this conversion), from which subsequent H_2 elimination affords the more stable iridium(I) complexes **7** and **8** (Scheme III).

The thermal reaction of $Ir^{III}H_2[C_6H_2(CH_2NMe_2)_3$-2,4,6](COD) (**15**), which also proceeds via C(aryl)–H reductive elimination, affords the intermediate IrH(COD)[1,3,5-$(Me_2NCH_2)_3C_6H_3$] (cf. **17a**/**b**). All three aryl C–H bonds are now equivalent and equally unfavorable for "re-metalation" due to the steric hindrance of the three bulky CH_2NMe_2 groups. Since "re-metalation" would only result in re-formation of the iridium(III) dihydride complex **15** (a reaction that is obviously thermodynamically unfavorable), the alternative pathway followed is dissociation of the neutral arene ligand 1,3,5-$(Me_2NCH_2)_3C_6H_3$ from the metal center.

Conclusions

Iridium(I) complexes of type $Ir^I[C_6H_2(CH_2NMe_2)$-2-R^1-4-R^2-6](COD) react with H_2 to form the unique octahedral iridium(III) dihydrides $Ir^{III}H_2[C_6H_2(CH_2NMe_2)$-2-$R^1$-4-$R^2$-6](COD), which display interesting reactivity patterns. From these reactions it can be concluded that, without altering the innermost ligand sphere of the metal center, intramolecular steric effects can drastically change the direction of H–H and C–H bond elimination/addition reactions in iridium(III) compounds. Whereas $Ir^{III}H_2$-$[C_6H_2(CH_2NMe_2)$-2-R^1-4-R^2-6](COD) complexes that have a proton as the R^2 group react further by simple H–H elimination, those where R^2 is a bulkier alkyl group react further by an exclusive C(aryl)–H reductive elimination process. Therefore, when discussing the electronic and thermodynamic factors of H–H and C–H bond activation, it is also important to take possible interligand repulsions into account.

Acknowledgment. Richard A. Nordemann and Miss Jacqueline M. A. Wouters are thanked for practical assistance. Professor K. Vrieze is thanked for helpful discussions.

Electronic Structure of Triple-Decker Sandwich Compounds with P_5, P_6, As_5, and C_nH_n as Middle Rings[†]

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Extended Hückel calculations on $CpNiCpNiCp^+$, $CpCoC_6H_6CoCp$, $CpCoC_7H_7CoCp$, $CpVC_6H_6VCp$, $C_6H_6CrC_6H_6CrC_6H_6$, $CpMoP_6MoCp$, $CpCrP_5CrCp$, and $CpMoAs_5MoCp$ ($Cp = \eta^5$-C_5H_5) have been carried out to find the relationship of the stability of the metal–ring combination with the number of valene electrons. The electron count varies from 34 electrons to 26 electrons depending on the magnitude of the interactions 4a–e. With the vanadium complex the e_2'' interaction, 4b, is substantial. With P_6, P_5 and As_5 ligands, the a_2'' interaction, 4e, also becomes very strong. $CpMoAs_5MoCp$ leads to a degenerate HOMO with three electrons leading to a distortion of the As_5 ring, with two long and three short As–As bonds. The isoelectronic P_5 compound does not have such a distortion as the HOMO is a nondegenerate MO with only one electron.

Triple-decker sandwiches, **1**, are formally obtained from metallocenes, **2**, by the additional sandwiching with a metal and a ring. The following metal and ring combinations are known among them: metal = V, Cr, Fe, Co, Ni, Mo, Pt; terminal ring = C_5H_5, C_6H_6, $C_2B_2SH_4$, $C_3B_2H_5$; middle ring = C_5H_5, C_6H_6, P_5, As_5, P_6, $C_2B_2SH_4$, $C_4B_2H_5$, $C_3B_2H_5$.[1-16] Table I lists these complexes with the number of valence electrons and the M–M distances wherever known. There are many interesting structural variations in these compounds. The M–M distance falls within the bonding range only with phosphorus and arsenic rings in the middle.[14-16] While most of the triple-decker sandwich compounds with C_nH_n, P_5, and P_6 as middle rings retain local C_n axis, the As_5 ring in $CpMoAs_5MoCp$ has a distorted geometry with two As–As bonds longer than the other three.[16] The structure appears as a combination of As_3 and As_2 as in **3**. The middle As in the As_3 group is farthest from the metals so that an η^4-description is often used for the As_5 ligand.

