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Gas-phase formation of mono- and dications from iron-subgroup decamethylmetallocenes and their calculation by the density functional method

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Abstract

The possibility of forming mono- $[C_5Me_5MC_5Me_4CH_2]^+$ (**1**) and dications $[1,2(CH_2)_2C_5Me_3MC_5Me_5]^{2+}$ (**2**) and 1,1′-$[M(C_5Me_4CH_2)_2]^{2+}$ (**3**) starting from iron subgroup decamethylmetallocenes (Fe (**a**), Ru (**b**), Os (**c**)) was studied using electron-impact mass-spectrometry. The peaks of both single (M^+) and doubly charged (M^{2+}) molecular ions are present in the mass-spectra of all compounds studied. The basic fragmentation patterns are the elimination of one (M^+) and two atoms of hydrogen (M^{2+}) to give the corresponding mono- (**1**) and dications (**2** and/or **3**). The density-functional method was used for ab initio calculations of the geometry and total energies of cations 1 and 2 and the *anti*, *syn*, and *gauche* conformers of **3** for comparison with the dication $[1,3\text{-}(CH_2)_2C_5Me_3MC_5Me_5]^{2+}$ (**2b′**). The calculation data for monocations **1a**–**c** are in a good agreement with the results of X-ray analysis of these cations except for the M–CH_2 interatomic distances and angles α, which are presumed to be most sensitive to phase changes. The relative order of stabilities of the mono- and dications was as follows: $\mathrm{F} < \mathrm{Ru} < \mathrm{Os}$. This order agrees with mass-spectrometric data. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Monocations $[C_5Me_5MC_5Me_4CH_2]^+$; Dications 1,1′-$[M(C_5Me_4CH_2)_2]^{2+}$ and $[1,2(CH_2)_2C_5Me_3MC_5Me_5]^{2+}$ (M = Fe, Ru, Os); Mass-spectrometry; Ab initio calculations; Relative stabilities

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1. Introduction

Interest in the chemistry of metallocenylmethyl cations rose after the discovery of ferrocene, which the ferrocenyl fragment can stabilize, carbocationic center [1]. Earlier we developed methods for preparing mono- $[C_5Me_5MC_5Me_4CH_2]^+$ (**1**) and dications $[1,2\text{-}(CH_2)_2\text{-}C_5Me_3MC_5Me_5]^{2+}$ (**2**) and 1,1′-$[M(C_5Me_4CH_2)_2]^{2+}$ (**3**) starting from decamethylmetallocenes of the iron subgroup (Fe (**a**), Ru (**b**), Os (**c**)) [2–7]. The preferred multi-step method for preparing cations **1**–**3** consisted of oxidation of decamethylmetallocenes by $BaMnO_4$ to give aldehydes and their subsequent transformation into the appropriate alcohols, which react with protic acids to give the primary monocations according to the scheme [2–4,7]:

$$C_5Me_5MC_5Me_5 \xrightarrow{BaMnO_4} C_5Me_5MC_5Me_4CHO \xrightarrow{LiAlH(^tBuO)3} C_5Me_5MC_5Me_4CH_2OH \xrightarrow{H^+} [C_5Me_5MC_5Me_4CH_2]^+ \qquad (1)$$

The oxidation of the decamethylmetallocenes produces the homo- and heteroannular aldehydes 1,2-$(CHO)_2C_5Me_3MC_5Me_5$ and 1,1′-$M(C_5Me_4CHO)_2$ as by-products. These were converted into dications **2** and **3** using the superacid CF_3SO_3H according to the same scheme [5,6].

