in the benzoate and the four compounds listed in Table VI. In short, weak association can be prevented by weak interference.

It is interesting to compare some of the structure parameters in this, the first isolated $Mo_2(O_2CR)_4$ molecule to be studied by X-ray crystallography, with those in the five associated $Mo_2(O_2CR)_4$ compounds previously studied crystallographically. The pertinent data on the latter are listed in Table VI. The only dimension that differs significantly from one of these associated compounds to another is the intermolecular Mo··O(b) distance, which is ca. 2.65 Å to two, ca. 2.87 Å in two others, and 2.71 Å in the fifth. However, this does not seem to induce, or correlate with, significant variations in any other distance. The Mo–Mo distances are all in the narrow range of 2.088–2.096 Å, with an average value of 2.092 Å. In each case the Mo–O(b) distances are ca. 0.03 Å longer than the Mo–O(nb) ones, and the latter, with the possible exception of the rather imprecise one in the CF_3 compound, are in the range 2.098–2.113 Å. In the present case, where all of the Mo–O distances are of the Mo–O(nb) type, the mean value is 2.098 ± 0.009 Å.

The only significantly different distance in the present case is the Mo–Mo distance, 2.082 (1) Å, which is 0.014 (2) Å shorter than that in the benzoate and 0.010 Å shorter than the average of all five listed in Table VI. Qualitatively, it is to be expected that the formation of weak intermolecular bonds would lengthen the Mo–Mo bond slightly, and a lengthening of 0.010–0.014 Å is indicated by the results reported here.

This present work is in excellent accord with the results of an electron diffraction study of the gaseous $Mo_2(O_2CCH_3)_4$ molecule,[11] where it was found that all bond lengths are essentially the same as those in the crystalline compound except for the Mo–Mo distance, which is 2.079 (3) Å. This is a decrease of 0.014 (3) Å from that in the crystalline compound, equal to the decrease we have found.

There has also been a gas-phase electron diffraction study of $Mo_2(O_2CCF_3)_4$, but here the uncertainty in the Mo–Mo bond length, 2.105 (9) Å, together with that in the crystallographic value, 2.090 (4) Å, is such that the difference between them has an esd of ca. 0.010 Å, which is sufficient to obscure the sort of 0.010-Å difference in the other direction that might have been anticipated.

Acknowledgment. We thank the National Science Foundation for financial support.

Registry No. $Mo_2(O_2Cbiph)_4$, 78764-18-8; $Mo_2(O_2CCH_3)_4$, 14221-06-8.

Supplementary Material Available: Tables of observed and calculated structure factors and least-squares planes and dihedral angles (Table V) (11 pages). Ordering information is given on any current masthead page.

---

[11] Fink, M.; Kelley, M., Department of Physics, University of Texas, Austin, TX, private communication.

Contribution from the Department of Chemistry,
Texas A&M University, College Station, Texas 77843

A Quadruply Bonded Dimolybdenum Compound Containing Only Chelating Ligands: Bis(diethyl-2-pyrazolylhydroxoborato)bis(diethyldi-2-pyrazolylborato)dimolybdenum

F. ALBERT COTTON,* BRIAN W. S. KOLTHAMMER, and GRAHAM N. MOTT

Received April 8, 1981

Another of the reaction products of $[Et_2B(pz)_2]^-$ (pz = 2-pyrazolyl) with $Mo_2(O_2CCH_3)_4$ has been isolated and identified by X-ray crystallography. It is the first reported Mo_2^{4+} complex containing exclusively chelating ligands, two of which are $[Et_2B(pz)_2]^-$ ions and two are $[Et_2B(OH)pz]^-$ ions. One ligand of each type is coordinated to each molybdenum atom, and the arrangement is such that the $N_3OMo\overset{4}{-}MoON_3$ core is essentially eclipsed; there is no crystallographic symmetry, but the overall ligand arrangement conforms to virtual C_2 symmetry, with the twofold axis a perpendicular bisector of the Mo–Mo bond. This bond has a length of 2.156 (1) Å. The compound crystallizes in space group $P2_1/n$ with unit cell dimensions of $a = 10.176$ (5) Å, $b = 20.984$ (4) Å, $c = 22.892$ (5) Å, $\beta = 91.70$ (0)°, $V = 4886$ (5) Å^3, and $Z = 4$. The manner in which the dipyrazolyl ligand is partly converted to the pyrazolyl hydroxo ligand is not known, but the process occurs even under carefully anaerobic conditions.

