Ab initio MO LCAO SCF simulation of molecular and electronic structure of η^5-π-$C_{60}H_5XCp$ (X = Fe, Si) complexes

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The problem of existence of η^5-π-complexes of unsubstituted fullerene I_h-C_{60} and its cyclopentadienyl type derivative $C_{60}H_5^{\cdot}$ is discussed. *Ab initio* MO LCAO SCF calculations of hypothetical sandwich systems η^5-π-$C_{60}H_5XCp$ (X = Fe (**1a**), Si (**1b**)), the cationic complex $C_{60}FeCp^+$ of unsubstituted C_{60}, and the $C_{60}H_5^{\cdot}$ radical were performed in the STO-3G and 3-21G basis sets. In the **1a**, **1b**, and $C_{60}H_5^{\cdot}$ systems, hydrogen atoms are attached to carbon atoms of fullerene I_h-C_{60} at α-positions relative to the same pentagonal face (*pent**). In η^5-complexes, XCp species are also coordinated to this face. According to calculations in the 3-21G basis set, the Fe—*pent** bond energy in complex **1a** is much higher than those of similar bonds in **1b** and in the η^5-π-$C_{60}FeCp^+$ cation (117 kcal mol^{-1} *vs.* 37 and 64 kcal mol^{-1}, respectively) and is 7 kcal mol^{-1} higher than the Fe—Cp bond energy in the classical sandwich system $FeCp_2$. The Fe...C_{pent^*} and Fe...C_{Cp} distances in complex **1a** are slightly shorter than the Fe...C distance in the ferrocene molecule. The spin populations in the $C_{60}H_5^{\cdot}$ radical are almost completely localized on the atoms of the *pent** face, which must favor the formation of η^5-π-complexes of this radical.

Key words: fullerene, π-complexes, sandwich systems with iron and silicon atoms, radicals; *ab initio* quantum-chemical calculations, MO LCAO SCF method.

The problem of existence of η^5- and η^6-complexes of unsubstituted fullerene I_h-C_{60} was studied in detail[1–4] (see also references cited in Ref. 1). Using semiempirical quantum-chemical methods (EHT, MNDO, MNDO/PM3), it was shown[1–4] that η^n-complexes of unsubstituted fullerene at $n = 5$ or 6 should be much less stable than analogous classical biscyclopentadienyl and bisarene compounds of transition or main group elements. One theoretically substantiated[2–4] procedure for stabilizing the η^5-bond between metal atoms (or XCp species) and the atoms of the selected pentagonal face (*pent**) in the carbon cage involves attachment of univalent functional groups (R) or atoms (H, Cl, and Br) to C atoms in the α-positions relative to the *pent** face. Recently, the efficiency of such a stabilization procedure was experimentally confirmed by synthesizing the first stable cyclopentadienyl-type complexes of pentaphenyl derivatives of fullerene I_h-C_{60}, *viz.*, half-sandwich $C_{60}Ph_5X$ (X = Li, In, Tl, Cu · PEt_3) molecules. The complex with X = Tl was studied by X-ray analysis.[5] Further calculations of such systems by the MNDO/PM3 [6] and MO LCAO SCF/3-21G* methods[7] showed that the results of numerical simulation are in good agreement with experimental data. In addition, it has been shown[6] that with R = H the half-sandwich complexes $C_{60}R_5X$ (X = In, Tl) must be more stable than with R = Ph.

The possibility for η^5-π-$C_{60}H_5XCp$ complexes with atoms of main group elements (X = Si, Ge, Sn) to exist was established by the MNDO/PM3 method.[3] Based on the results of calculations of the above systems, it was hypothesized that structurally similar η^5-π-complexes with transition metal atoms X must also exist and that the X—*pent** bonds in such complexes should be stronger than in the complexes with main group elements.

In this work, we simulated the geometry and electronic structure of hypothetical sandwich complexes η^5-π-$C_{60}H_5FeCp$ (**1a**) and η^5-π-$C_{60}H_5SiCp$ (**1b**) (Fig. 1), bent-sandwich complex η^5-π-$C_{60}H_5SiCp$ (**1c**, see Fig. 1), cation η^5-π-$C_{60}FeCp^+$, and radical $C_{60}H_5^{\cdot}$ and estimated their stability.

