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# A High-Precision Neutron Diffraction Investigation of the Prototype Biscyclopentadienyl Transition Metal Hydride $(\eta^5\text{-}C_5H_5)_2MoH_2$ and Resolution of the Structure in Terms of Modern Bonding Theory

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A high-precision single-crystal neutron diffraction determination of the crystal and molecular structure of $(\eta^5\text{-}C_5H_5)_2MoH_2$ has been carried out in order to resolve previous x-ray and neutron diffraction studies which produced structural models which are inconsistent with modern bonding theories. The complex crystallizes in space group $C2/c$ with cell parameters of $a = 14.311$ (7) Å, $b = 5.905$ (3) Å, $c = 10.440$ (5) Å, $\beta = 104.15$ (2)°, and $Z = 4$. Intensity data were measured for two independent octants out to $(\sin\theta)/\lambda = 0.72$. The structure was solved by direct methods and refinement led to final discrepancy indices of $R(F_o^2) = 0.074$ and $R_w(F_o^2) = 0.101$. The dihedral angle between the two cyclopentadienyl planes is 34.2°, and the C–C bond lengths within each ring are indicative of a completely delocalized $\pi$ system. We have unequivocally located and refined the coordinates of the metal-bonded hydrogen atom and obtained a Mo–H distance of 1.685 (3) Å and a H–Mo–H′ angle of 75.5 (3)°. The new structural parameters determined for $(\eta^5\text{-}C_5H_5)_2MoH_2$ are substantially different from those previously reported but are in excellent agreement with those predicted today for transition metal cyclopentadienyl hydrides.

## Introduction

The early transition metal complexes $(\eta^5\text{-}C_5H_5)_2ML_n$, $n = 1–3$, have been extensively studied both experimentally and theoretically.[2] The majority of these investigations were initiated in order to clearly establish which of two alternative molecular orbital schemes is more consistent with the experimental evidence. The first model, proposed by Ballhausen and Dahl[3] in 1961, correctly predicts the bent sandwich configuration of the cyclopentadienyl ligands about the metal. In addition, this qualitative model proposes that in M(IV) $d^1$ and $d^2$ $(\eta^5\text{-}C_5H_5)_2MH_2$ complexes the nonbonding electrons are in an orbital which bisects the two hydride ligands (Figure 1a). In 1967, Alcock[4] reported a $CH_3\text{–}Re\text{–}CH_3$ angle of 76° in the compound $(\eta^5\text{-}C_5H_5)(\eta^4\text{-}C_5H_5CH_3)Re(CH_3)_2$ which was inconsistent with the placement of the Ballhausen–Dahl nonbonding orbital. He therefore suggested a revised model which accommodated the nonbonding electrons in an orbital outside the $ML_2$ moiety (Figure 1b).

The accumulated crystallographic,[4–11] magnetic,[8–10,12,13] and photoelectron spectral[14,15] evidence at the present time clearly indicates the Ballhausen–Dahl model is not valid. The molecular orbital scheme[2,5,14,15] that emerges from these studies is in many respects similar to the qualitative, and therefore not entirely complete, model proposed by Alcock.[4] These MO descriptions provide the rationalization for two important structural observations relevant to these complexes: (1) in a series of M(IV) $(\eta^5\text{-}C_5H_5)_2ML_2$ complexes, the L–M–L angle should decrease in the transition metal series $d^0 \rightarrow d^1 \rightarrow d^2$; (2) the highest occupied molecular orbital (HOMO) in $d^1$ and $d^2$ systems contains partial $\pi^*$ antibonding character which has the effect of lengthening the M–L bond, if L is a $\pi$ donor, as the orbital is successively occupied.

The hydrides (L = H) are of particular interest as the simplest models for investigating the electronic structure and bonding in these compounds. Hydride ligands are particularly suitable because their small ligand displacement reduces steric interactions, and, secondly, in the total absence of $\pi$ bonding with the metal they can only participate as $\sigma$ donors. A review and discussion of the structural properties of the trihydrides $(\eta^5\text{-}C_5H_5)_2MH_3$ (M = Nb, Ta) have been recently given by Wilson et al.[11] However, the simplest $d^2$ biscyclopentadienyl compound, $(\eta^5\text{-}C_5H_5)_2MoH_2$, which has been the prototype model for many of the bonding theories, has never been fully characterized structurally.