Cations **1**, containing Ru and Os, were also prepared in a single-stage process by UV photolysis of the appropriate decamethylmetallocenes in the presence of the strong protic acids CF_3COOH and CF_3SO_3H [8]. It should be noted that a one-pot synthesis of these cations was carried out earlier by oxidation of the decamethylmetallocenes of ruthenium [9] and osmium

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[10] by silver salts. Recently dications **2** and **3** have also been obtained by dissolution of $(C_5Me_5)_2M$ (where M = Ru, Os) in oleum [11]. The salts of monocations **1a**–**c** are sufficiently stable and their structures were established by the X-ray analysis. The iron-containing cation **1a** with the counter-ion $[3,5\text{-}(CF_3)_2C_6H_3]_4B^-$ was also characterized by this method for the first time [12]. Dications **2** and **3** are less stable. According to NMR spectra, they are stable in the superacid CF_3SO_3H solution at temperatures from − 60 up to + 60°C. The *gauche* conformer is the most stable one in solution [6]. X-ray data for salts of cations **1** containing the whole iron subgroup showed that Ru- and Os-containing ions [3,4] are stabilized by the formation of a donor–acceptor σ-bond between the carbocation center and the metal to give metallonium (onium) compounds. The carbocation structure is more characteristic of the Fe-containing ion. In this cation the Fe–CH_2 bond is greatly elongated (2.56 Å). According to quantum-chemical calculations by the EHM method, less than 10% of the positive charge is located on the metal atom [13].

In the present report, the possibility of forming mono- and dications from decamethylmetallocenes of the iron subgroup in the gas phase was studied using electron-impact mass-spectrometry, and calculations of their geometry and complete energies were made by the density-functional method. This theoretical research is especially important for dications because their salts were not separated as pure substances and X-ray analyses were not carried out for them.

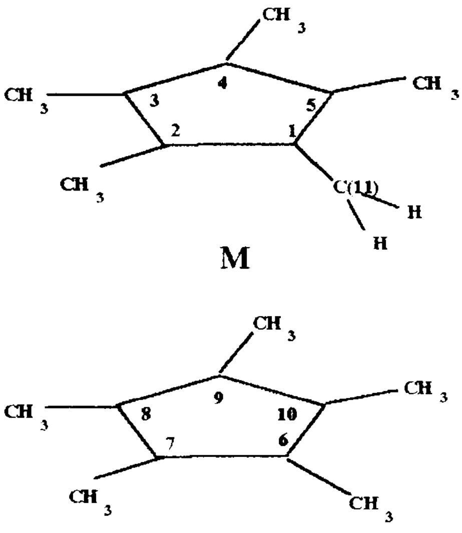
2. Results and discussion

The mass-spectra of all $(C_5Me_5)_2M$ (M = Fe,Ru,Os) contain peaks of both single- and doubly charged molecular ions. The metallocenes **1**–**3** fragment through the loss of hydrogen atoms, methyl groups and one ligand, giving rise to a series of ions $[M-n\mathrm{H}]^{k+}$, $[M-m\mathrm{Me}-n\mathrm{H}]^{k+}$ and $[\mathrm{M}\text{–}\mathrm{C_5Me_5}\text{–}m\mathrm{Me}\text{–}n\mathrm{H}]^{k+}$ ($n = 1$–8, $m = 1$–3, $k = 1,2$). The peak intensities depend on both the charge of the ion and the nature of metal atom. In particular, the first dehydrogenation step of the singly charged molecular ions involves elimination of one hydrogen atom. The intensities of peaks for $[M-\mathrm{H}]^+$ ions are 5–8 times greater than those of $[M-2\mathrm{H}]^+$. However, the doubly charged ions typically eliminate two hydrogen atoms to give only the $[M-2\mathrm{H}]^{2+}$ ions (Table 1). This indicates that the mono- and dications are highly stable. The geometrical and energetic characteristics of these ions were calculated using the density functional method.

The eclipsed conformation predominates for metallocene derivatives in the gas phase according to the electron diffraction data [14] and was chosen as the initial geometry for optimization of the energy. Our calculations of two conformations of decamethylrutenocene have shown that the eclipsed conformation (A) is energetically more favorable than the staggered conformation (B) (the difference in energy is 1.8 kcal mol^{-1}; the total energy values are E(A) = − 873.4846 a.u., E(B) = − 873.481 a.u.

The structures of the monocations of iron (**1a**), ruthenium (**1b**) and osmium (**1c**) are presented in the scheme. Their energetic and geometric parameters are listed in Table 2.

