

## Electronic absorption spectra of molybdenum(0) bisarene complexes, $(\eta^6\text{-Arene})_2\text{Mo}^0$

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### Abstract

The UV and visible absorption spectra of  $(\eta^6\text{-Arene})_2\text{Mo}^0$  (Arene = benzene (I), toluene (II), *m*-xylene (III), mesitylene (IV)) in the vapor phase and in the pentane solution have been investigated. Rydberg series converging to the ionization limit have been found in the spectra of vaporous complexes. The sharpest Rydberg bands correspond to the transitions  $4d(a_{1g}) \rightarrow Rnp(e_{1u})$  and  $4d(a_{1g}) \rightarrow Rnp(a_{2u})$ . The band arising from the  $4d(a_{1g}) \rightarrow R5s(a_{1g})$  Rydberg transition has been found in the vapor-phase spectra of the II and III complexes. Some weak bands in the vapor-phase spectra have been tentatively assigned to the  $4d(a_{1g}) \rightarrow Rnd$  transitions. Rydberg bands disappeared from the spectra on going from vapor phase to pentane solution. The ionization limits for I–IV are  $5.525 \pm 0.010$ ,  $5.375 \pm 0.010$ ,  $5.250 \pm 0.010$ ,  $5.137 \pm 0.010$  eV, respectively. These limits correspond to the ionization from the highest occupied molecular orbital  $4d(a_{1g})$  and are consistent with the first ionization potentials determined by photoelectron spectroscopy for the complexes I, II, and IV.

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### Introduction

The electronic absorption spectra of bisarene complexes of molybdenum(0) have received little attention. Only a few reports on the study of the  $(\eta^6\text{-Arene})_2\text{Mo}^0$  absorption spectra in the visible and near-UV region have appeared [1–5]. The solution spectra of these compounds were recorded by Fischer and Fritz [1] and by Andrews and Ozin [5], but the data published in 1961 [1] are at variance with data recently obtained [5]. The spectra of the products formed by the reaction of Mo atoms with the polymers containing phenyl groups have been investigated previously. Up to now the spectra of vaporous  $(\eta^6\text{-Arene})_2\text{Mo}^0$  complexes have not been obtained. On the other hand, we recently investigated the electronic absorption spectra of bis( $\eta^6$ -arene)chromium(0) and bis( $\eta^6$ -arene)vanadium(0) in the vapor phase [6–9]. It was found that Rydberg bands were present in these vapor-phase

spectra. Such bands were absent in the spectra of the  $(\eta^6\text{-Arene})_2\text{Cr}^0$  and  $(\eta^6\text{-Arene})_2\text{V}^0$  solutions. The disappearance of Rydberg bands, on going from the vapor-phase spectra to the solution ones, is caused by the scattering of a Rydberg electron in media with low electron mobility [10]. Since the electronic structures of  $(\eta^6\text{-Arene})_2\text{Cr}^0$  and  $(\eta^6\text{-Arene})_2\text{Mo}^0$  are similar [11,12], it was expected that Rydberg bands would be observed in the visible and near-UV vapor-phase absorption spectra of molybdenum(0) bisarene complexes. So we decided to investigate the electronic absorption spectra of  $(\eta^6\text{-Arene})_2\text{Mo}^0$  in the vapor phase and to compare them with the solution spectra as well as with the spectra of  $(\eta^6\text{-Arene})_2\text{Cr}^0$  [6-9].

## Experimental

The  $(\eta^6\text{-Arene})_2\text{Mo}^0$  complexes (Arene =  $\text{C}_6\text{H}_6$  (I),  $\text{CH}_3\text{C}_6\text{H}_5$  (II), 1,3- $(\text{CH}_3)_2\text{C}_6\text{H}_4$  (III), 1,3,5- $(\text{CH}_3)_3\text{C}_6\text{H}_3$  (IV)) were prepared by co-condensation of the molybdenum atoms with the vapors of the organic ligands at  $-196^\circ\text{C}$  [13]. All organometallic compounds obtained were purified by repeated vacuum sublimation.

The vapor-phase spectra of the I-IV complexes were recorded in a vacuum cell with a "Specord UV-Vis" (Carl Zeiss, Jena, G.D.R.) spectrometer at  $80\text{--}150^\circ\text{C}$ . For comparison, the absorption spectra of the complexes in n-pentane solution were recorded on the same spectrometer in the vacuum cell at room temperature. Errors in determination of the band positions were  $50\text{--}80\text{ cm}^{-1}$  for narrow bands and  $100\text{--}250\text{ cm}^{-1}$  for broad bands and shoulders.

