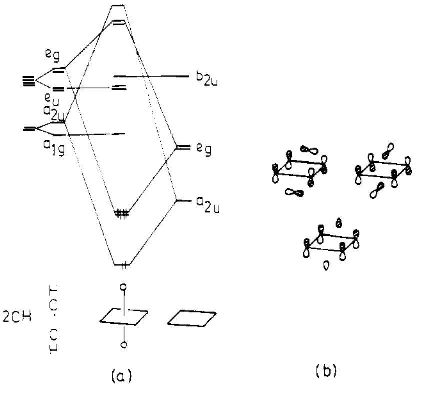


Figure 3. (a) Schematic interaction diagram between the e and lower a π orbitals of B_4H_4 and the orbitals of the CH groups. (b) The three stabilized orbitals resulting from the interaction of the ring and caps.

two-electron bonds between neighboring pairs of borons and hydrogens, there will be no electrons in the π orbitals of the B_4H_4 ring. The CH group has three electrons available for bonding. With two CH groups as in **2a**, there will be six electrons for ring–cap binding. The six-electron rule for *closo*-carboranes can be justified by an interaction diagram between the π orbitals of the ring and the orbitals of the cap, shown schematically in Figure 3a. As there are three stabilized orbitals (Figure 3b), systems with six electrons to bind the rings and caps are expected to be stable. All two-carbon carboranes considered here satisfy the six-electron rule. A similar six-electron rule has been sketched by Lipscomb.[5] Even though an electron-counting rule cannot explain the relative stabilities of isomers, the concept of caps and rings forming polyhedral molecules suggests a criterion for predicting the relative stabilities of *closo*-carboranes as we develop here.

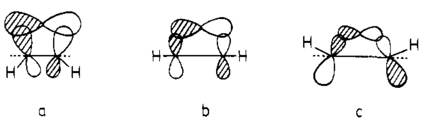


Figure 4. Diagrammatic presentation of the overlap of the orbitals of the cap with the π orbitals of the ring: (a) cap orbitals too large, resulting in the ring hydrogens bending away from the cap; (b) optimum situation; (c) cap orbitals too contracted, resulting in the ring hydrogens bending toward the cap.

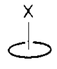
Table I. Out-of-Plane Bending (deg) of the Ring Hydrogens in Pyramidal Molecules (9) Comprised of Carbocyclic Rings and BH and CH Caps at STO-3G (3-21G) Levels[g]

	ring		
cap	C_3H_3	C_4H_4	C_5H_5
BH	31.8 (34.8)[a]	−1.2 (1.0)[c]	−8.1 (−4.4)[e]
CH	19.5 (19.5)[b]	−5.4 (−2.7)[d]	−11.7 (−8.2)[f]

[a] $C_3H_3BH^-$. [b] C_4H_4, T_d. [c] C_4H_4BH. [d] $C_4H_4CH^+$. [e] $C_5H_5BH^+$. [f] $C_5H_5CH^{2+}$. [g] See ref 6. Positive values indicate that the hydrogens are bent away from the cap.

Ring–Cap Matching and Isomer Stability

Recently the consequences of a six-electron rule was shown explicitly in pyramidal systems, **9**, with carbocyclic rings and



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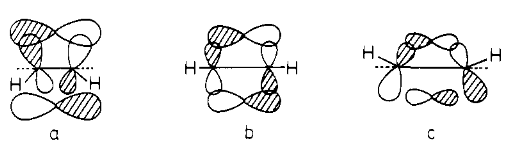
various caps.[6] The magnitude of interaction of a carbocyclic ring with a cap depends on the number of atoms in the ring (ring size) and the diffuse nature of the orbitals of the cap. Most stable arrangements are obtained when the overlap between the π orbitals of the ring and the orbitals of the cap is maximum. An estimate of this orbital compatibility may be inferred from the out-of-plane bending of the ring hydrogens.[6] When the ring is too large or the orbitals of the cap are too diffuse, the overlap between the ring π orbitals and the cap orbitals may be improved by out-of-plane bending of ring hydrogens (Figure 4), even though this leads to diminished ring hydrogen binding. The optimum ring–cap interaction will have maximum overlap without any ring hydrogen bending at all. This allows the selection of a ring of a particular size for a given cap and vice versa. The BH group has more diffuse orbitals than the CH group. BH would therefore prefer a larger ring than that preferred by CH. The out-of-plane bendings calculated for CH and BH caps with carbocyclic rings (Table I)[6] show the difference in the diffuse nature of orbitals of these two caps.

