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Theoretical Study of 3-Penten-2-one Complexes of Iron and Chromium Subgroup Metals with Various Modes of the Enone Coordination

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Abstract—The calculated parameters of the steric and electronic structure and shielding constants of η^2-(3-penten-2-one)Fe(CO)$_4$, η^2-(3-penten-2-one)M(CO)$_5$, η^4-(3-penten-2-one)Fe(CO)$_3$, and η^4-(3-penten-2-one)$\cdot$M(CO)$_4$ (M = Cr, Mo, W) nicely agree with the experiment. Coordination of the α-enone with transition metals significantly distorts the conjugation between the C=C and C=O bonds.

It is believed by some authors that the reactivity of a heteropolyene ligand is affected by π complexation with a transition metal only in η^n complexes with low n [1, 2]. In this case the metal is considered as a protective group blocking the most active multiple bond of the polyene. We have shown previously [3, 4] that α-enones containing one or several aromatic fragments, when coordinated in the η^2 or η^4 mode to Cr, Mo, or W, react with dialkyl hydrogen phosphites by the scheme of the Abramov reaction, whereas with free α-enones the process follows the pattern of the Pudovik reaction (hydrophosphorylation of the C=C bond).

The similar reactivity of the coordinated enones, independent of the coordination mode, cannot be explained in terms of the concept of the protective role of metal. Probably, bonding with the metal center affects the geometric and electronic structure of the α-enone ligand. To reveal changes in the structure of α-enones due to π complexation, we performed a theoretical study by the SBK (ECP) method of a series of heterodiene π complexes: η^2-(3-penten-2-one)-tetracarbonyliron(0); η^4-(3-penten-2-one)tricarbonyliron(0); η^2-(3-penten-2-one)pentacarbonylchromium(0), -molybdenum(0), and -tungsten(0); and η^4-(3-penten-2-one)tetracarbonylchromium(0), -molybdenum(0), and -tungsten(0).

To study the structural and energy parameters of the compounds, we chose the ECP (SBK) basis in which the electrons of the inner shells are described by the Stevens–Basch–Krauss model potential. In this method we used the 6–31G basis for hydrogen atoms and the quadro- and tri-zeta basis sets for the *s*, *p*, and *d* shells of heavy atoms. For heavy atoms we used the *d*-polarizing function. In this basis we performed the complete geometry optimization [5].

The magnetic properties of molecules were determined by the nonempirical method of gradient-invariant atomic orbitals (GIAO) used for calculating the shielding constants [6]. The GIAO method is based on the perturbation theory in calculations of the magnetic shielding. The procedure was developed by Ramsey [7–9] who obtained the following expression for the component of the nuclear magnetic shielding tensor for a particular case when the origin of the coordinate system is fixed on the nucleus under consideration:

$$\sigma_{\alpha\beta} = \sigma^d_{\alpha\beta} + \sigma^p_{\alpha\beta}$$

$$= \frac{\bar{e}^2}{2mc^2} \sum_i \langle \Psi_0 | r_i^{-3} (\vec{r}_i^{\,2} \delta_{\alpha\beta} - r_\alpha r_\beta) | \Psi_0 \rangle$$

$$- \frac{\bar{e}^2}{2mc^2} \sum_n (E_n - E_0)^{-1} \langle \Psi_0 | L_{n\alpha} | \Psi_n \rangle \langle \Psi_n | L_{n\beta} r_i^{-3} | \Psi_0 \rangle.$$

Here $\bar{e}$ and m are the electron charge and weight, respectively; $\vec{L}_n = [\vec{r}_n \times \vec{p}_n]$ is the orbital moment; in the latter expression $\vec{p}_n$ is the operator of the momentum of the nth electron, and E_n is the energy of the nth excited state.

The problem of the dependence on the position of the origin was solved by London who used the so-called gradient-invariant atomic orbitals, or London orbitals [10]. They have the form

$$\Psi'_v = \left\{ - \frac{i\bar{e}}{\hbar c} [\vec{A}_v \times r] \right\} \Psi_0.$$

where Ψ'_v is the orbital of the atom whose position in space is characterized by the vector $\vec{R}_\nu$, the position