## Results and discussion

The electronic absorption spectra of our  $(\eta^6\text{-Arene})_2\text{Mo}^0$  complexes recorded with pentane solutions are in good agreement with the data of Andrews and Ozin [5]. The solution spectrum of II is given in Fig. 1. The spectra of other molybdenum(0) bisarene complexes are similar. The solution spectra show a very strong peak A, a less intense band B, and a system of very weak bands, C (Fig. 1). The solution spectra resemble those of  $(\eta^6\text{-Arene})_2\text{Cr}^0$  [8,14,15], since the electronic

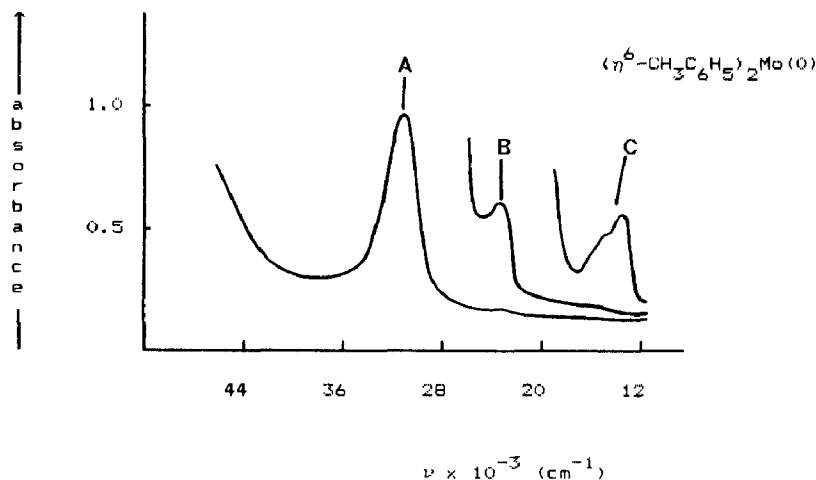


Fig. 1. Electronic absorption spectrum of II in pentane solution.

Table 1

Band maxima ( $\text{cm}^{-1}$ ) in the electronic spectra of the complexes I–IV in pentane solution

Band	I	II	III	IV
A	32000	31150	30350	30150
B	25530	25270	25000	24870
C	–	16270 <sup>a</sup>	16120 <sup>a</sup>	–
	–	15370 <sup>a</sup>	15170 <sup>a</sup>	15570 <sup>a</sup>
	–	13670	13650	13830

<sup>a</sup> Shoulder.

and molecular structure of molybdenum(0) and chromium(0) bisarene complexes are similar. The electronic configuration of bis( $\eta^6$ -benzene)molybdenum(0) in the ground state is  $^1A_{1g} \dots [\pi(e_{1g})]^4 [\pi(e_{1u})]^4 [4d(e_{2g})]^4 [4d(a_{1g})]^2 [4d(e_{1g})]^0 [\pi(e_{2u})]^0 \dots$  [11,16] (we have used the irreducible representations of  $D_{6h}$  point group to designate the symmetry of the ( $\eta^6$ -Arene) $_2\text{Mo}^0$  molecular orbitals (MO's) and electronic states). The peak A (Fig. 1) may be assigned to the symmetry allowed  $4d(e_{2g}) \rightarrow \pi(e_{2u})$  transition by analogy with ( $\eta^6$ -C<sub>6</sub>H<sub>6</sub>)Cr<sup>0</sup> [17]. The band B probably corresponds to a symmetry-forbidden transition whereas the system C probably arises from spin-forbidden transitions. It should be noted that the weak absorption bands in the solution spectra of I–IV are better resolved than those of ( $\eta^6$ -Arene) $_2\text{Cr}^0$  [8,14,15]. The frequencies of the bands A, B, and C are listed in Table 1. The introduction of methyl substituents into the benzene rings of ( $\eta^6$ -C<sub>6</sub>H<sub>6</sub>) $_2\text{Mo}^0$  most strongly influences the position of the A band (Table 1). The bands of system C undergo the smallest shifts.