The ring–cap matching becomes more critical when there are two caps interacting from either side of a ring. Bending of ring hydrogens cannot help now. If the caps are identical, the increase in overlap to one cap gained by ring hydrogen bending is canceled by the decrease in overlap caused to the other ring (**10**). The



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(5) (a) Lipscomb, W. N. *J. Chem. Phys.* **1958**, *28*, 170. (b) Moore, E. B., Jr.; John, L. L., Jr.; Lipscomb, W. N. *Ibid.* **1961**, *35*, 1329. Also see ref 2e and 3f.

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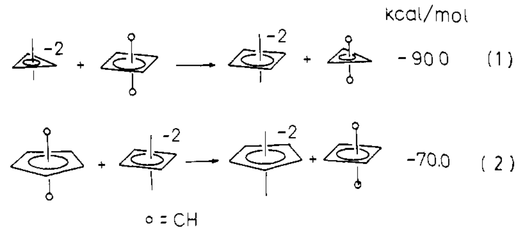
reported study (Table I) on pyramidal systems with carbocyclic rings gives us a guide in selecting the appropriate ring for BH or CH as a cap in carboranes. If allowance is made for the longer bonds (B–B > B–C > C–C) involved in the rings of carboranes the overlap of the BH cap with borocycles will decrease in the order of ring size as $5 > 4 \gg 3 \approx 6$. Similarly for CH having less diffuse orbitals it will be $4 > 3 > 5 \gg 6$. The correctness of this order is reinforced by the explanations it provides, as is discussed below. But a more direct check may be obtained from the reaction energies ((1) and (2)) calculated by using PRDDO

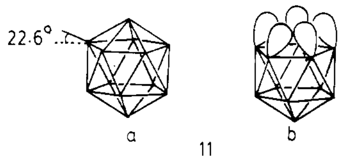


energies available from the literature.[3c] These reactions give the different preferences of BH and CH for three-, four-, and five-membered boron rings. The first reaction indicates that the BH cap prefers a four-membered ring over a three-membered ring. In other words, given a choice between three- and four-membered rings, CH would prefer the three-membered ring while BH would prefer the four-membered ring. The second equation shows in a similar way the preference of the BH cap for a five-membered ring relative to a four-membered ring; the CH cap is happier on a four-membered ring. In short, the cap having more diffuse orbitals prefers a larger ring.

With this background let us again look at the carboranes. In **1** the axial or trans position above and below the three-membered ring will be more appropriate for a CH than a BH cap. Hence **1a** is more stable than **1b** or **1c**. The octahedron, **2**, can be divided into rings and caps such that any two opposite groups can be considered as the caps. Hence a definite conclusion cannot be made regarding stabilities based on the ring–cap matching. Structure **6**, which can be considered as two caps interacting with a stack of two four-membered rings, also falls under the six-electron rule. The ring-cap matching criterion indicates that **6a** should be more stable than **6b** or **6c**. Available experimental and theoretical studies indicate that **6a** is the most stable isomer.[1,3]

Let us now consider isomers based on five-membered rings. According to the overlap criterion five-membered borocycles prefer BH rather than CH as caps. Hence **3a** is the least stable isomer of the four possibilities. It is calculated to be so.[3] When one CH cap is exchanged with a BH group from the ring as in **3b**, the system becomes more stable. The most stable isomers are **3c** and **3d**, where both caps are BH groups. These are the only ones known experimentally.[1] All theoretical and experimental studies support the relative stabilities we have deduced. The greater stability of **3c** over **3d** may be explained by the concept of bond separation energy or simply by the difference in bond energies involved.[1b,7]

The icosahedral carboranes cannot be divided uniquely into caps and rings; any two geometrically opposite vertices can constitute the caps with two five-membered rings in between (**7**). Since the CH group also has to be a cap for the five-membered ring, one may be tempted to conclude that icosahedral carboranes are not very stable. The orientation of the π orbitals, however, are very different in the pentagonal bipyramid (**3**) and in the icosahedron (**7**). The ring hydrogens of the five-membered ring in **3a** remain in the plane of the ring by symmetry. Any conceptual division of an ideal icosahedron into rings and caps would leave the ring hydrogens bent toward the caps by 22.6° (**11a**). As a result the ring π orbitals will be rehybridized, increasing the ring–cap overlap (**11b**). This explains the stability of icosahedral carboranes even when CH groups form caps on five-membered rings. Ring–cap matching does not provide a clear-cut distinction in stabilities of isomers here.