The data calculated for bonds in cations **1a**–**c** compare quite well with experimental data from X-ray analysis not only for the lengths C_{ring}–CH_3 bonds but also for ring C–C bonds (deviations do not exceed 0.08 Å) for the whole subgroup. The calculated lengths of the C(1)–C(11) bonds are somewhat different from X-ray results. Greater deviations (~ 0.1 Å) are observed for the calculated M–C_{ring} bonds. They are consistent with some distortion of the sandwich structure, judging from the shorter M–C(11) bonds and more longer M–C(14) bonds, which indicate that the cyclopentadienyl rings are slated. In all cases these rings are nonparallel. Deviations (~ 5°) are observed and practically coincide with the values of the dihedral angles (4.8° Fe, 6.8° Ru, 6.9° Os) between them for the same cations in the crystalline state [3,4,12].



1a, M=Fe ; 1b, M=Ru ; 1c, M=Os

However, the calculations and experimental results differ significantly for the M–CH_2 (i.e. M–C(11)H_2) bonds and α angles (the deviation angles of the C(1)–C(11) bonds from the plane of cyclopentadienyl ligand) in cations **1a**–**c**. In cation **1a** the length of the

Fe–C(11) bond decreases from 2.567 Å in the solid phase to 2.324 Å in the gas. According to the calculation, the angle α in cation **1a** is smaller than in cations **1b** and **1c**. This is different from the X-ray data and indicates that the M–C(11) bond in cation **1a** in the gas phase is stronger than in the crystalline state. The reasons for these discrepancies may be the fact that the structure of the cation in the gas phase is not influenced by the anion and the crystal environment but is influenced not only by the electronic effect of metal atom and its nucleophilicity (which has been repeatedly noted in the behavior of their cations in crystal and liquid phases), but also by its size. Thus, on the one hand, the nucleophilicity of the metal atoms increases from the top to the bottom in the subgroup sequence. This shortens the M–C(11) bond in the order Fe–Ru–Os. On the other hand, the very small atomic radius of the iron atom in comparison to Ru and Os should produce

Table 1
The intensity of peaks of single- (1+) and doubly charged (2+) ions in mass-spectra of $(C_5Me_5)_2M$ (M = Fe, Ru, Os)

	$(C_5Me_5)_2Fe$		$(C_5Me_5)_2Ru$		$(C_5Me_5)_2Os$	
	1+	2+	1+	2+	1+	2+
M	100	100	100	100	100	100
$M-\text{H}$	4.4		10.6		13.2	2.5
$M-2\text{H}$	1.5	13.8	2.5	14.7	1.6	40.3
$M-n\text{H}$	5.9	36.2	18.2	14.7	21.6	90.9
$M-m\text{Me}-n\text{H}$	7.3	24.9	73.8	69.0	74.7	177.4
$M-\text{C2H4}$		10.5	1.1		1.7	
C5Me5M–nMe–mH	7.2		36.9			

Table 2
The results of calculations for monocations **1a**–**c**. Comparison with the data of X-ray analysis of these ions in crystals