The electronic absorption spectra of ( $\eta^6$ -Arene) $_2\text{Mo}^0$  in the vapor phase (Figs. 2–5) differ strongly from those of the solutions. The B and C bands (Fig. 1) were not observed in the vapor-phase spectra because of their low intensity. The maxima of the peaks A in the spectra of vaporous I–IV are at 32300, 31450, 30600 and 29900  $\text{cm}^{-1}$ , respectively. The data listed in Table 1 show that in the most cases the A band maximum undergoes a small red shift on going from the vapor-phase

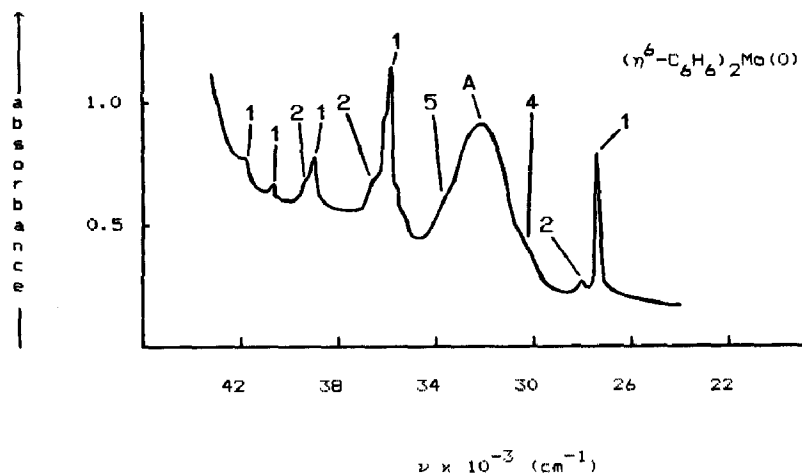


Fig. 2. Vapor-phase electronic absorption spectrum of I.

spectrum to the solution spectrum. Such behaviour is typical for the bands corresponding to valence-shell transitions [10]. However, the vapor-phase spectra show the comparatively narrow bands which disappear on going to the solution spectra (designated by the Arab numerals in Figs. 2–5). It was shown previously [6–9] that such disappearance of absorption bands may be indicative of their Rydberg origin. Indeed, we have established that bands 1 (Figs. 2–5) represent a Rydberg series converging to the ionization limit. The frequencies of these bands are given by the well-known Rydberg formula

$$\nu_n = E - R/(n - \delta)^2 \quad (\text{eq. 1})$$

where  $E$  is the ionization limit,  $R$  the Rydberg constant,  $n$  is a principle quantum number,  $\delta$  the quantum defect.

The band 1 frequencies observed and those calculated from eq. 1 are listed in Table 2. The calculation was carried out by a computer program which permitted us to select the  $E$  and  $\delta$  parameters such that the difference between the calculated and experimental frequencies was minimal. It is seen from the Table 2 that this difference is smaller than the error inherent in the determination of band positions (except for that of bands 1 with the longest wavelength). The calculated frequency for IV does not coincide with that observed for the second member of the series. The deviation of the positions of the first members of the Rydberg series from that determined by eq. 1 is typical for polyatomic molecules [10].

The calculated ionization limits (Table 2) are in good agreement with the first ionization potentials ( $IP$ ) determined from the photoelectron spectra for I, II and IV [11,12]. Thus, the  $E$  values (Table 2) represent the first  $IP$  of I–IV. Hence, the presence of the Rydberg series allows the first  $IP$  of the  $(\eta^6\text{-Arene})_2\text{Mo}^0$  complexes to be determined from the vapor-phase electronic absorption spectra. Thus, the first ionization potential of bis( $\eta^6\text{-}m\text{-xylene}$ )molybdenum(0) ( $5.250 \pm 0.010$  eV) has been determined for the first time in this work.

The first  $IP$  of  $(\eta^6\text{-Arene})\text{Mo}^0$  is assigned to the ionization from the  $4d(a_{1g})$  orbital. Consequently, the bands 1 (Figs. 2–5) correspond to the transitions from this MO. By analogy  $(\eta^6\text{-Arene})_2\text{Cr}^0$  and  $(\eta^6\text{-Arene})_2\text{V}^0$  [6–9], these bands can be

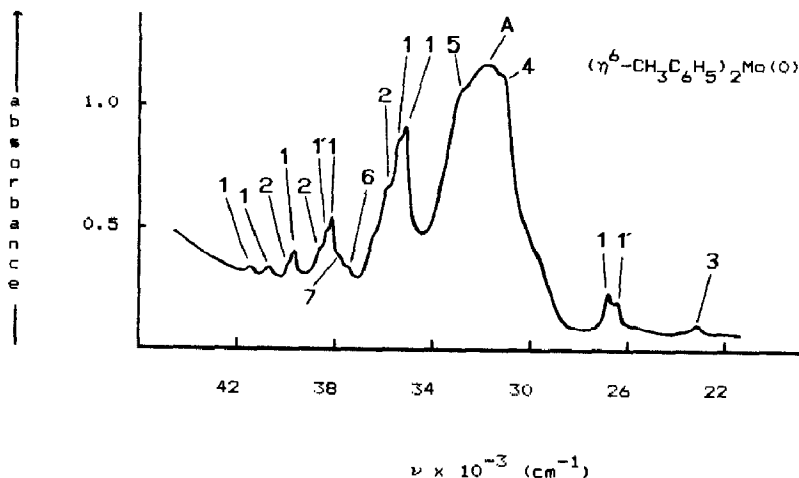


Fig. 3. Vapor-phase electronic absorption spectrum of II.