Calculation procedure

Calculations were performed by the MO LCAO SCF method in the RHF (for molecules with closed electron shells) and ROHF (for radicals) approximations with the minimum (STO-3G) and split-valence (STO-3-21G) basis sets using the GAMESS program package[8] on a DEC 3000 AXP-400X workstation.

Results and Discussion

Half-sandwich and sandwich complexes $XCp^{\cdot}$ and XCp_2 (X = Fe, Si). The results of calculations of these systems studied previously by other methods[9–17] are of

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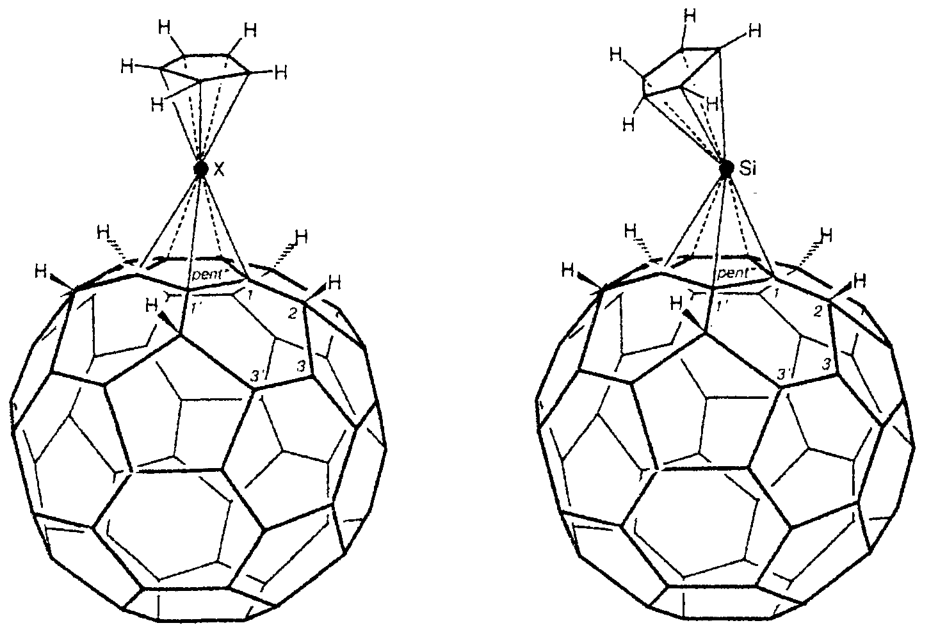


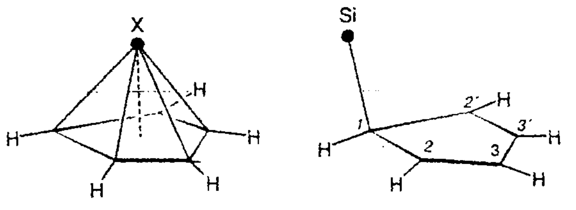
1a: X = Fe
1b: X = Si

1c

Fig. 1. Structures of η^5-π-complexes $C_{60}H_5XCp$ (**1a—c**); hereafter the atoms equivalent under C_{5v} symmetry differ in the number of primes.

auxiliary character and will be used below for comparing the energy and geometric characteristics of X—Cp bonds in half-sandwich and sandwich XCp' and XCp_2 complexes with analogous values for the X—*pent** bonds in complexes $C_{60}R_5X$ (Tables 1 and 2). In this work, we report only the data obtained in the STO-3-21G basis set, since our MO LCAO SCF/STO-3G calculations showed that the formation of XCp' and XCp_2 complexes from X and Cp species is energetically unfavorable despite the finding of corresponding local minima of the total energy.

According to calculations, the $FeCp^+$ (**2a**) and $SiCp^+$ (**2b**) cations have a half-sandwich structure with C_{5v} symmetry (Fig. 2). It was established that the ground state of radicals FeCp' (**3a**) and SiCp' (**3b**) is characterized by a multiplicity of 2. The former species has a η^5-half-sandwich structure, while the latter one has the structure of a σ-complex (both with C_s symmetry, see Fig. 2). The geometric parameters and bond orders in radical systems **3a,b** are listed in Table 2. The reduction in their symmetry is due to the Jahn—Teller effect, since each of the cations **2a,b** has a doubly degenerate LUMO energy level. The Fe—Cp bond in radical **3a** is much stronger than the Si—Cp bond in **3b**, which is indicated by their energies (see Table 1), X...C_{Cp} (X = Fe, Si) distances, and corresponding bond orders (*W*, see Table 2). The spin population distributions in radicals **3a,b** are listed in Table 3, from which it follows that the unpaired electrons in the radicals are almost completely localized on X atoms.