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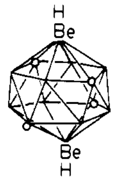
It is now easy to see why polyhedra based on six-membered rings (**4**, **8**) are absent among carboranes. CH does not have orbitals diffuse enough to have effective overlap with the π orbitals of a six-membered borocycle. Table I suggests that the ring hydrogens will have to be bent by large magnitudes toward the cap in six-membered rings. How can we improve the situation? The cap orbitals should be more diffuse so that there will be appreciable overlap between the cap orbitals and ring π orbitals. Thus replacement of the cap with BeH or Li, which have more diffuse orbitals, should help.[8] Of course, suitable replacements must be made in the rings to conserve the number of electrons. For example, a more realistic isoelectronic analogue of **8a** will be **12**, obtained by replacing two CH caps by BeH and four BH units of the ring by CH groups. Another method for stabilizing a 14-vertex polyhedron will be to use isolobal transition-metal groups as caps.[9] Transition-metal fragments isolobal to BH and CH groups (**13**) have highly diffuse orbitals. This is also shown by the out-of-plane bendings of the ring substituents commonly observed in transition-metal complexes with cyclopolyene ligands.[9e] Molecular orbital studies have indicated that five- and six-membered rings are appropriate ligands for transition metals; little out-of-plane bending of ring hydrogens is needed here.[9e] Thus transition-metal fragments can be used as caps for stabilizing a carborane skeleton of 14 vertices. With use of C_5H_5Fe, which is isoelectronic to BH^+, a possible compound will be $CpFeB_8C_4H_{12}FeCp$ (**14**). The two extra carbons here make the system neutral, and yet six electrons—two each from the C_5H_5Fe groups and one each from the CH groups—are available as before. The most stable arrangement will have the two C_5H_5Fe groups as the caps interacting with the six-membered rings. Interestingly enough a tetramethyl derivative of **14** has already been prepared. Thermal rearrangements indicate that the most stable isomer has the two C_5H_5Fe fragments as the caps, as verified by X-ray



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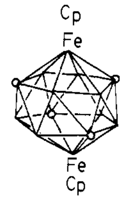

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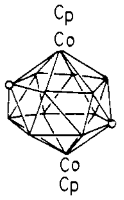

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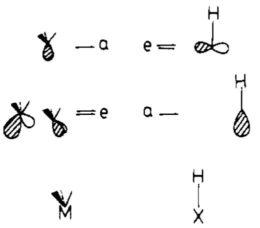

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(8) Atomic radii or the optimized exponents in a basis set indicates the expected trend of the diffuse nature of orbitals Li > Be > B > C.

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crystallography.[10] The corresponding cobalt analogue, as expected, has only two carbon atoms in the polyhedron (**15**).[10c]

Application of the concepts based on compatibility of orbitals of the rings and caps to borane anions, metal clusters, and organic reaction mechanisms are currently being investigated.

Conclusions

The electronic structure of *closo*-carboranes follows a six-electron rule. The relative stability of position isomers is determined by the matching of the rings and caps that formally constitute the carborane. CH prefers to be the cap on three- and four-membered boron rings. BH prefers to be the cap on five-membered rings. These preferences are dictated by the greater overlap enjoyed by a cap having more diffuse orbitals to the orbitals of a larger ring. The most stable isomer satisfies these preferences as far as possible. Even the BH group does not have orbitals sufficiently diffuse to be appropriate caps on six-membered borocycles. Caps can be selected to stabilize polyhedra based on larger rings.

Acknowledgment. We thank Professor Paul von Ragué Schleyer for constructive criticisms, helpful suggestions, and several enlightening discussions. The University of Hyderabad is thanked for providing research facilities.

Registry No. 1a, 20693-66-7; **1b**, 23777-70-0; **1c**, 30396-61-3; **2a**, 20693-67-8; **2b**, 20693-68-9; **3a**, 25036-79-7; **3b**, 25036-76-4; **3c**, 20693-69-0; **3d**, 30347-95-6; **6a**, 23653-23-8; **6b**, 41655-27-0; **6c**, 23704-81-6; **7a**, 20644-12-6; **7b**, 16872-09-6; **7c**, 16986-24-6; **12**, 83435-74-9; **14**, 83435-75-0; **15**, 52649-56-6.