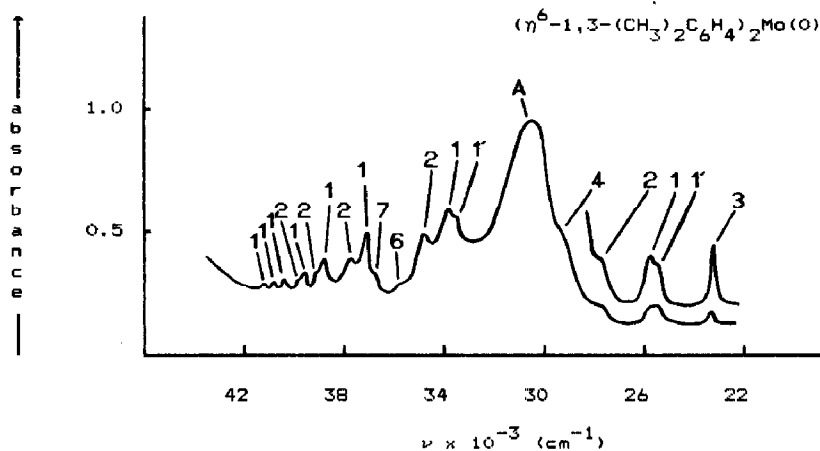


Fig. 4. Vapor-phase electronic absorption spectrum of III.

Table 2

Calculated (eq. 1) and observed  $\nu(\text{cm}^{-1})$  frequencies of bands 1, 1', 2 in the electronic spectra of I-IV complexes (Figs. 2-5).  $E$  (eV),  $n$ ,  $\delta$  (see eq. 1) and the observed  $R5p$  term values  $T(R5p)$  ( $\text{cm}^{-1}$ ) are presented. The values of the first ionization potentials  $IP_{a1g}$  (eV) determined by the photoelectron spectroscopy method [11] are also given

	I		II		III		IV	
	$\nu_{\text{calc}}$	$\nu_{\text{obs}}$	$\nu_{\text{calc}}$	$\nu_{\text{obs}}$	$\nu_{\text{calc}}$	$\nu_{\text{obs}}$	$\nu_{\text{calc}}$	$\nu_{\text{obs}}$
<b>Bands 1 (Figs 2-5)</b>								
$n$								
5	28200	27330	27120	26490	25970	25730	25920	25970
6	36040	36050	34880	34870	33820	33800	33240	31760
7	39350	39350	38160	38170	37120	37150	36380	36380
8	41040	41030	39850	39860	38820	38800	38010	37940
9	42030	42030 <sup>a</sup>	40830	40830	39800	39770	38960	38950
10	42660	-	41450	41430	40430	40430	39560	39560
11	43070	-	41870	-	40840	40870	39970	40030
12	43370	-	42160	-	41140	41140	40260	40300
$\delta$		2.41		2.40		2.41		2.34
$T(R5p)$		17230		16860		16600		15460
<b>Bands 1' (Figs. 2-5)</b>								
$n$								
5	-	-	27370	26250	25050	25530 <sup>a</sup>	-	-
6	-	-	34980	35100 <sup>a</sup>	33500	33500 <sup>a</sup>	-	-
7	-	-	38210	38330 <sup>a</sup>	36960	-	-	-
$\delta$				2.38		2.48		
$T(R5p)$				17100		16800		
<b>Bands 2 (Figs. 2-5)</b>								
$n$								
5	29630	28070?	28410	-	28130	27630 <sup>a</sup>	27030	26750 <sup>a</sup>
6	36600	36640 <sup>a</sup>	35380	35500 <sup>a</sup>	34690	34700	33670	33750
7	39620	39530 <sup>a</sup>	38410	38570 <sup>a</sup>	37570	37610	36590	36750 <sup>a</sup>
8	41190	-	39990	40060 <sup>a</sup>	39090	39130 <sup>a</sup>	38130	38200 <sup>a</sup>
9	42120	-	40910	-	39990	39930 <sup>a</sup>	39030	-
$\delta$		2.29		2.29		2.22		2.24
$T(R5p)$		16490		-		14700		14680
$E$	$5.525 \pm 0.010$		$5.375 \pm 0.010$		$5.250 \pm 0.010$		$5.137 \pm 0.010$	
$IP_{a1g}$	5.52 [11]		5.32 [11]		-		5.13 [11]	

<sup>a</sup> Shoulder.