Table 1. M–C and C–O bond lengths, Å

ECP/SBK[a]			Experiment[b]		Calculation[c]	
complex	M–C	C–O	M–C	C–O	M–C[d]	C–O
		M = Fe				
η^2-[$CH_3CH=CHC(O)CH_3$]$Fe(CO)_4$, *e*-CO	2.026	1.140	1.827[e]	1.152[e]	1.823/1.843[f]	1.162[f]
η^2-[$CH_3CH=CHC(O)CH_3$]$Fe(CO)_4$, *a*-CO	2.174					
η^4-[$CH_3CH=CHC(O)CH_3$]$Fe(CO)_3$	2.060	1.137				
		M = Cr				
η^2-[$CH_3CH=CHC(O)CH_3$]$Cr(CO)_5$, *e*-CO	1.961	1.151	1.914[g]	1.140[g]	1.770/1.861[h]	–
η^2-[$CH_3CH=CHC(O)CH_3$]$Cr(CO)_5$, *a*-CO	2.014					
η^4-[$CH_3CH=CHC(O)CH_3$]$Cr(CO)_4$	2.241	1.141				
		M = Mo				
η^2-[$CH_3CH=CHC(O)CH_3$]$Mo(CO)_5$, *e*-CO	2.076	1.144	2.063[i]	1.145[i]	2.005/2.065[h]	–
η^2-[$CH_3CH=CHC(O)CH_3$]$Mo(CO)_5$, *a*-CO	2.133					
η^4-[$CH_3CH=CHC(O)CH_3$]$Mo(CO)_4$	2.050	1.148				
		M = W				
η^2-[$CH_3CH=CHC(O)CH_3$]$W(CO)_5$, *e*-CO	2.070	1.150	2.058[i]	1.148[i]	2.020/2.057[h]	–
η^2-[$CH_3CH=CHC(O)CH_3$]$W(CO)_5$, *a*-CO	2.156					
η^4-[$CH_3CH=CHC(O)CH_3$]$W(CO)_4$	2.040	1.152				

[a] Results of this work. [b] Experimental data for internuclear distances in homoligand carbonyls $M(CO)_x$. [c] Results of the theoretical study of acetylene π complexes $(CH{\equiv}CH)M(CO)_x$. [d] The first figure corresponds to the carbon atom of CO axial with respect to coordinated acetylene, and the second figure, to equatorial CO molecules. [e] Data of gas-phase electron diffraction [14]. [f] BLYP–ECP calculations [15]. [g] Neutron diffraction data for the crystalline phase [16]. [h] MP2/II calculations [17]. [i] Data of gas-phase electron diffraction [18].

of the electron is described by the radius vector $\vec{r}$, and $\vec{A}_v = [\vec{H}\times\vec{r}]$ is the vector potential of the magnetic field on the nucleus. This method is widely used to describe the second-order magnetic properties of of atoms and molecules.

The GIAO calculations using the coupled Hartree–Fock method, performed for the first time by Ditchfield [11], allowed the requirements to the basis size to be considerably reduced. The GIAO method was substantially improved by using a procedure similar to analytical differentiation [12, 13].

The M–C bond lengths for coordinated carbonyl ligands, obtained by calculation and available from the literature, are given in Table 1. It is seen that the M–C bond lengths for equatorial CO groups are nicely consistent with the experimental values for homoligand carbonyl complexes of the corresponding chromium-subgroup metal complexes. Deviations from the experimental values are from 0.005 to 0.05 Å, which shows that the method is quite applicable for calculations of these organometallic compounds. According to [14], the metal–carbonyl ligand bond lengths in the equatorial plane of a π complex differ insignificantly from those in the homoligand carbonyl complexes. The M–C bond with the CO molecule in the trans position relative to the α-enone ligand is 0.05–0.1 Å longer than those with the equatorial CO molecules. This fact is consistent with the results of theoretical studies of the complexes $(alkyne)M(CO)_x$ [16, 18] and with the experimentally observed [15] trans influence of the unsaturated ligand in organometallic compounds, which is stronger than that of the carbonyl ligands. On the whole, the geometric parameters of the π complexes of chromium subgroup metals, determined by us, are better consistent with the experiment than the bond lengths obtained in the previous MP2/II calculations of organometallic compounds of chromium-subgroup metals [18].

The calculated M–C and C=O bond lengths in the iron complexes are worse consistent with the experiment than those in the complexes of the chromium-subgroup metals. The calculated M–C bond length for the equatorial CO molecule differs from the experimental value for $Fe(CO)_5$ by 0.2 Å; the C–O bond length also differs significantly (by 0.01 Å). This may be due to two factors: errors of the used method of the effective shell potential and different nature of iron π complexes as compared to those of chromium-subgroup metals.