2a: X = Fe (q = 1)
2b: X = Si (q = 1)
3a: X = Fe

3b

Fig. 2. Half-sandwich complexes XCp: cations **2a,b** with C_{5v} symmetry and radical species **3a,b** with C_s symmetry (q is the charge of the complex).

The structures of sandwich π-complexes XCp_2 (**4a—c**) are shown in Fig. 3. It should be noted that several isomers can exist with X = Si.[9—13] Here, we describe only two of them, $SiCp_2$ with D_{5d} symmetry (**4b**) and a bent-sandwich isomer with C_{2v} symmetry (**4c**), which is 7.1 kcal mol^{-1} more stable than the former (see Tables 1 and 2). The energy of complex $2\eta^1$-$SiCp_2$, in which the Si atom forms σ-bonds with each Cp ring, is 9.1 kcal mol^{-1} lower than that of **4b**. These values indicate that complexes $SiCp_2$ are structurally nonrigid.

With X = Fe, there exist only sandwich systems with parallel Cp rings: the complex $FeCp_2$ has D_{5d} or D_{5h} symmetry.[15—17] With X = Fe, the X—Cp bond in complexes XCp' and XCp_2 is much stronger than with X = Si. It should be noted that the geometric parameters

Table 1. Total (E_{tot}) and orbital energies (E_{HOMO} and E_{LUMO}), energy gaps ($\delta = E_{HOMO} - E_{LUMO}$), dissociation energies of X—*pent** and X—Cp bonds ($\Delta_{X-pent*}$ and Δ_{X-Cp}, respectively), and Mulliken effective atomic charges (q) in η^5-$C_{60}H_5XCp$, Cp, XCp, and XCp_2 systems calculated by the *ab initio* MO LCAO SCF method in the STO-3-21G basis set

Compound	Sym-metry	$-E_{tot}$ [a] /au	E_{HOMO} [b]	E_{LUMO} [b]	δ	$\Delta_{X-pent*}$	Δ_{X-Cp}	q/au [b]			
			eV			kcal mol^{-1}		X	C_{pent*}	C_{Cp}	H_{Cp}
$C_{60}H_5FeCp$ (**1a**)	C_{5v}	3709.4716	-7.68^1	0.30^2	8.0	117.3	—	1.61	−0.13	−0.40	0.26
$C_{60}H_5SiCp$ (**1b**)	C_{5v}	2740.5318	-7.69^1	0.29^2	8.0	36.6	—	1.04	−0.04	−0.34	0.25
$C_{60}H_5SiCp$ (**1c**)	C_s	2740.5409	-7.61^1	0.17^1	7.8	42.4	—	1.08	−0.21	-0.29^1 -0.32^2 -0.41^2	0.25^3 0.26^2
$FeCp^+$ (**2a**)	C_{5v}	1447.1017	-14.30^2	-5.26^1	9.0	—	—	1.41	—	−0.40	0.32
$SiCp^+$ (**2b**)	C_{5v}	478.3249	-15.7^2	-3.08^2	12.6	—	—	1.00	—	−0.35	0.35
$FeCp^{\cdot}$ (**3a**)	C_s	1447.5362	-2.42^1	1.43^2	3.8	—	64.3	0.59	—	-0.35^1 -0.37^2 -0.39^2	0.25
$SiCp^{\cdot}$ (**3b**)	C_s	478.5047	-2.18^1	0.97^1	3.2	—	36.6	0.40	—	-0.66^1 -0.28^2 -0.22^2	0.27^1 0.25^2 0.24^2
$FeCp_2$ (**4a**)	D_{5d}	1638.5937	-9.09^2	3.36^2	12.4	—	110.4	1.38	—	−0.40	0.26
$SiCp_2$ (**4b**)	D_{5d}	669.6681	-8.03^2	2.68^2	10.7	—	38.6	0.94	—	−0.34	0.24
$SiCp_2$ (**4c**)	C_s	669.6795	-8.08^1	2.22^1	10.3	—	45.7	0.93		-0.26^1 -0.49^2 -0.23^2	0.25^2 0.24^3
$[C_{60}H_5]^-$ (**5a**)	C_{5v}	2262.0394	-3.55^2	3.06^2	6.6	—	—	—	0.01	—	—
$[C_{60}H_5]^{\cdot}$ (**5b**)	C_s	2261.9686	-4.31^1	0.17^1	4.5	—	—	—	0.10^1 0.02^2 0.06^2	—	—
$C_{60}FeCp^+$ (**6**)	C_{5v}	3706.2520	-11.23^2	−4.022	7.2	64.3	—	1.77	−0.16	−0.40	0.29
Cp^-	D_{5h}	191.1094	-1.35^2	13.05^2	14.4	—	—	—	—	−0.30	0.10
$Cp^{\cdot}$	C_{2v}	191.1019	-3.80^1	4.66^1	8.5	—	—	—	—	-0.19^1 -0.27^2 0.23^2	0.25^1 0.24^4
C_{60}	I_h	2259.0477	-8.33^5	-0.63^5	7.7	—	—	—	0	—	—