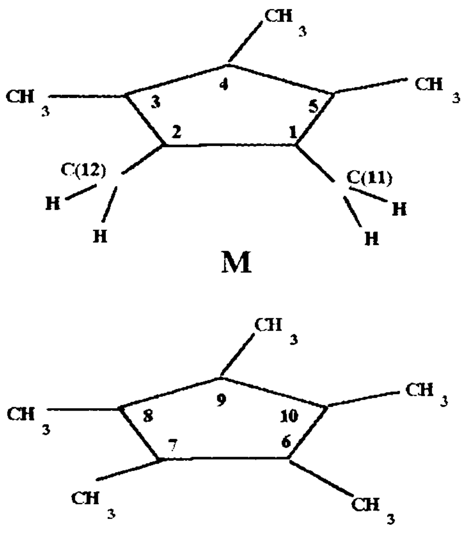
Parameters	**1a**		**1b**		**1c**	
	Theory	X-ray	Theory	X-ray	Theory	X-ray
Bond distances (Å)						
M–C(1)	2.020	1.968	2.156	2.066	2.158	2.069
M–C(2)	2.172	2.050	2.306	2.186	2.288	2.187
M–C(3)	2.290	2.116	2.424	2.266	2.402	2.264
M–C(4)	2.279	2.136	2.430	2.273	2.418	2.269
M–C(5)	2.164	2.054	2.318	2.178	2.314	2.181
M–C(6)	2.208	2.094	2.320	2.200	2.323	2.222
M–C(7)	2.151	2.104	2.282	2.211	2.269	2.225
M–C(8)	2.144	2.055	2.275	2.191	2.272	2.193
M–C(9)	2.158	2.010	2.285	2.190	2.295	2.194
M–C(10)	2.182	2.122	2.332	2.211	2.350	2.221
M–C(11)	2.324	2.567	2.410	2.270	2.341	2.244
C(1)–C(2)	1.494	1.449	1.499	1.461	1.501	1.470
C(1)–C(5)	1.495	1.416	1.498	1.453	1.500	1.461
C(1)–C(11)	1.415	1.370	1.424	1.401	1.442	1.426
C(2)–C(3)	1.441	1.378	1.446	1.404	1.455	1.403
C(3)–C(4)	1.474	1.457	1.477	1.436	1.478	1.439
C(4)–C(5)	1.441	1.419	1.445	1.417	1.452	1.413
C(6)–C(7)	1.468	1.431	1.478	1.428	1.484	1.449
C(6)–C(10)	1.459	1.430	1.457	1.423	1.457	1.435
C(7)–C(8)	1.460	1.370	1.464	1.418	1.471	1.414
C(8)–C(9)	1.470	1.400	1.474	1.442	1.476	1.451
C(9)–C(10)	1.460	1.410	1.466	1.423	1.479	1.432
Bond angles (°)						
M–C(1)–C(11)	83.2	98.9	81.9	–	78.4	–
M–C(11)–C(1)	59.7	49.2	62.3	–	64.5	–
α	34.0	23.6	32.4	40.3	36.9	41.8
γ	6.1	4.8	4.2	6.8	5.7	6.9
Total energy $-E$ *(a.u.)*						
	902.2612	–	872.6920	–	869.8436	–

the opposite effect. Thus, the Fe-containing cation **1a** appears to deviate from the general sequence.

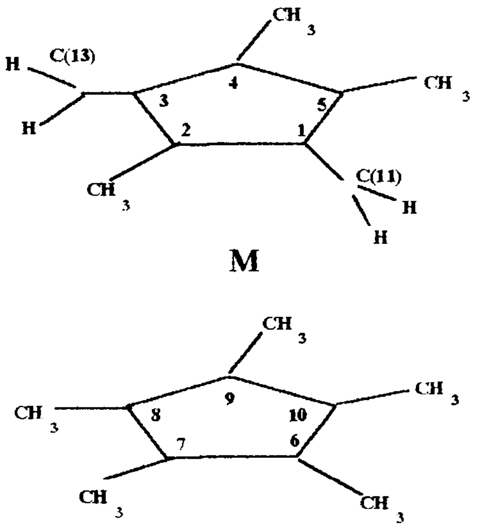
In summary, calculations for monocations **1a**–**c** agree well with geometric parameters of the sandwich structures of these cations that were found from X-ray studies. This is especially true for the C–C and M–C_{ring} bonds. The largest deviations have been observed for interatomic distances M–C(11) (i.e. M–CH_2) and angles α. This is connected presumably with the sensitivity of these parameters to the phase change because M–CH_2 bonds, in contrast with the usual ones, are donor-accepting, whereas the metal atom is positively charged. In crystals, the presence of anions in the salts of cations **1a**–**c** may influence strongly the interatomic distances and α angles.

The calculations that have been carried out for homoannular dications **2a**–**c** and various conformations of the heteroannular **3b** dications, which were generated [5,6,11] only in the liquid phase and thus were not investigated by X-ray methods, can provide useful information on their structures. In addition to the calculations for the dications listed above, the same procedure was performed for the homoannular Ru-containing dication, which has CH_2-groups in the *meta*-position (**2b**′).