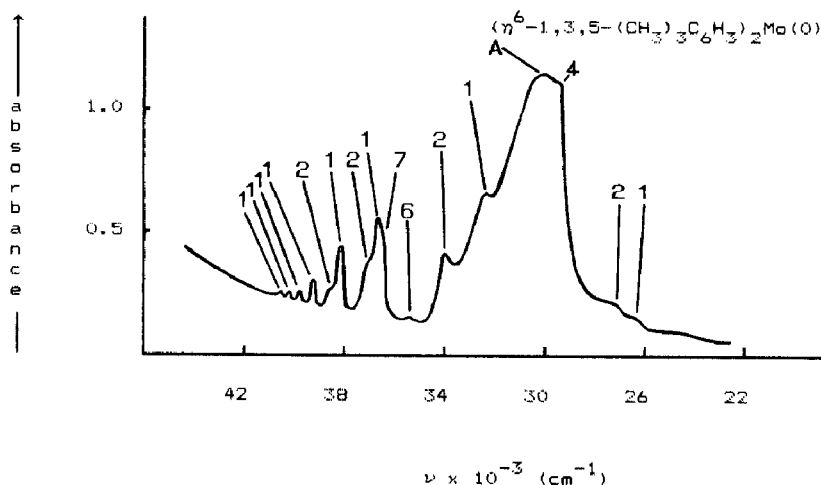


Fig. 5. Vapor-phase electronic absorption spectrum of IV.

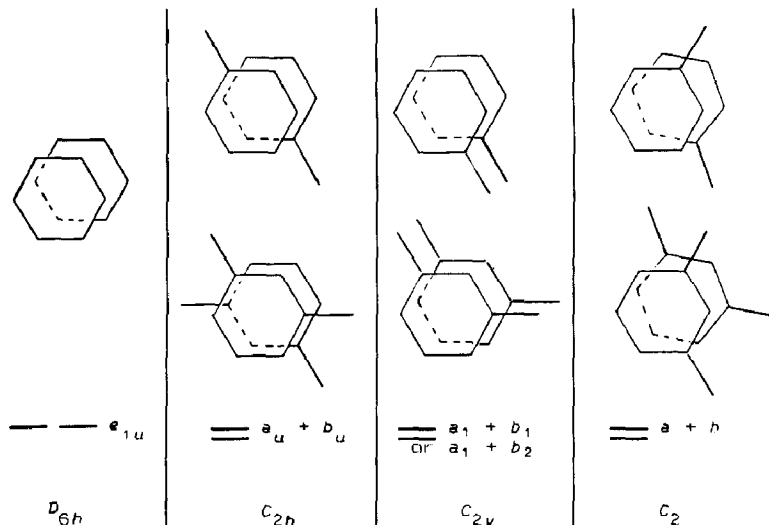
unambiguously assigned to the symmetry-allowed  $4d(a_{1g}) \rightarrow Rnp$  transitions. For the second member of this series in the  $(\eta^6\text{-C}_6\text{H}_6)_2\text{Mo}^0$  spectrum (Fig. 2), a vibrational structure with bands separated by  $\sim 250\text{ cm}^{-1}$  is observed. This value obviously corresponds to the frequency of the symmetrical metal-ring stretching, as in the case of  $(\eta^6\text{-C}_6\text{H}_6)_2\text{Cr}^0$  [6].