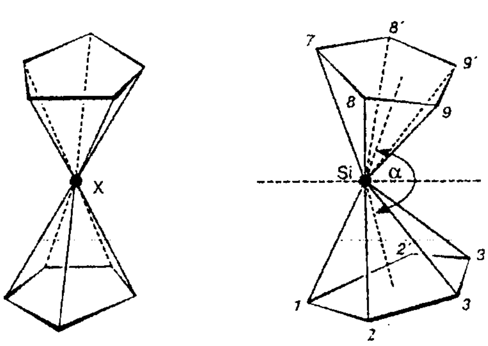
[a] Total energies of the atoms: $E_{tot}(Si, {}^3P_0) = -287.3444$ au, $E_{tot}(Fe, {}^5D_4) = -1256.3318$ au.

[b] Here and in Table 2 the upper index means the multiplicity of the given value.

found using the STO-3G basis set appeared to be closer to experimental data (see notes "*c*"—"*e*" to Table 2).

Anion $C_{60}H_5^-$ (**5a**, Fig. 4) was calculated previously by the MNDO[4,19] and MNDO/PM3 methods.[3,20] Our *ab initio* calculations performed assuming that the anion has C_{5v} symmetry showed that anion **5a** has a closed electron shell and is characterized by a rather high ionization potential and large energy difference between the LUMO (E_{LUMO}) and HOMO (E_{HOMO}) energy levels. The energy and charge characteristics of anion **5a** are listed in Table 1 and its geometric parameters are presented in Table 2.

The highest occupied level for anion **5a** appeared to be doubly degenerate, which is responsible (due to the Jahn—Teller effect) for symmetry reduction of the structure of the corresponding $C_{60}H_5^{\cdot}$ radical to C_s (**5b**, see Fig. 4). The spin populations in the radical **5b** are almost completely localized on the atoms of the *pent**



4a: X = Fe
4b: X = Si

4c

Fig. 3. Sandwich π-complexes **4a,b** with D_{5d} symmetry and a bent-sandwich complex **4c** with C_{2v} symmetry. The latter, in which the *3—3'* and *9—9'* edges are brought together, belongs to the *e—e* (edge-to-edge) type.[12]

Table 2. Interatomic distances (*d*/Å), bond orders (*W*/au), and the angle of the out-of-plane deviation of the C—H bond with respect to the Cp ring plane (φ/deg) in half-sandwich and sandwich complexes calculated by the *ab initio* MO LCAO SCF method in the STO-3-21G basis set