Introduction

Several years ago reactions of $Mo_2(O_2CCH_3)_4$ with di- and tripyrazolylborate ligands were investigated.[1] The following three reactions were reported:

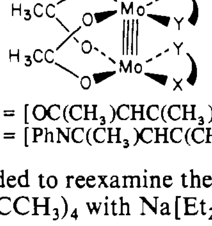
$$Mo_2(O_2CCH_3)_4 + 4Na[BEt_2(pz)_2] \rightarrow Mo_2(BEt_2(pz)_2)_4\ (\mathbf{1}) + 4CH_3CO_2Na \quad (1)$$

$$Mo_2(O_2CCH_3)_4 + 2Na[BEt_2(pz)_2] \rightarrow Mo_2(O_2CCH_3)_2(BEt_2(pz)_2)_2\ (\mathbf{2}) + 2CH_3CO_2Na \quad (2)$$

$$Mo_2(O_2CCH_3)_4 + 2K[BH(pz)_3] \rightarrow Mo(O_2CCH_3)_2(BH(pz)_3)_2\ (\mathbf{3}) + 2CH_3CO_2K \quad (3)$$

Products **2** and **3** were fully characterized by X-ray crystallography and shown to contain a cisoid $Mo_2(O_2CCH_3)_2$ unit with one chelating pyrazolylborate ligand on each metal atom. Attempts to obtain crystals of the blue compound, **1**, were unsuccessful, and at that time no further efforts were planned.

Since then two other reactions[2,3] of $Mo_2(O_2CCH_3)_4$ with chelating ligands have been examined, but in each case only two chelating ligands could be introduced, giving the products **4**[2] and **5**.[3]



4, X-Y = $[OC(CH_3)CHC(CH_3)O]^-$
5, X-Y = $[PhNC(CH_3)CHC(CH_3)O]^-$

We recently decided to reexamine the earlier work on the reaction of $Mo_2(O_2CCH_3)_4$ with $Na[Et_2B(pz)_2]$ in the hope

---

[1] Collins, D. M.; Cotton, F. A.; Murillo, C. A. *Inorg. Chem.* **1976**, *15*, 1862.

[2] Garner, C. D.; Parker, S.; Walton, I. B.; Clegg, W. *Inorg. Chim. Acta* **1978**, *31*, L451.

[3] Cotton, F. A.; Ilsley, W. H.; Kaim, W. *Inorg. Chim. Acta* **1979**, *37*, 267.

Table I. Crystallographic Data and Enraf-Nonius CAD-4 Data Collection Procedures

formula	$Mo_2O_2N_{14}C_{38}B_4H_{66}$	V, Å^3	4886 (5)
mol wt	986.17	β, deg	91.70 (0)
space group	$P2_1/n$	Z	4
a, Å	10.176 (5)	ρ_c, g/cm^3	1.340
b, Å	20.984 (4)	μ(Mo Kα), cm^{-1}	5.545
c, Å	22.892 (5)		

cryst sizes, mm	0.65 × 0.5 × 0.5 (1), 0.60 × 0.5 × 0.5 (2)
radiation	graphite-monochromated Mo Kα ($\lambda\alpha$ = 0.710 73 Å)
collection range	$+h,+k,\pm l$; $0 < 2\theta \leqslant 50°$
aperture width, deg	$1.50 + 1.0 \tan\theta$
prescan rejection limit	2.0
max counting time, s	30
prescan acceptance limit	0.02
X-ray exposure time, h	19 (1), 42 (2)
cryst dec	50% (1), 36% (2)
no. of unique data	7291
no. of data $I < 3\sigma(I)$	5100
p	0.05
no. of variables	511
R_1	0.044
R_2	0.056
esd	1.579
largest shift	0.41
largest peak, e/Å^3	0.63