The principle quantum number, which corresponds to the metal  $d$  orbital forming the nonbonding highest occupied  $a_{1g}$  MO of the bisarene complex, increases by 1 on going from  $(\eta^6\text{-Arene})_2\text{Cr}^0$  to  $(\eta^6\text{-Arene})_2\text{Mo}^0$ . This should result in increase in the quantum defect for Rydberg transitions from the  $a_{1g}$  orbital by  $\sim 1$  [10]. A comparison of the data in Table 2 with those previously published [7–9] shows that  $\delta$  does increase by  $\sim 1$  on going from bis( $\eta^6$ -arene)chromium(0) to bis( $\eta^6$ -arene)molybdenum(0) (the quantum defects for the series of bands 1 in the spectra of  $(\eta^6\text{-Arene})_2\text{Cr}^0$  (Arene =  $\text{C}_6\text{H}_6$ ,  $\text{CH}_3\text{C}_6\text{H}_5$ ,  $1,3\text{-(CH}_3)_2\text{C}_6\text{H}_4$ , and  $1,3,5\text{-(CH}_3)_3\text{C}_6\text{H}_3$ ) are 1.35, 1.40, 1.40, and 1.60, respectively [7–9]). The first members of the Rydberg series are usually characterized by the term values ( $T_n = R/(n - \delta)^2$ ), i.e. the difference between the ionization limit and Rydberg band frequency [10]. Since the change in the  $n$  and  $\delta$  values on going from  $\text{Cr}^0$  to  $\text{Mo}^0$  complex is nearly the same, the term values for the first member of the Rydberg series in the  $(\eta^6\text{-Arene})_2\text{Cr}^0$  and  $(\eta^6\text{-Arene})_2\text{Mo}^0$  spectra should be similar. Indeed, the term values for longest wavelength in bands 1 (the  $4d(a_{1g}) \rightarrow R5p$  transition) in the spectra of I–IV (Table 2) are very close to those for the  $3d(a_{1g}) \rightarrow R4p$  transition in the  $(\eta^6\text{-Arene})_2\text{Cr}^0$  spectra ( $17290$ ,  $17150$ ,  $16590$ , and  $14910\text{ cm}^{-1}$  for Arene =  $\text{C}_6\text{H}_6$ ,  $\text{CH}_3\text{C}_6\text{H}_5$ ,  $1,3\text{-(CH}_3)_2\text{C}_6\text{H}_4$ , and  $1,3,5\text{-(CH}_3)_3\text{C}_6\text{H}_3$ , respectively [9]).

The  $np$  Rydberg orbitals are split into MO's of the  $a_{2u}$  and  $e_{1u}$  type under a  $D_{6h}$  symmetry group. This should result in the existence of two  $4d(a_{1g}) \rightarrow Rnp$  Rydberg series in the  $(\eta^6\text{-Arene})_2\text{Mo}^0$  spectra. The second series can be composed of the bands 2 (Figs. 2–5). The frequencies of these bands are described by the Rydberg formula when the  $E$  values obtained for the bands 1 (Table 2) are used. The differences between the quantum defects for bands 1 and 2 (Table 2) are close to those for the  $np(\pi_u)$  and  $np(\sigma_u)$  Rydberg series in the  $\text{CO}_2$  absorption spectrum

[18]. So it can be suggested that for  $(\eta^6\text{-C}_6\text{H}_6)\text{Mo}^0$  the bands 1 correspond to the  $4d(a_{1g}) \rightarrow Rnp(e_{1u})$  transitions while the bands 2 arise from the  $4d(a_{1g}) \rightarrow Rnp(a_{2u})$  transitions.

The molecular symmetry is reduced from  $D_{6h}$  to  $C_{2h}$ ,  $C_{2v}$  or  $C_2$  on going from I to II and III. This reduction in symmetry removes the degeneracy of the  $np(e_{1u})$  Rydberg orbitals:



As a result of this splitting, the addition peaks may appear near the bands 1. Indeed, bands 1' adjoining the bands 1 are observed in the spectra of II and III (Figs. 3 and 4). The bands 1' for II form the Rydberg series converging to the first  $IP$  (Table 2). Similar bands were clearly seen in the spectra of vaporous bis( $\eta^6$ -*o*-xylene)chromium(0) and bis( $\eta^6$ -*m*-xylene)chromium(0) [7-9]. The appearance of the bands 1' in the spectra of II and III confirms the assignment of the bands 1 in the  $(\eta^6\text{-C}_6\text{H}_6)_2\text{Mo}^0$  spectrum to the  $4d(a_{1g}) \rightarrow Rnp(e_{1u})$  transitions. Thus, the bands 1, 1' in the spectra of II, III (Figs. 3 and 4) correspond to the bands 1 (Fig. 2) which are split because of the reduction in molecular symmetry. However, the degeneracy of the  $Rnp(e_{1u})$  orbitals remains in bis( $\eta^6$ -mesitylene)molybdenum(0) (point group  $D_{3d}$ ,  $D_{3h}$  or  $D_3$ ). In accord with this fact, bands 1' are not observed in the spectrum of IV (Fig. 5).