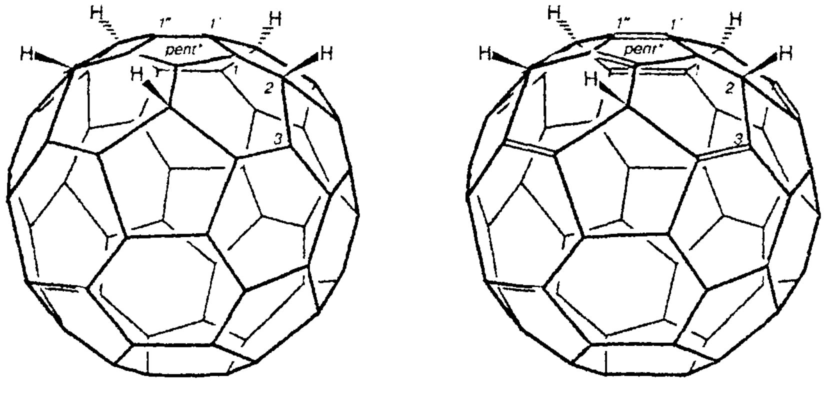
Compound	*d*(C—C) [*W*]		*d*	*d*(X—C) [*W*]		*d* [*W*]		φ
	*pent**	Cp	C(1)—C(2)	*pent**	Cp	X—*pent**	X—Cp	
$C_{60}H_5FeCp$ (**1a**)	1.408 [1.269]	1.418 [1.250]	1.500 [0.904]	2.163 [0.171][a]	2.185 [0.212]	1.801 [0.855]	1.721 [1.060]	1.4
$C_{60}H_5SiCp$ (**1b**)	1.401 [1.328]	1.414 [1.303]	1.498 [0.881]	2.489 [0.106][b]	2.474 [0.133]	2.183 [0.530]	2.160 [0.665]	−1.9
$C_{60}H_5SiCp$ (**1c**)	1.422 [1.367]^2	1.420 [1.342]^2	1.493 [0.894]	2.350 [0.160]^2	2.315 [0.185]^2	[0.533]	[0.657]	—
	1.433 [1.295]^2	1.431 [1.268]^2		2.488 [0.086]^2	2.425 [0.112]^2			
	1.441 [1.252]^1	1.436 [1.232]^1		2.568 [0.041]^1	2.497 [0.063]^1			
$FeCp^+$ (**2a**)	—	1.422 [1.206]	—	—	2.151 [0.299]	—	1.778 [1.499]	4.8
$SiCp^+$ (**2b**)	—	1.425 [1.205]	—	—	2.268 [0.305]	—	1.917 [1.515]	2.2
$FeCp^{\cdot}$ (**3a**)	—	1.415 [1.292]^2	—	—	2.431 [0.171^2	—	2.122 [0.931]	3.3^1
		1.418 [1.275]^2			2.404 [0.182]^2			3.9^2
		1.420 [1.267]^1			2.361 [0.198]^1			4.9^2
$SiCp^{\cdot}$ (**3b**)	—	1.449 [1.078]^2	—	—	2.075 [0.459]^1	—	[1.017]	—
		1.392 [1.407]^2			2.497 [0.216]^2			
		1.404 [1.366]^1			3.027 [0.063]^2			
$FeCp_2$ (**4a**)	—	1.417 [1.256]	—	—	2.204 [c] [0.205]	—	1.846 [e] [1.025]	2.3
$SiCp_2$ (**4b**)	—	1.413 [1.305]	—	—	2.553 [d] [0.141]	—	2.252 [0.705]	1.3
$SiCp_2$ (**4c**)	—	1.445 [1.114]^1	—	—	2.276 [0.272]^2	—	—	—
		1.414 [1.266]^2			2.715 [0.088]^2			
		1.399 [1.389]^2			2.946 [0.010]^1			
$[C_{60}H_5]^-$ (**5a**)	1.399 [1.384]	—	1.507 [0.890]	—	—	—	—	—
$[C_{60}H_5]^{\cdot}$ (**5b**)	1.457 [1.129]^2	—	1.506^1	—	—	—	—	—
	1.343 [1.659]^2		1.510^2					
	1.488 [1.099]^1		1.519^2					
$C_{60}FeCp^+$ (**6**)	1.460 [1.102]	1.419 [1.225]	1.366 [1.491]	2.220	2.157 [0.258]	1.840	1.788 [1.290]	1.6
Cp^-	—	1.406 [1.387]	—	—	—	—	—	0
$Cp^{\cdot}$	—	1.484 [1.099]^1	—	—	—	—	—	0
		1.348 [1.674]^2						
		1.451 [1.137]^2						

Note. The numbering of atoms is shown in Figs. 1—5.