This is not to say that the structure of $(\eta^5\text{-}C_5H_5)_2MoH_2$ has not been investigated; however, none of the studies reported to date has been unambiguous with respect to the precise location of the hydride ligands and determination of the equality of the C–C distances in the cyclopentadienyl ligands. From an x-ray diffraction study, Gerloch and Mason[16] were able to determine the relative configuration of the cyclopentadienyl ligands and, by doing so, provide conclusive evidence of a bent sandwich complex. However, they also report an estimated Mo–H distance of 1.2 Å, which appeared to support early models[17,18] of metal–hydrogen bonding in which the hydride atom is "embedded" in the metal orbitals. While Gerloch and Mason[16] characterized this apparent agreement as "fortuitous", Abrahams and Ginsburg[19] demonstrated conclusively that from the x-ray film data it was impossible to locate the metal-bonded hydrogen atoms. A more recent structural study, based on profile analysis of a neutron diffraction powder pattern of $(\eta^5\text{-}C_5H_5)_2MoD_2$, has been cited in the literature.[20] The reported Mo–D distance is 1.96 Å with a D–Mo–D angle of 83.2°. These values are considered anomalous with respect to the structural parameters of other metal–hydride complexes[11] and clearly there is a need for accurate structural parameters as has been expressed by many investigators.[2,14,16]

In view of the lack of precise data on the metal dihydrides, which is still needed today in order to reconcile certain aspects of bonding theory with experimental data, we have carried out a highly precise molecular structure determination of $(\eta^5\text{-}C_5H_5)_2MoH_2$ using single-crystal neutron diffraction techniques. The results of this study and the interpretation of the molecular structure in terms of modern bonding theory are reported here.

## Experimental Section

**Data Collection.** The complex was prepared under an argon atmosphere from the reaction of anhydrous $MoCl_5$, sodium cyclopentadienide, and excess sodium borohydride in 1,2-dimethoxyethane.[21] A crystal of approximate dimensions 5.5 × 3.0 × 1.7 mm and weighing ~44 mg was sealed in a lead-glass capillary under vacuum. With the crystal mounted in a general orientation, all data were collected using an Electronics and Alloys four-circle goniostat at the CP-5 reactor at Argonne National Laboratory in a manner previously described.[22] From a search of reciprocal space, a total of 14 reflections were located and automatically centered. They were then indexed and transformed, using the program BLIND,[23] into the same monoclinic $C$-centered cell reported for the x-ray analysis,[16] and an initial

**Table I**

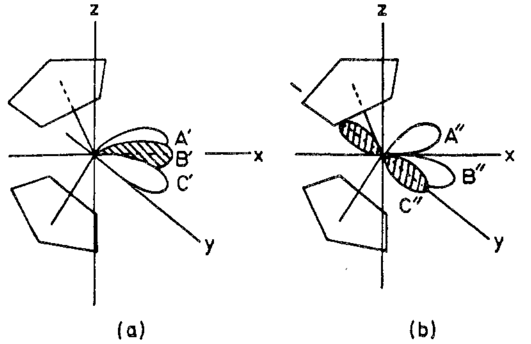
Final Positional and Thermal Parameters for $(\eta^5\text{-}C_5H_5)_2MoH_2$

| Atom | $x^a$ | $y$ | $z$ |
|---|---|---|---|
| Mo | 0.0 | 0.3317 (3) | 0.25 |
| C(1) | −0.1029 (1) | 0.0556 (2) | 0.2694 (2) |
| C(2) | −0.1488 (1) | 0.1883 (3) | 0.1568 (1) |
| C(3) | −0.1645 (1) | 0.4059 (3) | 0.2047 (1) |
| C(4) | −0.1284 (1) | 0.4093 (3) | 0.3431 (1) |
| C(5) | −0.0897 (1) | 0.1938 (3) | 0.3852 (2) |
| H(1) | −0.0814 (3) | −0.1201 (6) | 0.2673 (5) |
| H(2) | −0.1705 (2) | 0.1320 (8) | 0.0562 (4) |
| H(3) | −0.1982 (2) | 0.5483 (7) | 0.1456 (4) |
| H(4) | −0.1287 (3) | 0.5518 (7) | 0.4070 (4) |
| H(5) | −0.0586 (3) | 0.1468 (8) | 0.4857 (4) |
| H(6) | −0.0264 (2) | 0.5572 (6) | 0.1488 (3) |