Table I. Currently Known Triple-Decker Sandwich Compounds with Metal–Metal Distances, Number of Valence Electrons, and References

compound	M–M dist[a]	no. of valence electrons	ref
(1) $CpNiCpNiCp^+$	3.580	34	1
(2) $CpCoC_6R_6CoCp$		34	3
(3) $CpVC_6R_6VCp$	3.400	26	2
(4) $C_6H_6CrC_6H_6CrC_6H_6$	3.338	30	4
(5) $CpFe(C_2B_2SR_4)FeCp$	3.236	30	6
(6) $(C_2B_2SR_4)Co(C_2B_2SR_4)Co(C_2B_2SR_4)$		30	7
(7) $CpM(C_3B_2R_5)M'Cp$			
(a) M = Ni, M′ = Ni	3.416	33	8
(b) M = Fe, M′ = Co	3.337	32	8
(c) M = Fe, M′ = Co	3.204	30	8
(d) M = Co, M′ = Co		31	8
(8) $CpCo(C_3B_2R_5)CoCp$	3.140	30	9
(9) $CpRh(C_4B_2R_6)RhCp^{2+}$	3.440	30	10
(10) $CpM(C_3B_2R_5)M'(C_3B_2R_5)$			
(a) M = Co, M′ = Pt		30	11
(b) M = Ni, M′ = Pt		31	11
(c) M = Co, M′ = Ni		30	11
(11) $(C_6H_5R)Fe(C_3B_2H_5)Ni(C_3B_2H_5)$		30	12, 13
(12) $CpMoP_6MoCp$	2.648	28	14
(13) $CpMoAs_5MoCp$	2.762	27	16
(14) $CpCrP_5CrCp$	2.728	27	15

[a] Distances in Å.

The number of electrons around the metals also varies considerably. If only the π-electrons of the ligands are included in the electron count, there are 26 electrons in the vanadium complex $C_5H_5VC_6H_6VC_5H_5$ and 34 electrons in the nickel complex $C_5H_5NiC_5H_5NiC_5H_5^+$. There are any number of complexes with intermediate electron counts of 28 and 30 (Table I). Several theoretical studies have

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[†] Dedicated to Professors P. T. Narasimhan and M. V. George, I. I. T. Kanpur, on their sixtieth birthdays.

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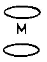
Table II. Calculated M-M Distances (Å) Using Average Metal-Ligand Distances (X = C, P, As)

compound	distances		
	M-X	X-X	M-M
(1) CoC_5H_5Co	2.19	1.40	3.675
(2) CoC_6H_6Co	2.19	1.40	3.368
(3) CoC_7H_7Co	2.19	1.40	2.969
(4) CoC_8H_8Co	2.19	1.40	2.409
(5) CrP_5Cr	2.29	2.17	2.720
(6) MoP_6Mo	2.54	2.17	2.648
(7) $MoAs_5Mo$	2.54	2.51	2.762

appeared on these triple-decker sandwich complexes. Hoffmann and co-workers gave a detailed description of the electronic structure of triple-decker sandwiches based on extended Hückel calculations on $CpNiCpNiCp^+$.[17] Complexes with 30 or 34 valence electrons were predicted to give stable closed-shell species. Nonempirical Fenske–Hall calculations on $C_5H_5VC_6H_6VC_5H_5$[18] gave an energy level ordering different from the general scheme based on the extended Hückel calculations on $C_5H_5NiC_5H_5NiC_5H_5^+$. Semiempirical INDO studies on triple-decker sandwiches with heterocyclic middle rings have been used to correlate electronic structure with reversible redox reactions and C–H bond activation possible with the $C_3B_2H_6$ ligand.[19] Extended Hückel calculation on bipyramidal skeletons[20] have been carried out to understand the variation in the electron counts in triple-decker sandwich compounds.