For 1,2-homoannular dications **2a**–**c**, the C(1)–C(11) bond length increases characteristically down the subgroup. These bonds are slightly shorter than those of the corresponding mono-cations **1a**–**c** (Table 3). The interatomic distances M–C(1) also grow linearly in the subgroup and are slightly longer than the lengths of corresponding M–C(1) bonds in monocations **1a**–**c**. The heteroannular dications typically have exocyclic M–CH_2 bonds that are slightly longer than those in homoannular dications. This suggests that the M–CH_2 bond in the last compounds is stronger. In the series of homoannular dications **2a**–**c**, the distances between the metal atom and atom C(11) of the exocyclic bond decrease smoothly. These distances slightly exceed the corresponding values for monocations of the corresponding metals. This bond strength is assumed to be slightly weaker than in the monocations. For homoannular dications **2a**–**c**, the M–C(11) bond length typically decreases from top down in the subgroup. This bond is longer than in corresponding monocations. The differences are insignificant for the Ru- and Os-containing cations (0.046 and 0.060 Å, respectively) and are substantial for Fe-containing cation (~ 0.170 Å).



2a, M=Fe ; 2b, M=Ru ; 2c, M=Os



2b’ , M=Ru

In Ru-containing dication **2b**, the metal atom interacts with two vicinal CH_2 groups whereas in dication **2b**′, the Ru–C(1) and Ru–C(3) distances differ substantially and are equal to 2.194 and 2.608 Å, respectively. For **2b**′ a very short C(3)–C(13) bond (1.387 Å) is observed. The α angle does not differ from zero. Thus, in dication **2b**′, the C(13)H_2 group does not interact with the central metal atom. Homoannular 1,3-dication **2b**′ turns out to be energetically less stable than homoannular 1,2-dication **2b** (the energy difference is 15.7 kcal mol^{-1}). Consequently, it is not surprising that the oxidation of decamethylrutenocene in a superacid gives rise to **2b** instead of **2b**′.

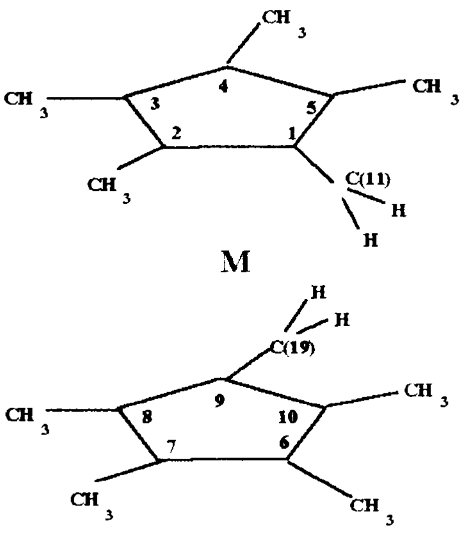
The presence of a C(13)H_2 unit lying practically in the plane of the cyclopentadienyl ring results in the strong alternating of the C–C bonds in the ring. Such

Table 3
The results of calculations for homoannular 1,2-dications of iron, ruthenium and osmium **2a**–**c**, 1,3-dication of ruthenium **2b′**, and of heteroannular dication of ruthenium **3b** for different conformers