Anisotropic Thermal Parameters $(\times 10^4)^b$ for $(\eta^2\text{-}C_5H_5)_2MoH_2$

| Atom | $\beta_{11}$ | $\beta_{22}$ | $\beta_{33}$ | $\beta_{12}$ | $\beta_{13}$ | $\beta_{23}$ |
|---|---|---|---|---|---|---|
| Mo | 21.0 (5) | 125 (4) | 53 (1) | 0.0 (0) | 8.5 (6) | 0.0 (0) |
| C(1) | 35.2 (6) | 170 (3) | 148 (2) | −15 (1) | 30.2 (8) | 5 (2) |
| C(2) | 25.9 (5) | 297 (5) | 102 (2) | −15 (1) | 6.5 (7) | −47 (2) |
| C(3) | 26.4 (5) | 269 (4) | 99 (1) | 23 (1) | 9.1 (6) | 9 (2) |
| C(4) | 36.6 (6) | 268 (4) | 91 (1) | 14 (1) | 26.5 (7) | −20 (2) |
| C(5) | 40.3 (6) | 271 (4) | 92 (2) | 4 (1) | 28.3 (7) | 41 (2) |
| H(1) | 73 (2) | 197 (8) | 265 (7) | −14 (3) | 55 (3) | 2 (6) |
| H(2) | 59 (2) | 629 (19) | 130 (4) | −39 (5) | 2 (2) | −125 (8) |
| H(3) | 56 (2) | 437 (14) | 159 (4) | 67 (4) | 9 (2) | 72 (6) |
| H(4) | 78 (2) | 404 (13) | 159 (4) | 31 (4) | 53 (3) | −74 (7) |
| H(5) | 85 (2) | 570 (17) | 122 (4) | 17 (5) | 41 (3) | 106 (7) |
| H(6) | 63 (2) | 292 (9) | 140 (4) | 21 (3) | 24 (2) | 79 (5) |

[a] $x, y, z$ are fractional coordinates. [b] Anisotropic temperature factors of the form $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$.



(a) (b)

**Figure 1.** Metal hydride orbitals available to monodentate ligands according to (a) Ballhausen and Dahl[3] and (b) Alcock.[4] For $(\eta^5\text{-}C_5H_5)_2ML_2$ complexes, the shaded orbital is the LUMO in $d^0$ systems and the HOMO in $d^1$ and $d^2$ systems.

orientation matrix was obtained. A least-squares fit of the angles $2\theta$, $\chi$, and $\phi$ of 17 strong reflections ranging in $2\theta$ from 40 to 60° ($\lambda$ 1.142 (1) Å)[22] yielded $a$ = 14.311 (7) Å, $b$ = 5.905 (3) Å, $c$ = 10.440 (5) Å, $\beta$ = 104.15 (2)°, and $V_c$ = 855.5 Å$^3$. With four formula weights of $(C_5H_5)_2MoH_2$ per unit cell, the calculated density is 1.77 g/cm$^3$. Intensity data were measured for two independent octants out to $(\sin\theta)/\lambda = 0.72$ using the $\theta$–$2\theta$ step-scan mode, with 0.1° step intervals and preset scan ranges of 40–70 steps. The data were corrected for absorption ($\mu_{\text{calcd}}$ = 2.34 cm$^{-1}$) with transmission coefficients ranging from 0.48 to 0.69, and a set of $F_o^2$ values, where $F_o$ is the observed structure factor amplitude, was obtained. The variances of $F_o^2$ were calculated using the expression $\sigma^2(F_o^2) = \sigma_c^2(F_o^2) + (0.03F_o^2)^2$, where $\sigma_c^2(F_o^2)$ is determined from counting statistics and 0.03 is an added factor deduced from the 3% maximum variation of the intensities of two reference reflections which were measured periodically throughout the data collection.