In this paper we compare the variations in the electronic structures of 1 as a function of the metal and the middle ring. A better understanding of (a) the requirements for M–M bonding and its consequences, (b) reasons for the distortion of As_5 as a middle ring, and (c) number of valence electrons required for stability will be sought in this study. Our analysis uses wave functions generated by using extended Hückel calculations[21,22] but relies on symmetry, electronegativity, and the extent of overlap of orbitals whenever possible.

1



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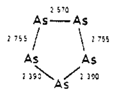

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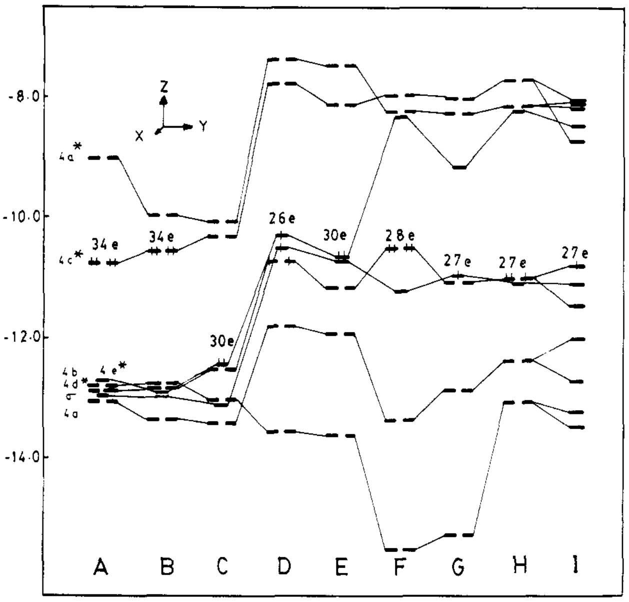

Figure 1. Correlation of the energy levels of the triple-decker sandwich compounds A, $CpNiCpNiCp^+$, B, $CpCoC_6H_6CoCp$, C, $CpCoC_7H_7CoCp^{5+}$, D, $CpVC_6H_6VCp$, E, $C_6H_6CrC_6H_6CrC_6H_6$, F, $CpMoP_6MoCp$, G, $CpCrP_5CrCp$, H, $CpMoAs_5MoCp$ (symmetric), and I, $CpMoAs_5MoCp$ (distorted), with electron count ranging from 34 to 26.

Relation between the Metal-Metal Distance and the Size of the Middle Ring in Triple-Decker Sandwich Compounds

With use of average metal–ligand distances available from literature, anticipated M–M distances have been calculated for representative triple-decker sandwich compounds (Table II). With C_nH_n rings in the middle, M–M distances fall in the bonding range only for $n > 7$. There are no known complexes with planar C_7H_7 rings in the middle. Larger rings become practical with heavier metal atoms. Thus M–M distances are short with the central rings P_6, P_5, and As_5. The electron count for a closed-shell system depends on the individual metal as well as the metal–metal distance. An interaction diagram between $C_5H_5Ni\cdots NiC_5H_5$ and C_5H_5 had shown that the major binding of the middle ring with the metals takes place through the e_1'' orbitals.[17] The lower lying d orbitals (remnants of the t_{2g} set) are not affected by this considerably. The interaction diagram leads to the 30- and 34-electron count for stable closed-shell species because the antibonding character of the e_1' level is not very high.[17] Four other types of interactions, 4b–e, are dormant with this combination of metal and ligands. The interaction between e_2'' orbitals (4b) increases when the e_2'' MOs of the ring is lower in energy and when the M–M distances are shorter. An increase in the size of the middle ring, as shown below, achieves both of these. The $e_2'' - e_2''$ energy difference decreases with an increase in metal orbital en-