of finding a way to isolate and prove the structure of the $Mo_2(Et_2B(pz)_2)_4$ molecule, which we believed to be the only compound of the Mo_2^{4+} unit, or indeed any other multiply bonded M_2^{n+} unit, to contain only chelating ligands.[4] We have, in fact, demonstrated the existence of such a compound, but not the one we had in view at the outset.

Experimental Section

All manipulations were carried out under an atmosphere of dry argon. Solvents were dried over Na–K alloy or P_2O_5, distilled immediately before use, and transferred by syringe.

Synthesis and Crystallization of $Mo_2[Et_2B(pz)_2]_2[Et_2B(OH)pz]_2 \cdot 2CH_3CN$. Reaction of $Mo_2(O_2CCH_3)_4$[5] (0.43 g, 1 mmol) with 1.36 g (6 mmol) of $Na(pz)_2BEt_2$[6] in refluxing toluene by the method of Collins et al.[1] afforded, following chromatography on Florisil with benzene, a single intense blue band. After elution and removal of solvent the oily residue was dissolved in a minimum of acetonitrile. Crystallization overnight at −10 °C produced large moderately air-sensitive turquoise crystals.

The elemental composition of the isolated crystals was shown by X-ray crystallography (vide infra) not to be the expected tetrakis(diethyldipyrazolylborato)dimolybdenum complex, $Mo_2[Et_2B(pz)_2]_4$, as suggested by Collins et al.[1] but rather the complex $Mo_2[Et_2B(pz)_2]_2[Et_2B(OH)pz]_2 \cdot 2CH_3CN$ containing two partially hydrolyzed pyrazolylborate ligands; presumably adventitious water in the acetonitrile was responsible. A number of further attempts to crystallize the unhydrolyzed compound have been unsuccessful.

Collection and Reduction of X-ray Data. Crystals of the title complex were mounted in capillary tubes with use of degassed epoxy cement. Despite this, decomposition caused by either oxidation or solvent loss occurred and a multiple data set was necessary. Data were collected on two approximately equidimensional crystals, and the two sets of data were matched on the basis of three intensity standards [2,12,−10; 2,10,−9; 3,7,−11]. At the outset of each data collection counting statistics for these standard reflections differed by less than 1% between the two crystals, and the successful refinement of structure indicated the reliability of the method used.

Intensity data were collected at room temperature on an Enraf-Nonius CAD-4 automated diffractometer where automatic location and centering of 25 reflections (23° ≤ 2θ ≤ 31°) provided the unit cell parameters presented in Table I. A preliminary survey of the intensity data established systematic absences in $h0l$ for $h + l = 2n$ and $0k0$ for $k = 2n$, indicating the space group $P2_1/n$. The intensity data were collected to $2\theta = 50°$ by using the ω–2θ method and a scan range determined by $\Delta\omega = (0.85 + 0.35 \tan\theta)°$ with a 25% extension at either end for background determination. Standard data collection procedures have been previously summarized,[7] and the specific CAD-4 operating parameters used here are presented in Table I. Of the 7291 symmetry-independent reflections measured, all those with intensities $I \geq 3\sigma(I)$ (5100) were used in subsequent calculations. Standard deviations were estimated from counting statistics. Data were reduced to unscaled, observed structure factor amplitudes after correction for Lorentz and polarization factors. With $\mu = 5.545$ cm^{-1} no absorption correction was deemed necessary.