In addition to the $C$ centering, for which $hkl$, $h + k = 2n + 1$, are extinct, examination of the data revealed systematic extinctions for $h0l$, $l = 2n + 1$. As also determined by Gerloch and Mason[16] from the x-ray analysis, these extinctions are consistent with the space groups $C2/c$ [$C_{2h}^6$, No. 15][24a] or $Cc$ [$C_s^4$, No. 9].[24a] However, the statistical distribution of the intensities of the normalized structure factors $|F_o|$, as determined by the program MULTAN, is clearly characteristic of a centrosymmetric structure for the neutron data. Therefore, the monoclinic space group $C2/c$ was chosen and was additionally justified by the satisfactory least-squares refinement ultimately obtained.

**Table II.** Root-Mean-Square Amplitudes of Vibration (Å)

| Atom | Min | Intermed | Max |
|---|---|---|---|
| Mo | 0.143 (2) | 0.149 (2) | 0.166 (2) |
| C(1) | 0.152 (2) | 0.192 (2) | 0.277 (2) |
| C(2) | 0.152 (2) | 0.207 (2) | 0.260 (2) |
| C(3) | 0.149 (2) | 0.226 (2) | 0.230 (2) |
| C(4) | 0.157 (2) | 0.219 (2) | 0.231 (2) |
| C(5) | 0.165 (2) | 0.204 (2) | 0.248 (2) |
| H(1) | 0.183 (4) | 0.254 (3) | 0.372 (5) |
| H(2) | 0.189 (4) | 0.273 (4) | 0.365 (5) |
| H(3) | 0.179 (4) | 0.293 (4) | 0.320 (5) |
| H(4) | 0.184(4) | 0.295 (4) | 0.317 (5) |
| H(5) | 0.201 (4) | 0.284 (4) | 0.347 (5) |
| H(6) | 0.189 (4) | 0.248 (3) | 0.297 (4) |

**Solution and Refinement of the Structure.** The initial locations of the molybdenum and the five independent carbon atoms were obtained by direct methods using MULTAN. Least-squares refinement[25] of their positional and isotropic thermal parameters led to discrepancy factors[26] of $R(F_o) = 0.422$, $R(F_o^2) = 0.592$, and $R_w(F_o^2) = 0.682$. The positions of the six hydrogen atoms were determined from a Fourier map of the nuclear scattering density with phases determined from the positional coordinates of the six nonhydrogen atoms. In the final stages of refinement, all atoms were treated with anisotropic thermal parameters and the data were corrected for secondary extinction[27,28] with a refined isotropic extinction coefficient of $g = 0.39\ (2) \times 10^4$. Correction factors ranged from 1.00 to 2.50 although for only 18 reflections were the factors greater than 1.25. The final discrepancy indices for all 1327 independent reflections are $R(F_o) = 0.095$, $R(F_o^2) = 0.074$, and $R_w(F_o^2) = 0.101$. The final scale factor is 1.365 (6), and the standard deviation of an observation of unit weight is 0.982. Positional and anisotropic thermal parameters from the final least-squares cycle are presented in Table I, and the root mean squares of the amplitudes of vibration are given in Table II.

## Discussion

A stereoscopic view of the $C$-centered centrosymmetric unit cell is shown in Figure 2, and a view of the molecule with the