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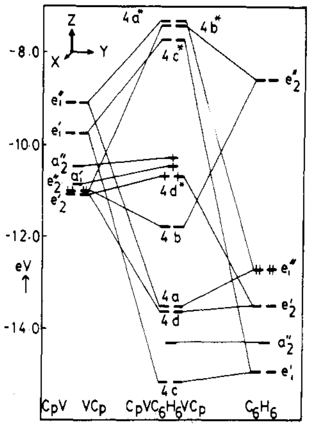
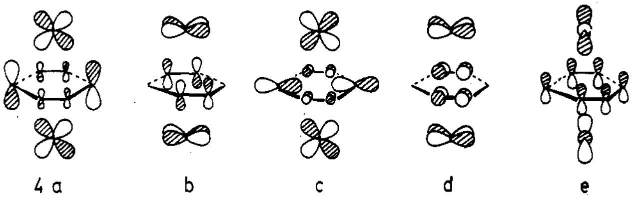


Figure 2. Construction of the orbitals of $CpVC_6H_6VCp$ from the fragments $CpV\cdots VCp$ and C_6H_6.

ergies. Thus metals lying on the left-hand side of the periodic table favors this interaction. We shall first consider the electronic structure of the model compounds $C_5H_5CoC_6H_6CoC_5H_5$, $C_5H_5CoC_7H_7CoC_5H_5$, $C_5H_5VC_6H_6VC_5H_5$, and $C_6H_6CrC_6H_6CrC_6H_6$ which would bring many of the interactions in 4 into focus. Derivatives of most of these compounds have been known experimentally.[2-5]



Electronic Structure of 1 with a Carbocyclic Ligand

There is very little difference between the electronic structure of $C_5H_5NiC_5H_5NiC_5H_5^+$ and the corresponding cobalt complex. Figure 1 gives a correlation of the frontier orbitals of $CpNiCpNiCp^+$ with $CpCoC_6H_6CoCp$, $CpCoC_7H_7CoCp$, $CpVC_6H_6VCp$, and $C_6H_6CrC_6H_6CrC_6H_6$. The 30- and 34-electron count found for Ni complexes remain valid for the cobalt complexes except for the fact that the e_1', 4c, orbitals go up in energy, as the middle ring becomes C_7H_7. Thus there is less chance of a 34-electron count with CoC_7H_7Co system. The situation is very different in $C_5H_5VC_6H_6VC_5H_5$ which is similar in MO energies to that of $C_6H_6CrC_6H_6CrC_6H_6$. Figure 2 gives an interaction diagram between the fragments $C_5H_5V\cdots VC_5H_5$ and C_6H_6. The magnitude of the H_{ii}'s corresponding to vanadium d orbitals is rather small so that the $CpV\cdots VCp$ fragment molecular orbitals are in between the e_1'' and e_2'' MOs of C_6H_6. In addition the V AOs are more diffuse in character leading to greater spread of the frontier levels in the fragment itself. The e_2'' is closer in energy to the e_2'' of the C_6H_6 so that 4b represents a strong interaction. The corresponding FMO overlap is reasonably large (0.19, entries corresponding to $\langle e_2''\rangle$, Table III). This is a two electron-two orbital interaction, lowering the metal e_2'' orbital energy. The e_1' MOs of C_6H_6 are stabilized by the interaction with the e_1' MOs of $CpV\cdots VCp$ fragment resulting in the donation of four σ-electrons to the metal (4c). With these C_6H_6 can be considered as a 10-electron donor. This is also observed in chromium compound. The a_1' and a_2'' orbitals of the t_{2g} group are slightly pushed up. Catching up with this is the e_2' MOs of the fragment pushed up by the corresponding e_2' MOs of the C_6H_6 ring. This interaction depends on the size of the middle ring, as seen in the overlaps given in Table III ($\langle e_2'\rangle$). The result is a close bunch of four frontier MOs. With the 26 valence electrons (30 valence electrons, including σ-electrons) in $CpVC_6H_6VCp$ we should anticipate a quintet corresponding to four unshared electrons. This is in accordance with the experimental observations and the Fenske–Hall calculations but differs from level ordering obtained from EH calculations on $CpNiCpNiCp^+$.[18] We find that if the same model compound is used, the energy levels are very similar from both the Fenske–Hall and EH methods, for this system. The bonding in $C_6H_6CrC_6H_6CrC_6H_6$ follow along the same lines. There are four electrons more in this system, leading to a closed-shell configuration of 30 electrons, filling all valence MOs (Figure 1) (or 34 electrons assuming benzene as a 10-electron donor). The concept of donation of σ-electrons is not new in organo transition-metal chemistry. The initial processes in the activation of C–H and C–C bonds are indeed donation of σ-electrons to the metal. However, only the unique symmetry conditions present in the benzene complex provides possibility for the donation of the σ C–C bonding electrons of a η^6-benzene ring to metals.