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Surface Organometallic Chemistry: Formation of $HFe_3(CO)_{11}^-$ from $Fe_3(CO)_{12}$ and $Fe(CO)_5$ on Silica, Alumina, Magnesia, and Zinc Oxide

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Received November 30, 1981

Abstract: This paper describes, at a molecular level, the organometallic chemistry that occurs during the adsorption of $Fe_3(CO)_{12}$ and $Fe(CO)_5$ on silica, alumina, magnesia, and zinc oxide. $Fe(CO)_5$ and $Fe_3(CO)_{12}$ are only weakly adsorbed on silica. In contrast on alumina, magnesia, and zinc oxide there is formation of the anionic hydride $HFe_3(CO)_{11}^-M^+$ (M = Al, Mg, Zn), which has been characterized in the adsorbed state by infrared, UV, and ^{1}H NMR spectroscopy and which has been extracted from the surface by ion exchange with Et_4NCl. The results indicate that the surface hydroxyl group of alumina, magnesia, or zinc oxide can make a nucleophilic attack at the coordinated CO as it occurs in solution with formation of the stable surface hydrido cluster. The result is also the first example of a grafted cluster where the grafting occurs by ionic interaction with a surface cation of the oxide lattice. It is possible that the anionic cluster interacts with such a surface cation via the oxygen lone pair of the bridging carbonyl ligand.

Surface organometallic chemistry can be considered as a major aspect of surface science and heterogeneous catalysis. Because of the intrinsic difficulties in the study of surface chemistry, few basic phenomena or elementary steps have been elucidated at a molecular level. Direct interaction between molecular cluster carbonyls and the surface hydroxyl groups of highly divided oxides is a possible approach to study the reactivity of metal–metal or metal–ligand bonds of carbonyl clusters toward the hydroxyl groups of a surface.

Surface hydroxyl groups of alumina can oxidize zerovalent rhodium in $Rh_6(CO)_{16}$ to surface $Rh^I(CO)_2$ complex with simultaneous release of hydrogen,[2] but surface hydroxyl groups of silica cannot oxidize zerovalent rhodium of $Rh_4(CO)_{12}$ or $Rh_6(CO)_{16}$.[3] Surface hydroxyl groups of silica, alumina, and magnesia can oxidatively add to the Os–Os bonds of $Os_3(CO)_{12}$ or $Os_3(CO)_{10}(CH_3CN)_2$ with formation of the grafted cluster (H) $Os_3(CO)_{10}$ (O-M) (M = Si, Al, Mg).[4-9]

We report here on the reactivity of $Fe_3(CO)_{12}$ (and $Fe(CO)_5$) with the hydroxyl groups of silica, alumina, magnesia, and zinc oxide. In some cases the OH groups of the oxide behave as

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[1] For typical results related to surface organometallic chemistry, see for example (a) C. M. Friend, R. M. Gavin, E. L. Muetterties, and M. C. Tsai, *J. Am. Chem. Soc.* **102**, 1717 (1980); (b) C. M. Friend, J. Stein, and E. L. Muetterties, *ibid.*, *103*, 767 (1981); (c) C. M. Friend and E. L. Muetterties, *ibid.*, *103*, 773 (1981); (d) Y. I. Yermakov, *Catal. Rev. Sci. Eng.*, **13**, 77 (1976); (e) D. G. H. Ballard, *Adv. Catal.*, **23**, 267 (1973); (*f*) A. Brenner and R. Burwell, *J. Catal.*, **52**, 353 (1978); (g) E. L. Muetterties, *Angew. Chem., Int. Ed. Engl.*, **17**, 545 (1978); (h) J. M. Basset, Y. Ben Taarit, J. L. Bilhou, J. Bousquet, R. Mutin, and A. Theolier, *Proc. Int. Cong. Catal. 6th* **1**, 570 (1977); (i) F. Correa, R. Nakamura, R. E. Stimson, R. L. Burwel Jr., and D. F. Shriver, *J. Am. Chem. Soc.*, **102**, 5114 (1980); (j) W. M. Bowser and W. H. Weinberg, *ibid.*, **103**, 1453 (1981); (k) W. M. Bowser and W. H. Weinberg, *ibid.*, **102**, 4720 (1980).

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