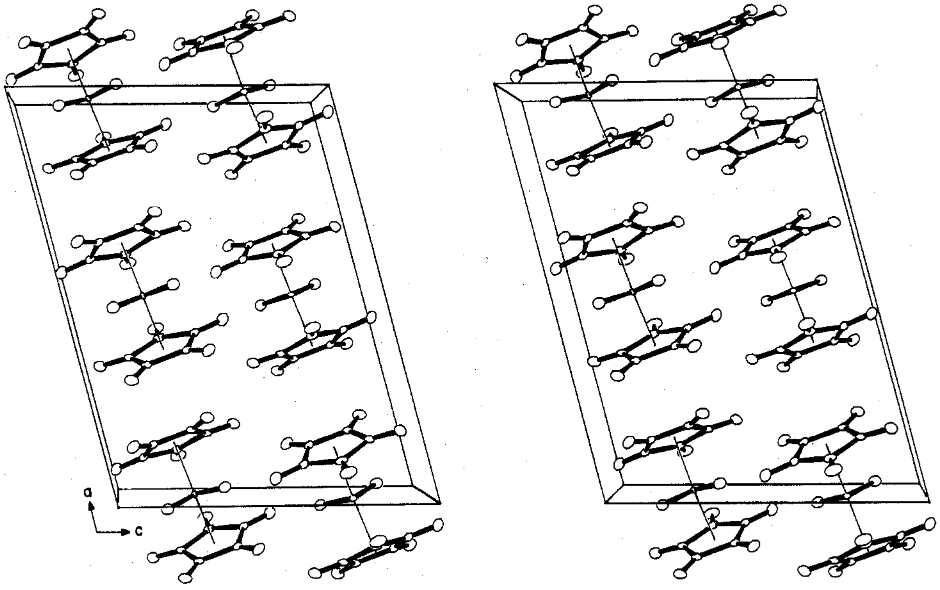


**Figure 2.** A stereoscopic view of the unit cell of $(\eta^5\text{-}C_5H_5)_2MoH_2$.

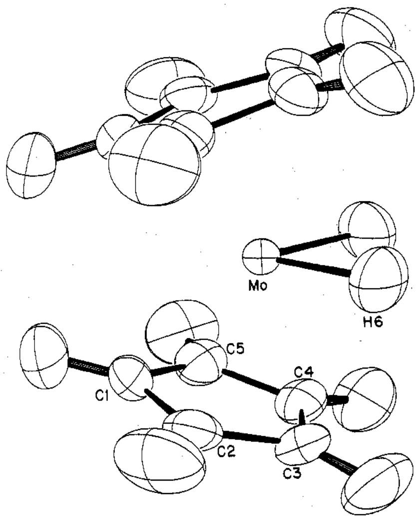


**Figure 3.** A perspective view of the $(\eta^5\text{-}C_5H_5)_2MoH_2$ molecule with the atom labeling scheme. The hydrogen atoms H(1)–H(5) are bonded to carbon atoms C(1)–C(5), respectively.

atom labeling scheme is shown in Figure 3. The closest intermolecular contacts are between H(5)···H(5), H(5)···H(6), and H(1)···H(6) at distances of 2.38, 2.40, and 2.47 Å, respectively. Therefore, the molecular packing is assumed to be primarily dictated by van der Waals forces. There is relatively good agreement between the positional parameters of the Mo and the $\pi$-$C_5H_5$ ring from the neutron and x-ray studies,[16] although some of the differences are significant (vide infra).

The principal intramolecular bond lengths and angles are presented in Table III. With the Mo atom occupying a special position 0, $y$, $^1/_4$, the molecule is required (crystallographically) to possess twofold symmetry. The two cyclopentadienyl rings are oriented in an eclipsed configuration, such that the molecule also possesses two noncrystallographic mirror planes. Each cyclopentadienyl ring is essentially planar (Table IV) and the dihedral angle between the two planes is 34.2°. This produces a "bending angle" of 145.8°, which is significantly larger than the range of 130–135° generally observed[6-10] for other $(\eta^5\text{-}C_5H_5)_2ML_2$ complexes. Lauher and Hoffman[2] postulate a larger bending angle with poorer $\pi$-acceptor and better $\sigma$-donor ability of the ligand L. Prout et al.[6] have noted from their structural studies that reduced ligand–ring repulsion