Table III. Fragment Molecular Orbital Overlaps between the Interacting Orbitals of $C_nH_nM\bullet\bullet\bullet MC_nH_n$ and the Middle Rings As Shown in 4

compound	4a[c] $\langle e_1''\rangle$	4b $\langle e_2''\rangle$	4c $\langle e_1'\rangle$	4d $\langle e_2'\rangle$	4e $\langle a_2''\rangle$
(1) CpCoCpCoCp[a]	0.2929	0.1510	0.0853	0.0630	0.0049
(2) $CpCoC_6H_6CoCp$	0.2864	0.1504	0.1145	0.0591	0.0340
(3) $CpCoC_7H_7CoCp$[a]	0.2863	0.1903	0.1862	0.1078	0.1312
(4) $CpVC_6H_6VCp$	0.2856	0.1963	0.0872	0.0882	0.1109
(5) $C_6H_6CrC_6H_6CrC_6H_6$	0.3591	0.1701	0.1668	0.1152	0.0759
(6) $CpCrP_5CrCp$	0.3723	0.2465	0.2733	0.1907	0.3208
(7) $CpMoP_6MoCp$	0.2308	0.2833	0.3235	0.2423	0.3456
(8) $CpMoAs_5MoCp$[b]	0.2882	0.2291	0.2999	0.2055	0.3585

[a] Not known experimentally. [b] Calculated by keeping local C_5 axis for As_5 ring. [c] $\langle e_1''\rangle$ is used instead of $\langle e_1''|e_1''\rangle$ to save space throughout the paper.

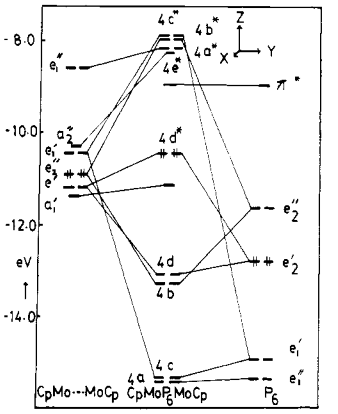


Figure 3. Construction of the orbitals of $CpMoP_6MoCp$ from the fragments $CpMo\cdots MoCp$ and P_6.