The limitations of the method of the effective shell

Table 2. Theoretical[a] and experimental[b] ^{1}H and ^{13}C NMR chemical shifts in π complexes of 3-penten-2-one and 4-methyl-3-penten-2-one with molybdenum and chromium

Complex	δ, ppm				δ_C, ppm					
	>C=CH–		–C(O)–CH_3		>*C*=CH–		>C=*C*H–		μ–CO[c]	
	calcd.	exptl.	calcd.	exptl.	calcd.	exptl.	calcd.	exptl.	calcd.	exptl.
η^2-(Enone)$Cr(CO)_5$	3.92	3.86	2.02	2.18	66	63	85	85	188/204	191/200
η^2-(Enone)μ°$(CO)_5$	3.68	3.74	2.00	2.13	70	68	78	80	193/211	195/207
η^4-(Enone)$Mo(CO)_4$	3.50	3.45	2.15	2.07	72	75	95	93	192	196

[a] The chemical shifts were calculated by the GIAO method, with the geometry of the 3-penten-2-one π complexes optimized by the SBK method. [b] The chemical shifts were determined experimentally for π complexes of 4-methyl-3-penten-2-one. [c] The first figure corresponds to the axial CO molecule, and the second, to the equatorial CO molecule.

potential in calculations of the geometric and energy parameters of compounds of Period III elements [16, 17] was repeatedly noted in the literature. The errors originate from unjustified complete neglect of the interaction of the inner electron shells of the heavy atom with the valence shells of ligands for elements with small atomic radii. Thus, the method of the effective shell potential gives more accurate results for elements of Period IV and especially Period V. Indeed, the geometric parameters obtained by us for organometallic compounds of molybdenum and tungsten are better consistent with the experiment than those for the chromium compounds.

Another cause of the observed effect is more significant rearrangement of the iron carbonyl complex on coordination of α-enone. As a result, the M–CO bond lengths in the π complex significantly differ from those in $Fe(CO)_5$. This assumption is supported by the fact that the calculated length of the bond between iron and the carbon atom of the enone double bond (2.100 Å) is close to the length of the bond with the carbon atom of coordinated acetylene (2.140 Å) reported in [16].

The chemical shifts of the carbon and hydrogen atoms in chromium and molybdenum complexes of 3-penten-2-one, calculated by us from the chemical shielding parameters by the GIAO method and determined experimentally for π complexes of 4-methyl-3-penten-2-one, synthesized by us, are listed in Table 2. The calculated chemical shifts of the carbon atoms of the CO group and double bond and of the vinyl protons are well consistent with the experiment. The random deviations of the calculated values from the experiment may be due to limited accuracy of the calculation procedure and also to the fact that the calculations and experimental determinations were performed with different (though structurally related) α-enones. Thus, the SBK and GIAO methods used for optimization of the geometric structure of molecules allow adequate determination of the geometric and physicochemical parameters of organometallic π compounds.

The bond lengths, bond orders, and bond and torsion angles in free and coordinated 3-penten-4-one, calculated by us, are listed in Table 3. Coordination brings about significant changes in the geometric and electronic structure of the α-enone. For the η^2 complexes, the length of the double bond increases by 0.05–0.15 Å; this increase is especially pronounced in elements with smaller atomic radii. Thus, in η^2-(3-penten-2-one)tetracarbonyliron(0) the length of the coordinated double bond is 1.521 Å, which corresponds to the length of the C–C bond between sp^3-hybridized carbon atoms. The order of the C=C bond decreases on coordination, especially in the iron and chromium complexes. This is probably due to the fact that the radius of Period III elements allows chemical bonding between the metal and π ligand by both donor and acceptor mechanisms. The chromium and iron complexes, in terms of the Dewar–Chatt–Duncanson model are structurally more similar to the metallacyclopropane boundary resonance structure. For elements of Periods IV and V, the transfer of the π-antibonding electrons of the enone ligand to the vacant *d* orbitals of Mo or W becomes the predominant process; as a result, the bond orders and bond angles in 3-penten-2-one η^2-coordinated to W do not change significantly relative to the free state. In all the η^2 complexes of 3-penten-2-one, except that with W, the planarity of the C=C–C=O fragment is distorted: The torsion angle between the C=C and C=O ring planes is 15.5°–32°. This fact, along with a significant decrease in the bond orders, suggests distor-