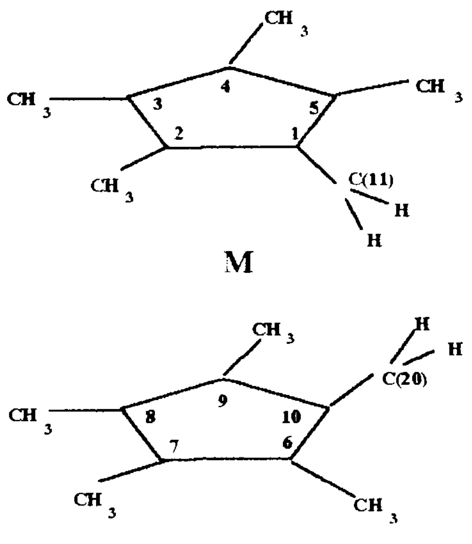
Parameters	**2a**	**2b**	**2c**	**2b′**	**3b**		
					anti	*gauche*	*syn*
Bond distances (Å)							
M–C(1)	2.064	2.200	2.195	2.194	2.189	2.194	2.192
M–C(2)	2.063	2.192	2.182	2.386	2.355	2.293	2.354
M–C(3)	2.362	2.634	2.528	2.608	2.535	2.427	2.422
M–C(4)	2.537	2.901	2.751	2.607	2.521	2.475	2.432
M–C(5)	2.365	2.654	2.558	2.450	2.321	2.365	2.358
M–C(6)	2.231	2.356	2.384	2.353	2.513	2.350	2.176
M–C(7)	2.220	2.291	2.293	2.336	2.501	2.453	2.359
M–C(8)	2.168	2.272	2.263	2.318	2.329	2.416	2.464
M–C(9)	2.165	2.289	2.292	2.276	2.181	2.293	2.429
M–C(10)	2.177	2.335	2.357	2.274	2.324	2.187	2.328
M–C(11)	2.504	2.456	2.401	2.401	2.515	2.586	2.687
M–C(12)	2.511	2.456	2.395	–	–	–	–
M–C(13)				2.603			
M–C(16)	–	–	–	–	–	–	2.619
M–C(19)	–	–	–	–	2.482	–	–
M–C(20)	–	–	–	–	–	2.547	–
C(1)–C(2)	1.513	1.513	1.514	1.467	1.499	1.494	1.497
C(1)–C(5)	1.479	1.477	1.481	1.511	1.491	1.501	1.498
C(1)–C(11)	1.403	1.417	1.432	1.426	1.414	1.408	1.412
C(2)–C(3)	1.480	1.478	1.482	1.492	1.450	1.458	1.445
C(2)–C(12)	1.401	1.417	1.433	1.506	1.513	1.510	1.509
C(3)–C(4)	1.452	1.453	1.460	1.507	1.468	1.476	1.493
C(4)–C(5)	1.452	1.452	1.458	1.421	1.465	1.447	1.443
C(6)–C(7)	1.467	1.477	1.477	1.456	1.467	1.449	1.498
C(6)–C(10)	1.466	1.460	1.461	1.490	1.468	1.501	1.498
C(7)–C(8)	1.470	1.480	1.486	1.480	1.453	1.476	1.445
C(8)–C(9)	1.469	1.469	1.475	1.466	1.499	1.460	1.488
C(9)–C(10)	1.471	1.478	1.480	1.476	1.491	1.495	1.448
Bond angles (°)							
M–C(1)–C(11)	90.41	82.46	79.90	80.06	85.71	88.98	93.92
M–C(11)–C(1)	55.50	62.64	64.14	64.16	60.20	58.02	54.48
M–C(2)–C(12)	90.83	82.79	80.08	–	–	–	–
M–C(12)–C(2)	55.24	62.30	63.83	–	–	–	–
M–C(3)–C(13)				127.18			
M–C(13)–C(3)				35.01			
M–C(6)–C(16)	–	–	–	–	–	–	91.14
M–C(16)–C(6)	–	–	–	–	–	–	56.16
M–C(9)–C(19)	–	–	–	–	84.37	–	–
M–C(19)–C(9)	–	–	–	–	61.00	–	–
M–C(10)–C(20)	–	–	–	–	–	87.33	–
M–C(20)–C(10)	–	–	–	–	–	59.04	–
α (1)	25.03	24.62	31.24	28.30	28.30	25.91	19.43
α (2)	24.58	24.30	31.11	–	–	–	–
α (3)	–	–	–	0.40	–	–	–
α (6)	–	–	–	–	–	–	23.88
α (9)	–	–	–	–	30.15	–	–
α (10)	–	–	–	–	–	27.87	–
γ	7.9	4.3	5.3	8.4	0.4	5.5	0.9
Total energy $-E$ *(a.u.)*	901.2885	871.7266	868.8789	871.7016	871.7115	871.7266	871.6978

alternating is not observed in the case of dication **2b** (see Table 3).