**Table III.** Principal Intramolecular Distances and Angles for $(\eta^5\text{-}C_5H_5)_2MoH_2$

| Atoms | Distance, Å | Atoms | Angle, deg |
|---|---|---|---|
| Mo–H(6) | 1.685 (3) | H(6)–Mo–H(6) | 75.5 (3) |
| Mo–C(1) | 2.238 (2) | C(1)–C(2)–C(3) | 106.7 (1) |
| Mo–C(2) | 2.277 (2) | C(2)–C(3)–C(4) | 108.9 (1) |
| Mo–C(3) | 2.326 (2) | C(3)–C(4)–C(5) | 108.9 (1) |
| Mo–C(4) | 2.325 (2) | C(4)–C(5)–C(1) | 106.8 (1) |
| Mo–C(5) | 2.277 (2) | C(5)–C(1)–C(2) | 108.7 (1) |
| C(1)–C(2) | 1.432 (2) | C–C–C (av)[a] | 108.0 (5) |
| C(2)–C(3) | 1.416 (2) | | |
| C(3)–C(4) | 1.410 (2) | | |
| C(4)–C(5) | 1.415 (2) | | |
| C(5)–C(1) | 1.433 (2) | | |
| C–C (av)[a] | 1.421 (5) | | |
| C(1)–H(1) | 1.084 (4) | | |
| C(2)–H(2) | 1.073 (4) | | |
| C(3)–H(3) | 1.084 (4) | | |
| C(4)–H(4) | 1.075 (4) | | |
| C(5)–H(5) | 1.071 (4) | | |
| C–H (av)[a] | 1.077 (3) | | |

[a] The esd's for the mean values are calculated according to $[\Sigma_n(x_i - \bar{x})^2/n(n-1)]^{1/2}$, where $\bar{x}$ represents the mean value of an observation $x_i$.

**Table IV.** Least-Squares Planes and the Distances of the Atoms from the Planes[a]

(a) Cyclopentadienyl Ring Defined by Carbon Atoms: $0.9491X + 0.2939Y - 0.1130Z = -2.2575$

(b) Cyclopentadienyl Ring Defined by Carbon and Ring Hydrogen Atoms: $0.9501X + 0.2894Y - 0.1162Z = -2.2798$

| Atom | Dist from plane (a) | Dist from plane (b) |
|---|---|---|
| C(1) | −0.004 (1) | 0.006 (1) |
| C(2) | 0.004 (1) | 0.013 (1) |
| C(3) | −0.002 (1) | 0.000 (1) |
| C(4) | 0.000 (1) | −0.002 (1) |
| C(5) | 0.002 (1) | 0.005 (1) |
| H(1) | −0.010 (4) | 0.005 (4) |
| H(2) | −0.029 (4) | −0.015 (4) |
| H(3) | −0.003 (4) | −0.003 (4) |
| H(4) | 0.015 (4) | 0.007 (4) |
| H(5) | −0.017 (4) | −0.016 (4) |
| Mo | 1.9415 (4) | 1.9463 (4) |

[a] The plane equations have the form $AX + BY + CZ = D$, where $X$, $Y$, and $Z$ are coordinates (Å) referred to the orthogonal axes $a$, $b$, and $c^*$.

due to smaller ligands leads to larger bending angles. Both of these interpretations appear to be valid for $(\eta^5\text{-}C_5H_5)_2MoH_2$, since, by comparison, the bending angle in $(\eta^5\text{-}C_5H_5)_2MoCl_2$ is 130°.[6]

From the early x-ray analysis of $(\eta^5\text{-}C_5H_5)_2MoH_2$,[16] it was proposed that there is localization of the $\pi$-electron density in the cyclopentadienyl rings, in which C–C bond lengths ranged from a minimum of 1.34 (4) Å to a maximum of 1.51 (5) Å. Abrahams and Ginsberg[19] pointed out that the differences in C–C bond distances were not significant in terms of the quoted errors, and, in fact, the C–C bond lengths derived from the neutron data range only from 1.410 (2) to 1.433 (2) Å, indicating a completely delocalized $\pi$ system. Although the rings are slightly titled (10°) such that the Mo–C distances range from 2.238 (2) to 2.326 (2) Å, the bonding is still indicative of pentahapto coordination.[29] The Mo to cyclopentadienyl ring distance along the vector normal to the ring plane is 1.94 Å (Table IV), as compared to 1.97 Å in $(\eta^5\text{-}C_5H_5)_2MoCl_2$.[6]