The long-wave bands 3 appear in the vapor-phase spectra on going from I to II and III (Figs. 2-4). These bands are absent in the solution spectra. The observed frequencies of the bands 3 and the calculated values of  $(n - \delta)$  are given in Table 3. The differences between the  $E$  values and the band 3 frequencies of II and III are 20100 and 19130  $\text{cm}^{-1}$ , respectively. The bands characterized by similar term values were observed in the vapor-phase spectra of bis( $\eta^6$ -toluene)chromium(0) and bis( $\eta^6$ -*m*-xylene)chromium(0) [7-9]. For  $(\eta^6\text{-Arene})_2\text{Mo}^0$ , the  $4d(a_{1g}) \rightarrow R5s(a_{1g})$  Rydberg transition has the longest wavelength. The bands 3 (Figs. 3 and 4) can be unambiguously assigned to this transition. The  $4d(a_{1g}) \rightarrow R5s(a_{1g})$  transition is symmetry-forbidden for I and IV, but becomes allowed when the symmetry is reduced to  $C_{2v}$  or  $C_2$ . The bands 3 (Figs. 3 and 4) and corresponding peaks in the spectra of  $(\eta^6\text{-Arene})_2\text{Cr}^0$  [7-9] clearly have the longest wavelengths of the known

Table 3

The frequencies of bands 3–7 ( $\text{cm}^{-1}$ ) in the electronic spectra of I–IV (Figs. 2–5). The values of  $(n - \delta)$  calculated from  $E$  (Table 2) are given in parentheses

Band	I	II	III	IV
3	–	23250 (2.34)	23200 (2.40)	–
4	31370 (2.88)	31140 (3.00)	29700 (2.95)	29470 (3.03)
5	33610 (3.17)	32430 (3.17)	–	–
6	–	37290 (4.26)	35660 (4.06)	35050 (4.15)
7	–	37850 (4.47)	36430 (4.31)	35950 (4.47)

Rydberg bands in the spectra of polyatomic molecules, which is due to the very low ionization potentials of  $(\eta^6\text{-Arene})_2\text{Cr}^0$  and  $(\eta^6\text{-Arene})_2\text{Mo}^0$ .

In addition to the bands 1, 1', 2, and 3, there are the weak features 4–7 in the spectra of I–IV (Figs. 2–5). Their frequencies and the relevant  $(n - \delta)$  values are given in Table 3, which shows that the bands of the same name have similar  $(n - \delta)$  values. This probably indicates that the Rydberg transitions from  $4d(a_{1g})$  orbital are responsible for the bands 4–7 since the  $(n - \delta)$  values (Table 3) were calculated from the ionization limits listed in Table 1. It seems that the assignment of bands 4 and 5 to the  $4d(a_{1g}) \rightarrow R5d$  transitions and bands 6 and 7 to the  $4d(a_{1g}) \rightarrow R6d$  transitions is the most probable. Similar bands were observed in the spectra of  $(\eta^6\text{-Arene})_2\text{Cr}^0$  and  $(\eta^6\text{-Arene})_2\text{V}^0$  [7–9].

Thus, a study of the  $(\eta^6\text{-Arene})_2\text{Mo}^0$  electronic absorption spectra in the vapor phase and in pentane solution has shown that Rydberg transitions from the highest occupied  $4d(a_{1g})$  MO make a significant contribution to the vapor-phase spectra. A sharpness of the corresponding Rydberg bands is due to the nonbonding character of  $4d(a_{1g})$  orbital. Rydberg transitions from the  $4d(e_{2g})$  orbital which is bonding [16,19] do not give sharp bands in the  $(\eta^6\text{-Arene})_2\text{Mo}^0$  spectra. There is a marked similarity between the Rydberg patterns in the vapor-phase spectra of  $(\eta^6\text{-Arene})_2\text{Mo}^0$  and those of  $(\eta^6\text{-Arene})_2\text{Cr}^0$ , which is clearly attributable to their very similar electronic structures.

The existence of the  $4d(a_{1g}) \rightarrow Rnp$  Rydberg series permits the first ionization potential of bis( $\eta^6\text{-arene}$ )molybdenum(0) complexes ( $IP_{a_{1g}}$ ) to be readily determined. The  $IP_{a_{1g}}$  values calculated as the convergence limits of the  $np$  Rydberg series are more accurate than those obtained from the photoelectron spectra (for some  $(\eta^6\text{-Arene})_2\text{Cr}^0$  complexes, the  $IP_{a_{1g}}$  values determined by the photoelectron spectroscopy [11,12,20,21] differ by 0.05–0.07 eV).