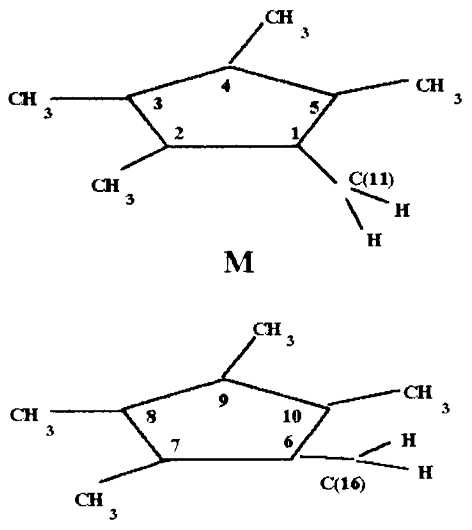
The values of the α angle for the dications are smaller than the respective values for monocations **1**. For example, for homoannular dication of osmium this value is equal to 31.1° (for the monocation, 36.9°). In the series of heteroannular Ru-containing conformers **3b**, the α angles decrease smoothly in the sequence: *anti*, *gauche*, *syn*.



3b-anti (M=Ru)



3b-gaush (M=Ru)



3b-syn (M=Ru)

In order to estimate the relative stabilities of monocations **1** of the iron subgroup in the gas phase, we calculated enthalpies of the hypothetical reaction of the neutral decamethylmetallocene with the proton which yield the hydrogen molecule. By optimizing the geometry in calculations using the BLYP/LanL2DZ method, the following values for the total energies of a hydrogen molecule and the decamethylmetallocenes of Fe, Ru and Os were obtained: -1.1638; -903.0607; -873.4858; -870.6302 a.u. By setting the enthalpy of this process equal to 0 for iron compounds, the calculations give the following enthalpies: Fe (0.0 kcal mol^{-1}) > Ru (-3.6 kcal mol^{-1} > Os (-6.8

kcal mol^{-1}). A similar sequence of stabilities is obtained for dications of metallocenes **2a**–**c**: Fe (0.0 kcal mol^{-1}) > Ru (−4.6 kcal mol^{-1}) > Os (−5.0 kcal mol^{-1}).

These sequences agree well with the mass-spectral data. It follows from Table 1 that the peak intensities for $[M-\mathrm{H}]^+$ and $[M-2\mathrm{H}]^{2+}$ ions, which are characteristic of the stabilities of the corresponding cations, increase in the same sequence.

The relative stabilities of the Ru-containing dications with homoannular and heteroannular structures are as follows: homoannular 1,2- (0.0 kcal mol^{-1}) > heteroannular *gauche*- (0.4 kcal mol^{-1}) > heteroannular *anti*- (9.5 kcal mol^{-1}) > homoannular 1,3- (15.7 kcal mol^{-1}) > heteroannular *syn*- (18.1 kcal mol^{-1}). It follows from the calculations that the homoannular 1,2-dication and the heteroannular dication with the *gauche* conformation have the same relative stabilities. We concluded that the *gauche* conformer is more stable than the *anti* and *syn* conformers based on earlier calculations of the potential energies of rotation of Cp-rings (EHM method) by Hoffmann, where the observed preference for the gauche conformer was explained by the interaction of the CH_2-cation 2p-orbitals with 3d-orbitals of the metal atom [5,6].

3. Experimental

The mass-spectra of $(C_5Me_5)_2M$ (M = Fe,Ru,Os) were measured on an MS-890 instrument at ionizing voltage 70 V and ionization chamber temperature 250°C. The spectra were adjusted to a monoisotopic form using the program AELITA [15].

The mono- and dications formed from decamethylmetallocenes in the gas phase were calculated using density functional theory (BLYP) [16,17] and the program GAUSSIAN-98 [18] on CRAY J-90 supercomputers (National Energy Research Supercomputer Center, Berkley, CA). The geometric structures of ions were optimized using Dunning–Hay DZ basis sets [19] and pseudo-potentials LanL2 for iron, ruthenium, and osmium [18]. A similar level of calculations was used successfully by one of us in previous studies of the geometrical and electronic structures of heavy metal complexes [20,21].

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