[a—e] Corresponding values obtained from calculations in the STO-3G basis set: [a] 2.151 Å; [b] 2.419 Å; [c] 2.132 Å (the experimental value[18] is 2.064 Å); [d] 2.437 Å (the experimental value[14] is 2.42 Å for $Si(CMe)_{10}$); [e] 1.758 Å (the value obtained from calculations in the DZ basis set[14] is 1.9 Å and the experimental value[18] is 1.65 Å).

face and are comparable with those in the Cp radical (see Table 3). It should be noted that in the case of anion **5a** the energy of the HOMO with e_1 symmetry (−3.5 eV) is much lower than in the case of the Cp^- anion (−1.4 eV) and that the C—C bonds in the *pent** cycle are shorter than in the cyclopentadienyl anion (*i.e.*, the structure **5a** has a "more localized" π-system compared with the unsubstituted fullerene I_h-C_{60}). These peculiarities of the geometry and electronic structure of anion **5a** must favor η^5-coordination of radical **5b** to the XCp group. Our results (see Tables 1 and 2) are in agreement with the previously reported data obtained from *ab initio* calculations in the 3-21G* basis set[7] and by the MNDO/PM3[20,3] and MNDO methods.[4,19]

Complexes η^5-$C_{60}H_5XCp$ (X = Fe (1a), Si (1b,c)) (see Fig. 1). Calculations of molecules **1a,b** were performed assuming that they have C_{5v} symmetry, with the initial geometry of the framework and XCp fragments taken from calculations of the structure **5a** and complexes XCp_2, respectively. Full optimization of the geometry of system **1b** performed earlier[3] by the MNDO/PM3 method confirms that it corresponds to a local minimum on the PES. The structure of complex **1c** (see Fig. 1), calculated assuming that it has C_s



5a **5b**

Fig. 4. Structures of anion $C_{60}H_5^-$ (**5a**) with C_{5v} symmetry and radical $C_{60}H_5^{\cdot}$ (**5b**) with C_s symmetry (for the geometric parameters, see Table 2).

Table 3. Spin populations (ρ) on the atoms in radicals calculated by the *ab initio* MO LCAO SCF method in the STO-3-21G basis set

Radical	ρ/au			
	C(1)	C(2)	C(3)	X
$C_{60}H_5^{\cdot}$	0.71	0.01	0.11	–
$Cp^{\cdot}$	0.64	0.02	0.16	–
$FeCp^{\cdot}$	0.00	0.00	0.00	0.98
$SiCp^{\cdot}$	0.00	0.00	0.02	0.95

symmetry, also corresponds to a local minimum whose energy is 5.2 kcal mol^{-1} lower than that of isomer **1b**. Complex **1c** can be considered as a bent sandwich similar to complex **4c**. The results of our *ab initio* calculations with the STO-3-21G basis set (see Tables 1 and 2) show that systems **1a**—**c** are fairly stable, have closed electron shells, high ionization potentials, and wide energy gaps (δ).

As should be expected, complex **1a** with the transition element atom is much more stable than the derivatives **1b**,**c** containing Si atoms. This is explained by the fact that there are bonding MOs of e_1 symmetry with appreciable contributions from d_{xz}- and d_{yz}-AOs of the Fe atom among occupied frontier orbitals of complex **1a**, whereas the analogous MOs of complex **1b** are antibonding MOs and are composed only of the ligand AOs. The found energies of the X—*pent** bond are 117.3 (**1a**), 36.6 (**1b**), and 42.4 kcal mol^{-1} (**1c**). Comparison of the Fe...C_{pent*} and Fe...C_{Cp} distances in molecule **1a** shows that the former is shorter than the latter (2.163 Å *vs.* 2.185 Å, respectively) and both of them are shorter than the Fe...C distance in the sandwich complex $FeCp_2$ (2.204 Å). This correlates with an increase in the strength of the Fe—*pent** bond in the molecule **1a** as compared to that of the Fe—Cp bond in $FeCp_2$. Analogously, the Si...C distances in complex **1b** are shorter than in $SiCp_2$; the energies of the Si—*pent** bond in **1b** and Si—Cp bond in $SiCp_2$ are close (see Table 1). The energies of heterolytic dissociation of complexes **1a** and **1b** into anions **5a** and corresponding cations **2a** and **2b** are 207.2 and 105.2 kcal mol^{-1}, respectively.