With the neutron data we are able to unequivocally locate and refine the metal-bonded hydrogen atom and obtain a Mo–H(6) distance of 1.685 (3) Å and a H(6)–Mo–H(6)′ angle of 75.5 (3)°. The relevant metal–hydride distances for $(\eta^5\text{-}C_5H_5)_2NbH_3$ and $(\eta^5\text{-}C_5H_5)_2TaH_3$ are Nb–H = 1.69 (4) Å and Ta–H = 1.774 (3) Å.[11] The small H(6)–Mo–H(6)′ angle of 75.5 (3)° provides additional evidence that the Ballhausen–Dahl[3] model is not valid, since this model requires a lone pair of electrons in an orbital highly localized between the two hydrogen atoms. Based on experimental data and theoretical calculations, it is now generally accepted that as the number of d electrons increases from 0 to 2, the L–M–L angle should decrease. Lauher and Hoffman[2] predicted a H–M–H angle of ~78° for a $d^2$ molecule, which is in relatively good agreement with our observed value of 75.5 (3)° in $(\eta^5\text{-}C_5H_5)_2MoH_2$.

It is of particular interest to relate our structural results to the MO calculations performed by Petersen et al.[14] on $(\eta^5\text{-}C_5H_5)_2MoH_2$. These calculations reveal that the predominant contributions to the completely occupied HOMO are from the Mo $4d_{z^2}$ and $4d_{x^2-y^2}$ AOs. (The $x$, $y$, $z$ axes of the coordinate system used by Petersen et al.[14] correspond to the $z$, $x$, $y$ axes, respectively, shown in Figure 1.) Since structural parameters were not available, the calculations were performed for three different sets of estimated Mo–H distances and H–Mo–H angles. Examination of the variation of the ratio of percent $4d_{z^2}$ to percent $4d_{x^2-y^2}$ contribution to the HOMO revealed that the ratio is relatively insensitive to Mo–H distance but increases significantly as the H–Mo–H angle decreases. For the hypothetical case where Mo–H = 1.75 Å and H–Mo–H = 82.0°, the calculated ratio is 80.7/5.5 = 14.6. Therefore, with the observed H(6)–Mo–H(6)′ angle of 75.5 (3)°, it can be postulated the HOMO is more than 80% localized along the $y$ axis of Figure 1, as originally predicted by Alcock.[4]

In conclusion, the structural parameters which we have determined for $(\eta^5\text{-}C_5H_5)_2MoH_2$ are substantially different from those reported earlier,[16,20] but completely in accord with currently accepted views[2,14] of the electronic and molecular structural properties of early transition metal cyclopentadienyl hydrides.

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**Supplementary Material Available:** A listing of structure factor amplitudes (7 pages). Ordering information is given on any current masthead page.

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(25) All least-squares refinements were based on the minimization of $\sum w_i|F_o^2 - S^2F_o^2|$ where $S$ is the scale factor and the individual weights $w_i = 1/\sigma^2(F_o^2)$. The neutron scattering amplitudes[24b] used in this study were $\bar{b}_{Mo} = 0.66$, $\bar{b}_C = 0.663$ and $\bar{b}_H = -0.372$ (all in units of $10^{-12}$ cm).

(26) $R(F_o) = \sum||F_o| - |F_c||/\sum|F_o|$, $R(F_o^2) = \sum|F_o^2 - F_c^2|/\sum F_o^2$, and $R_w(F_o^2) = [\sum w_i|F_o^2 - F_c^2|^2/\sum w_i F_o^4]^{1/2}$.

(27) The Zachariasen approximation[28a] was used for the overall isotropic $g$ parameter as defined and scaled by Coppens and Hamilton.[28b] The $|F_o|$ values were corrected for extinction from the expression $|F_o|_{cor} = |F_o|(1 + \bar{T}2g\lambda^3|F_c|^2/V^2 \sin 2\theta)^{-1/4}$, where $|F_c|$ is on an absolute scale, $\lambda$ is the wavelength (Å), $g$ the refined extinction parameter, $\bar{T}$ the mean absorption-weighted path length in the crystal in centimeters (calculated simultaneously during the computation of absorption corrections), and $V$ the unit cell volume (Å$^3$).

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