Table 3. Bond orders, bond and torsion angles, and interatomic distances in free and coordinated 3-penten-2-one, calculated by the SBK method

Complex	Bond order					Bond and torsion angles, deg				
	C^4–C^5	C^3–C^4	C^2–C^3	C^2–O	C^1–C^2	$C^5C^4C^3$	$C^4C^3C^2$	$C^1C^2C^3$	C^1C^2O	$C^3C^4C^2O$
–	1.032	1.940	0.906	2.047	1.036	122.2	123.1	114.9	123.1	0
η^2-$[CH_3CH{=}CHC(O)CH_3]Fe(CO)_4$	1.066	0.951	1.012	1.831	1.012	118.7	119.9	116.7	122.0	15.5
η^2-$[CH_3CH{=}CHC(O)CH_3]Cr(CO)_5$	1.047	1.580	0.899	2.014	0.963	116.8	115.9	120.8	119.4	32.1
η^2-$[CH_3CH{=}CHC(O)CH_3]Mo(CO)_5$	1.021	1.791	0.863	2.021	1.005	118.7	116.9	121.0	119.4	29.8
η^2-$[CH_3CH{=}CHC(O)CH_3]W(CO)_5$	1.027	1.831	0.911	2.016	1.000	125.3	121.4	118.5	121.3	2.4
η^4-$[CH_3CH{=}CHC(O)CH_3]Fe(CO)_3$	1.001	1.085	1.485	1.141	1.034	118.4	116.8	121.5	116.5	3.2
η^4-$[CH_3CH{=}CHC(O)CH_3]Cr(CO)_4$	1.049	1.487	0.933	1.090	0.972	114.0	122.3	123.6	119.4	9.1
η^4-$[CH_3CH{=}CHC(O)CH_3]Mo(CO)_4$	1.038	1.563	0.881	1.741	0.970	114.9	116.2	118.6	121.3	11.7
η^4-$[CH_3CH{=}CHC(O)CH_3]W(CO)_4$	1.061	1.241	0.886	1.642	1.036	124.0	130.8	126.1	115.4	73

Complex	Interatomic distance, Å				
	C^1–C^2	C^2–O	C^2–C^3	C^3–C^4	C^4–C^5
–	1.506	1.219	1.485	1.336	1.481
η^2-$[CH_3CH{=}CHC(O)CH_3]Fe(CO)_4$	1.516	1.263	1.510	1.521	1.523
η^2-$[CH_3CH{=}CHC(O)CH_3]Cr(CO)_5$	1.507	1.238	1.506	1.484	1.541
η^2-$[CH_3CH{=}CHC(O)CH_3]Mo(CO)_5$	1.508	1.233	1.509	1.390	1.524
η^2-$[CH_3CH{=}CHC(O)CH_3]W(CO)_5$	1.531	1.233	1.501	1.370	1.510
η^4-$[CH_3CH{=}CHC(O)CH_3]Fe(CO)_3$	1.522	1.357	1.467	1.518	1.522
η^4-$[CH_3CH{=}CHC(O)CH_3]Cr(CO)_4$	1.516	1.355	1.390	1.510	1.538
η^4-$[CH_3CH{=}CHC(O)CH_3]Mo(CO)_4$	1.533	1.248	1.487	1.387	1.524
η^4-$[CH_3CH{=}CHC(O)CH_3]W(CO)_4$	1.463	1.264	1.536	1.406	1.566

tion of conjugation between the double bonds in the α-enone.

The changes in the geometric and electronic structure of the α-enone on η^4 coordination are much more difficult to interpret. The length of the double bond increases, especially in the Fe (1.518 Å) and Cr (1.510 Å) complexes; in the W (1.406 Å) and Mo (1.387 Å) complexes this effect is considerably less pronounced. The bond orders also decrease, and the C–C and C–O bonds in the enone η^4-coordinated to Fe and W can be regarded as single bonds. For the Cr and Mo η^4 complexes, the order of the C=C bond is close to 1.5. Thus, in the η^4 complexes the order of the C=C bond is lower than in the η^2 complexes. The order of the C=O bond also decreases, especially in the Fe and Cr complexes. As in the case of η^2 coordination, the planarity of the C=C–C=O fragment is distorted: The C=C–C=O torsion angle varies from 3° to 73°, monotonically increasing with increasing radius of the metal atom. That is, in the η^4 complexes with Mo and W the α-enone molecule significantly changes its geometry to provide binding with the metal center via both double bonds.