Let us denote the total orders of X—C "bonds" with carbon atoms of the *pent** face and Cp ring as *W*(X—*pent**) and *W*(X—Cp), respectively. From the data in Table 2 it follows that *W*(Fe—*pent**) > *W*(Si—*pent**) and *W*(Fe—Cp) > *W*(Si—Cp). These inequalities correspond to the above estimates of the energies of X—*pent** and X—Cp bonds. It is hoped that, in fullerene complexes **1a**—**c**, the X...C distances calculated in the STO-3G basis set will be in better agreement with experimental data (see notes "*a*" and "*b*" to Table 2), analogously to XCp_2 sandwiches. Calculations in the STO-3G basis set show that in this case the bond orders *W*(X—C) change in parallel with the lengths of the X—C "bonds," *viz.*, $W(X—C_{pent*}) > W(X—C_{Cp})$ for complexes **1a**,**b** and $W(X—C_{pent*}) > W(X—C)$ for XCp_2.

The effective charges on the X atoms in half-sandwich complexes $XCp^{\cdot}$ and XCp^+ and in sandwich systems XCp_2 and $C_{60}H_5XCp$ are positive, the charge on the Fe atom being larger than on the Si atom. The electron density transfer in complexes **1a**,**b** is more pronounced than in corresponding XCp_2 molecules (see Table 1).

Cation η^5-$C_{60}FeCp^+$ (6). Optimization of the geometry of complex **6** assuming that it has C_{5v} symmetry has led to a local energy minimum to which the structure shown in Fig. 5 corresponds.

Cation **6** has a closed electron shell (see Table 1); however, it is less stable than complex **1a**, since it is characterized by a relatively low energy of the X—C_{60} bond (64.3 kcal mol^{-1}), estimated as the abstraction energy of cation $FeCp^+$. The Fe...*pent** distance in cation **6** is 0.04 Å longer than in complex **1a** and the

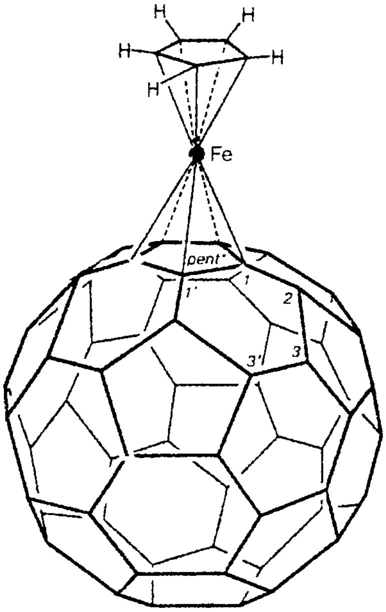


Fig. 5. Structure of η^5-π-complex $C_{60}FeCp^+$ (**6**) with C_{5v} symmetry.

Fe...Cp distance in this system is also lengthened as compared with the analogous distance in $FeCp^+$ (see Table 2).

* * *

The results of our calculations demonstrate the efficiency of attachment of H atoms to carbon atoms of fullerene C_{60} in the α-positions relative to the *pent** face for stabilizing the Fe—*pent** bond in the complexes of the unsubstituted I_h-C_{60} cluster. Based on these results, one can also conclude that *complex* η^5-π-$C_{60}H_5FeCp$ *is comparable to the ferrocene molecule in stability and must be much more stable than analogous silicon complexes and cationic complex* η^5-π-$C_{60}FeCp^+$ *of unsubstituted fullerene* C_{60}. On the contrary, complex η^5-π-$C_{60}H_5SiCp$ is less stable than the $SiCp_2$ molecule (the energy difference is 1.4 kcal mol^{-1}), while no local minima of the total energy were found for complex η^5-π-$C_{60}SiCp^+$ and $C_{60}XCp^{\cdot}$ (X = Fe, Si) radicals.

Previously, mention has been made that in $n\eta^5$-π-$C_{60}X_n$ (X = Li,[23] In,[24] SiCp[1]; n = 1 to 12) systems, in which the X atoms or species are coordinated to the pentagonal faces, the average energy of the X—C_{60} bond increases as n increases. It is hoped that $n\eta^5$-π-$C_{60}(FeCp)_n$ complexes also possess this property and that complex $12\eta^5$-π-$C_{60}(FeCp)_{12}$ with FeCp species η^5-coordinated to all pentagonal faces will also be stable.

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