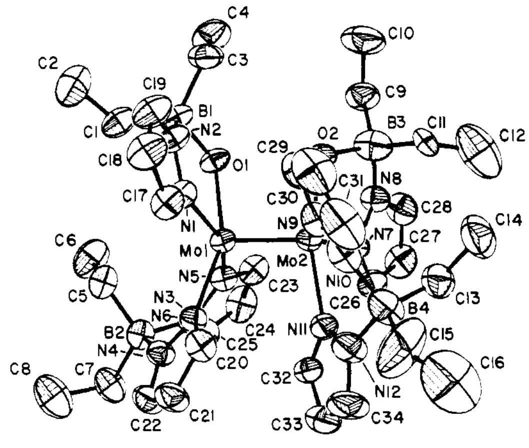


Figure 1. Computer-drawn representation of the entire $Mo_2[Et_2B(pz)_2]_2[Et_2B(OH)pz]_2$ molecule, showing the atom labeling scheme. Each atom is represented by its ellipsoid of thermal vibration scaled to enclose 40% of the electron density.

Solution and Refinement of the Structure. The structure was solved by Patterson and Fourier methods and refined[7] by full-matrix least squares. The positions of the two molybdenum atoms were obtained through a three-dimensional Patterson synthesis. Three cycles of isotropic least-squares refinement gave values of $R_1 = 0.32$ and $R_2 = 0.41$ where the R_i are defined as

$$R_1 = \sum(||F_o| - |F_c||)/\sum|F_o|$$

$$R_2 = [\sum w(|F_o| - |F_c|)^2/\sum w(|F_o|)^2]^{1/2}$$

Subsequent least-squares cycles and difference Fourier maps located all anticipated atoms except for two incomplete pyrazole rings. The only located atoms in both of these expected rings proved to be oxygen and require reformulation of the complex as $Mo_2[Et_2B(pz)_2]_2[Et_2B(OH)pz]_2$. Two acetonitrile molecules of crystallization completed the total of 60 nonhydrogen atoms; however, the relatively large isotropic thermal parameters of one of these solvent molecules suggested that decomposition by partial loss of solvent may have occurred during data collection. All nonsolvent and nonhydrogen atoms were anisotropically refined to discrepancy indices of $R_1 = 0.097$ and $R_2 = 0.126$. Hydrogen atoms (except those on the acetonitrile molecules) were introduced at calculated positions and their contributions included in F_c values, but they were not refined. Inclusion of these atoms in the refinement gave convergence at $R_1 = 0.044$ and $R_2 = 0.056$. The error in an observation of unit weight was 1.579, and the largest shift/error ratio in the final cycle was 0.02. A final difference synthesis showed random fluctuations not exceeding ±0.63 e/Å^3.

Final positional and thermal parameters are given in Table II. Values of F_o vs. F_c for the 5100 observed data are available as supplementary material.

Results and Discussion

The complete molecular structure is shown in Figure 1, where the labeling scheme for the atoms is defined. Because

---

(4) A possible exception is the $[Mo_2(en)_4]^{4+}$ ion, which has never been characterized structurally: Bowen, A. R.; Taube, H. *Inorg. Chem.* **1974**, *13*, 2245.

(5) Brignole, A. B.; Cotton, F. A. *Inorg. Synth.* **1972**, *13*, 87.

(6) Trofimenko, S. *J. Am. Chem. Soc.* **1967**, *89*, 6288.

(7) Bino, A.; Cotton, F. A.; Fanwick, P. E. *Inorg. Chem.* **1979**, *18*, 3558. All crystallographic computing was performed on a PDP 11/60 computer at the Molecular Structure Corp., College Station, TX, using a modified version of the Enraf-Nonius structure determination package.