The regression analysis of the ionization limits we have determined here (Table 2) shows that there is a linear correlation between the  $IP_{a_{1g}}$  of  $(\eta^6\text{-Arene})_2\text{Mo}^0$  and the number of methyl groups introduced into each benzene ring ( $m_{\text{Me}} = 0, 1, 2, 3$ ):

$$IP_{a_{1g}} (\text{eV}) = (5.515 \pm 0.012) - (0.129 \pm 0.006)m_{\text{Me}}; r = 0.998 \quad (2)$$

The  $IP_{a_{1g}}$  values for the derivatives of bis( $\eta^6\text{-benzene}$ )molybdenum(0) with tetra-, penta-, and hexamethylsubstituted ligands can be estimated by use of (eq. 2). These values should be  $\sim 5.00$ ,  $\sim 4.87$ , and  $\sim 4.74$  eV, respectively. It should be noted, however, that this estimation neglects the mutual influence of methyl groups. This influence can occur in the polysubstituted derivatives of  $(\eta^6\text{-C}_6\text{H}_6)_2\text{Mo}^0$ . It is seen from Table 2 that the introduction of one  $\text{CH}_3$  group into each ring of I causes



slightly stronger change in  $E$  than the introduction of a methyl substituent into each ring of III. This effect may intensify on going to the tetra-, penta-, and hexamethylsubstituted ligands. Hence, the extrapolation of (eq. 2) probably gives depressed values of  $IP_{a_{1g}}$ .

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### References

- 1 E.O. Fischer and H.P. Fritz, *Angew. Chem.*, 73 (1961) 355.
- 2 C.G. Francis and P.L. Timms, *J. Chem. Soc., Dalton Trans.* (1980) 1401.
- 3 C.G. Francis, H. Huber and G.A. Ozin, *Inorg. Chem.*, 19 (1980) 219.
- 4 G.A. Ozin and C.G. Francis, *J. Mol. Struct.*, 59 (1980) 55.
- 5 M.P. Andrews and G.A. Ozin, *Inorg. Chem.*, 25 (1986) 2587.
- 6 G.A. Domrachev, S.Yu. Ketkov and G.A. Razuvaev, *J. Organomet. Chem.*, 328 (1987) 341.
- 7 S.Yu. Ketkov, G.A. Domrachev and G.A. Razuvaev, *Metalloorg. Khim.*, 1 (1988) 40 (in Russian).
- 8 S.Yu. Ketkov, *Electronic Absorption Spectra of Chromium and Vanadium Bisarene Complexes*, Ph.D. Thesis, Moscow, 1988.
- 9 S.Yu. Ketkov, G.A. Domrachev and G.A. Razuvaev, *J. Mol. Struct.*, 195 (1989) 175.
- 10 M.B. Robin, *Higher Excited States of Polyatomic Molecules*, Vol. 1, Academic Press, New York, 1974, 374 pp.
- 11 S. Evans, J.C. Green, S.E. Jackson and B. Higginson, *J. Chem. Soc., Dalton Trans.*, (1974) 304.
- 12 J.C. Green, *Struct. Bond. (Berlin)*, 43 (1981) 37.
- 13 F.W.S. Benfield, M.L.H. Green, J.S. Ogden and D. Young, *J. Chem. Soc., Chem. Commun.*, (1973) 866.
- 14 R.D. Feltham, *J. Inorg. Nucl. Chem.*, 16 (1961) 197.
- 15 G.A. Domrachev, S.Yu. Ketkov and Yu.A. Shevelev, *Koord. Khim. (Russ.)*, 13 (1987) 1633.
- 16 D.M.P. Mingos, in: G. Wilkinson, F.G.A. Stone and E.W. Abel (Eds), *Comprehensive Organometallic Chemistry*, Vol. 3, Oxford, Pergamon Press, 1982, p. 1.
- 17 J. Weber, M. Geoffroy, A. Goursot and E. Penigault, *J. Am. Chem. Soc.*, 100 (1978) 3995.
- 18 C. Cossart-Magos, M. Jungen and F. Launay, *Mol. Phys.*, 61 (1987) 1077.
- 19 D.W. Clack and K.D. Warren, *Struct. Bond. (Berlin)*, 39 (1980) 1.
- 20 M.F. Guest, I.H. Hillier, B.R. Higginson and D.R. Lloyd, *Mol. Phys.*, 29 (1975) 113.
- 21 D.E. Cabelli, A.H. Cowley and J.J. Lagowski, *Inorg. Chim. Acta*, 57 (1982) 195.