Electronic Structure of 1 with P_6, P_5, and As_5 as the Middle Rings

Figure 1 indicates a 28-electron count for closed-shell species with phosphorus and arsenic rings. How this comes about is seen from the interaction diagram for $C_5H_5MoP_6MoC_5H_5$ (Figure 3). The standard Mo–P distance in combination with the P–P distances leads to a rather close Mo–Mo distance of 2.648Å. Consequently there are substantial Mo–Mo interactions in the $C_5H_5Mo\cdots MoC_5H_5$ fragment. The a_1'' and a_2'' orbitals of the t_{2g} realm are substantially split. The e_1' and e_1'' formed from the frontier orbitals interact even stronger, e_1'' going away from the bonding range. The fragment $C_5H_5Mo\cdots MoC_5H_5$ has an occupancy of σ^2, δ^4, and δ^{*4}. The unoccupied e_1' and a_2'' are only slightly higher. Of these the a_1' orbital is only slightly affected by the interaction with the σ orbitals of P_6. The e_2' MOs interact with e_2' orbitals of the P_6 substantially, but the bonding as well as antibonding combinations are occupied, 4d. The e_2'' interaction is very strong (see the corresponding overlap, Table III), pushing the antibonding combination up, 4b. However, the crucial difference that leads to a 28-electron count is the result of the a_2'' being pushed up by the interaction with the low-lying a_2'' orbital (which is not shown in Figure 3). This again is a result of the shorter M–M distance and the more diffuse nature of the P atoms and consequent large overlap between the FMOs. Considering C_6H_6 as a 10-electron donor, as was explained in vanadium compound, the P_6 compound will become a 32-electron compound and the P_5 and As_5 compounds 31-electron compounds. The extent of overlap between e_1' MOs in these compounds is significantly large as seen in Table III. The general level pattern remains the same for the As_5 and P_5 complexes with one major difference There is one electron less in both P_5 and As_5 complexes. The three electrons in the degenerate MO of $CpMoAs_5MoCp$ leads to a Jahn–Teller distortion of the central ring that is clearly seen in the X-ray structure of the compound, $C_5H_5MoAs_5MoC_5H_5$. A Walsh diagram (Figure 1, extreme right) indicates that among the many variations in energy levels, the prominent one is the splitting of the degenerate HOMO, one going up in energy and the other down. There is a net gain because there is only one electron to occupy the higher level. The corresponding P_5 compound, $C_5H_5CrP_5CrC_5H_5$, may be free of a similar distortion because the HOMO is a nondegenerate singly occupied orbital. This, however, could not be confirmed from the X-ray analysis available as there was high disorder in the crystal.[15] If there are 28 electrons, no distortion is expected as seen in $CpMoP_6MoCp$.

Conclusions

Molecular orbital studies using extended Hückel calculations on the triple-decker sandwich compounds $CpCoC_6H_6CoCp$, $CpVC_6H_6VCp$, $C_6H_6CrC_6H_6CrC_6H_6$, $CpMoP_6MoCp$, $CpMoAs_5MoCp$, and $CpCrP_5CrCp$ revealed the following. The bonding between $C_nH_nM\cdots MC_nH_n$ and the middle ring is controlled by a combination of individual interactions, 4a–e, each of which contributes differently in individual examples. The strength of each interaction (4a–e) depends on the metal and the size of the middle ring and leads to the observed electron counts of 34, 30, 28, and 26 valence electrons. The three electrons in the degenerate HOMO of $CpMoAs_5MoCp$ in the symmetric structure lead to a Jahn–Teller distortion in the As_5 ring. Such a distortion in P_5 ring is absent in $CpCrP_5CrCp$ because the HOMO is nondegenerate.

Acknowledgment. We thank the university of Hyderabad computer center for computations. A.C.R. thanks CSIR for financial assistance. A reviewer pointed out the appropriateness of treating C_6H_6 as a 10-electron donor in triple-decker sandwich compounds, and we thank him for this and other useful comments.

Appendix

Atomic parameters for all the atoms used in the extended Hückel calculations are taken from previous studies (carbon, hydrogen, vanadium, chromium, molybdenum,[25] arsenic,[24] phosphorus,[23] cobalt, and nickel[17]). Geometrical parameters are taken from the experimental structures wherever known (Table I). All C–H and P–P distances used in the calculations are 1.08 and 2.17 Å, respectively. For the symmetrical As_5 geometry an As–As distance of 2.509 Å is used.

Registry No. $CpNiCpNiCp^+$, 53664-04-3; $CpCoC_6H_6CoCp$, 114563-62-1; $CpCoC_7H_7CoCp^+$, 114563-63-2; $CpVC_6H_6VCp$, 86409-35-0; $C_6H_6CrC_6H_6CrC_6H_6$, 114580-89-1; $CpMoP_6MoCp$, 114551-20-1; $CpCrP_5CrCp$, 114551-21-2; $CpMoAs_5MoCp$, 82638-64-0; $CpV\cdots VCp$, 114551-22-3; $CpMo\cdots MoCp$, 114551-23-4; C_6H_6, 71-43-2; P_6, 15924-07-9; P_5, 15924-07-9; As_5, 114551-25-6.

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