Changes occurring in the geometric and electronic structure of η^4-coordinated 3-penten-2-one as compared to the free ligand suggest distortion of the conjugation between the double bonds. Thus, we can conclude that the main factor responsible for changes in the reactivity of α-enones at π coordination [2–4] is distortion of the conjugation in the heterodiene.

To check this assumption, we estimated the energy differences between the conformations of 3-penten-2-one in the free state and in the complex. We found that on coordination the enthalpy of formation of the enone increases, with the destabilization varying within 9–67 kJ mol^{-1}; this fact unambiguously indicates that the energy gain due to conjugation of the double bonds is lost.

For η^2 complexes the destabilization energy decreases, and for the η^4 complexes increases with increasing radius of the metal. This fact suggests that the most significant changes in the reactivity of heterodienes at η^2 and η^4 coordination should be observed in the case of metal atoms of small and large radius, respectively.

EXPERIMENTAL

The IR spectra were taken on a Specord M-80 spectrophotometer (mulls in mineral oil). The ^{1}H NMR spectra were recorded on Varian Unity-300 (299.94 MHz), Bruker-100 (100 MHz), and Bruker Gemini-200 (199.827 MHz) spectrometers at 25°C in C_6D_6, $CDCl_3$, and CD_3OD; the chemical shifts were determined relative to the residual proton signals of the deuterated solvents. The solution concentrations were 0.7–1.5 wt %. The ^{13}C NMR spectra were taken on a Varian Unity-300 spectrometer (75.4 MHz); the chemical shifts were determined relative to the $CDCl_3$ signals. Calculations by the GAUSSIAN 94 program [6] were performed in the Institute of Organic and Physical Chemistry, Russian Academy of Sciences (Moscow).

All experiments were performed in an argon atmosphere.

η^2-(4-Methyl-3-penten-2-one)pentacarbonylchromium(0). To a solution of 0.56 ml of 4-methyl-3-penten-2-one in 7 ml of THF, we added 1 g of $Cr(CO)_6$. The mixture was irradiated with UV light from a highpressure mercury lamp for 8 h. The colorless crystalline product that precipitated on cooling was filtered off and washed with hexane; yield 35%, mp 172–176°C (dec.). IR spectrum, ν, cm^{-1}: 1560 (coordinated C=C bond), 1720 (C=O bond in 4-methyl-3-penten-2-one, not involved in coordination), 1990, 1970, 1940, 1920, 1900 (coordinated CO molecules). ^{1}H NMR spectrum, δ, ppm: 3.86 (C=CH bond coordinated to Cr). ^{13}C NMR spectrum, δ_C, ppm: 191, 200 (coordinated CO molecules), 63, 85 (coordinated C=C bond).

η^2-(4-Methyl-3-penten-2-one)pentacarbonylmolybdenum(0) was prepared similarly from 0.56 ml of 4-methyl-3-penten-2-one in 7.0 ml of THF and 1 g of $Mo(CO)_6$. Yellowish substance, yield 42%, mp 168–171°C (dec.). IR spectrum, ν, cm^{-1}: 1555 (coordinated C=C bond), 1720 (C=O bond in 4-methyl-3-penten-2-one, not involved in coordination), 1995, 1980, 1960, 1930, 1910 (coordinated CO molecules). ^{1}H NMR spectrum, δ, ppm: 3.74 (C=CH bond coordinated to Mo). ^{13}C NMR spectrum, δ_C, ppm: 195, 207 (coordinated CO molecules), 68, 80 (coordinated C=C bond).

η^4-(4-Methyl-3-penten-2-one)tetracarbonyltungsten(0). A mixture of 1 g of $Mo(CO)_6$, 6 ml of acetonitrile, and 0.56 ml of 4-methyl-3-penten-2-one was refluxed under argon for 2 h. The resulting light yellow crystalline precipitate was filtered off and washed with hexane; yield 68%, mp 173–177°C (dec.). IR spectrum, ν, cm^{-1}: 1575 (coordinated C=C bond), 1700 (coordinated C=O bond in 4-methyl-3-penten-2-one), 1990, 1970, 1920, 1900 (coordinated CO molecules). ^{1}H NMR spectrum, δ, ppm: 3.45 (C=CH bond coordinated to molybdenum). ^{13}C NMR spectrum, δ_C, ppm: 196 (coordinated CO molecules), 75, 93 (coordinated C=C bond).

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