Table II. Positional and Thermal Parameters and Their Estimated Standard Deviations for $Mo_2[Et_2B(pz)_2]_2[Et_2B(OH)pz]_2 \cdot 2CH_3CN^{a,b}$

atom	*x*	*y*	*z*	*B*(1,1)	*B*(2,2)	*B*(3,3)	*B*(1,2)	*B*(1,3)	*B*(2,3)
Mo(1)	0.00175 (5)	−0.17582 (2)	−0.25149 (2)	2.39 (2)	2.62 (2)	2.98 (2)	0.00 (2)	−0.43 (2)	−0.08 (2)
Mo(2)	−0.03984 (5)	−0.16130 (2)	−0.16063 (2)	2.48 (2)	2.64 (2)	2.99 (2)	−0.17 (2)	−0.23 (2)	0.14 (2)
O(1)	−0.1164 (4)	−0.2586 (2)	−0.2694 (2)	2.8 (2)	2.8 (2)	5.0 (2)	0.1 (1)	−0.6 (2)	−0.7 (1)
O(2)	−0.1576 (4)	−0.2443 (2)	−0.1511 (2)	2.4 (2)	2.7 (1)	4.9 (2)	0.0 (1)	0.5 (2)	0.2 (1)
N(1)	0.1442 (5)	−0.2532 (2)	−0.2478 (2)	2.9 (2)	3.4 (2)	3.5 (2)	0.5 (2)	−0.3 (2)	−0.1 (2)
N(2)	0.0928 (5)	−0.3126 (2)	−0.2576 (2)	4.0 (3)	2.9 (2)	4.4 (2)	0.7 (2)	−0.8 (2)	−0.5 (2)
N(3)	0.1558 (5)	−0.1083 (2)	−0.2676 (2)	3.1 (2)	3.1 (2)	3.2 (2)	−0.2 (2)	−0.2 (2)	0.1 (2)
N(4)	0.1569 (5)	−0.0706 (2)	−0.3162 (2)	3.9 (3)	3.3 (2)	3.0 (2)	−0.5 (2)	−0.4 (2)	0.5 (2)
N(5)	−0.1341 (5)	−0.1109 (2)	−0.2967 (2)	2.8 (2)	3.2 (2)	3.5 (2)	0.1 (2)	−0.4 (2)	0.0 (2)
N(6)	−0.0899 (5)	−0.0686 (2)	−0.3373 (2)	3.8 (3)	3.4 (2)	3.4 (2)	0.2 (2)	−0.6 (2)	0.2 (2)
N(7)	−0.2333 (5)	−0.1205 (2)	−0.1526 (2)	3.0 (2)	2.8 (2)	4.2 (2)	−0.0 (2)	0.4 (2)	0.2 (2)
N(8)	−0.3279 (5)	−0.1642 (2)	−0.1386 (2)	2.5 (2)	3.8 (2)	4.9 (2)	−0.1 (2)	0.2 (2)	0.2 (2)
N(9)	0.1183 (5)	−0.2042 (2)	−0.1111 (2)	3.1 (2)	5.3 (2)	3.3 (2)	0.4 (2)	−0.5 (2)	0.6 (2)
N(10)	0.1969 (5)	−0.1728 (3)	−0.0711 (2)	3.4 (3)	6.7 (3)	4.0 (2)	−0.8 (2)	−0.4 (2)	0.9 (2)
N(11)	0.0496 (5)	−0.0697 (2)	−0.1449 (2)	4.0 (3)	3.6 (2)	3.3 (2)	−1.1 (2)	−0.1 (2)	−0.4 (2)
N(12)	0.1377 (6)	−0.0573 (3)	−0.1012 (2)	5.9 (3)	6.0 (3)	3.7 (2)	−3.0 (2)	−1.1 (2)	0.1 (2)
C(1)	−0.0433 (7)	−0.3268 (3)	−0.3553 (3)	4.8 (4)	3.9 (3)	5.1 (3)	0.2 (3)	−1.3 (3)	−1.1 (2)
C(2)	0.0317 (9)	−0.3837 (4)	−0.3778 (4)	8.5 (6)	6.9 (4)	6.1 (4)	1.7 (4)	−0.1 (4)	−1.4 (3)
C(4)	−0.2608 (8)	−0.3934 (3)	−0.2751 (4)	4.5 (4)	5.5 (3)	8.7 (5)	−1.8 (3)	−0.4 (4)	−2.0 (3)
C(3)	−0.1207 (8)	−0.3819 (3)	−0.2524 (3)	5.8 (4)	2.9 (3)	6.5 (4)	−0.3 (3)	0.4 (3)	0.6 (3)
C(5)	0.0534 (7)	−0.1475 (3)	−0.3953 (3)	3.9 (3)	5.1 (3)	3.8 (3)	0.8 (3)	−0.5 (3)	−0.5 (2)
C(6)	−0.0605 (9)	−0.1625 (4)	−0.4374 (3)	7.2 (5)	7.0 (4)	5.1 (3)	0.7 (4)	−1.9 (3)	−1.6 (3)
C(7)	0.0693 (7)	−0.0211 (3)	−0.4147 (3)	4.6 (4)	6.3 (3)	4.0 (3)	0.1 (3)	−0.1 (3)	1.6 (3)
C(8)	0.1793 (9)	−0.0311 (4)	−0.4563 (3)	6.8 (5)	10.3 (5)	5.7 (4)	−0.0 (5)	0.1 (4)	3.0 (4)
C(9)	−0.3982 (7)	−0.2832 (3)	−0.1426 (3)	3.9 (3)	4.4 (3)	6.8 (4)	−1.4 (3)	0.6 (3)	−0.4 (3)
C(10)	−0.3784 (9)	−0.3517 (4)	−0.1234 (4)	7.9 (5)	5.1 (4)	10.2 (6)	−2.9 (4)	0.8 (5)	0.7 (4)
C(11)	−0.2461 (8)	−0.2347 (3)	−0.0503 (3)	4.4 (4)	4.2 (3)	3.1 (3)	−0.5 (3)	1.0 (3)	0.9 (2)
C(12)	−0.3363 (11)	−0.2061 (6)	−0.0106 (4)	8.0 (6)	16.1 (8)	7.4 (5)	−0.0 (6)	−0.7 (5)	4.9 (5)
C(13)	0.0248 (8)	−0.1076 (3)	−0.0136 (3)	6.9 (5)	5.7 (3)	3.8 (3)	−1.5 (3)	−0.3 (3)	0.3 (3)
C(14)	0.0251 (9)	−0.1534 (4)	0.0389 (3)	8.9 (6)	9.4 (5)	4.1 (3)	−2.3 (5)	0.5 (4)	0.7 (3)
C(15)	0.2943 (12)	−0.0788 (5)	−0.0105 (4)	15.8 (8)	11.8 (6)	5.5 (4)	1.9 (6)	−5.5 (4)	−3.4 (4)
C(16)	0.2651 (13)	−0.0324 (7)	0.0268 (5)	10.2 (8)	17 (1)	12.0 (8)	−0.5 (8)	−1.8 (7)	3.6 (7)
C(17)	0.2705 (6)	−0.2610 (3)	−0.2335 (3)	2.4 (3)	4.8 (3)	5.2 (3)	0.5 (3)	−0.5 (3)	−0.5 (3)
C(18)	0.3029 (7)	−0.3242 (3)	−0.2337 (3)	4.3 (4)	5.0 (3)	6.7 (4)	1.7 (3)	−0.9 (3)	−0.0 (3)
C(19)	0.1887 (7)	−0.3557 (3)	−0.2485 (3)	5.4 (4)	3.7 (3)	6.7 (4)	1.7 (3)	−1.1 (3)	−0.4 (3)
C(20)	0.2654 (6)	−0.0940 (3)	−0.2364 (3)	2.6 (3)	5.3 (3)	3.6 (3)	−0.3 (3)	−0.8 (2)	0.3 (2)
C(21)	0.3370 (7)	−0.0482 (3)	−0.2642 (3)	3.8 (3)	5.3 (3)	4.9 (3)	−2.0 (3)	−0.1 (3)	0.1 (3)
C(22)	0.2648 (7)	−0.0345 (3)	−0.3139 (3)	4.4 (3)	4.7 (3)	4.0 (3)	−1.5 (3)	0.3 (3)	0.5 (2)
C(23)	−0.2640 (7)	−0.0991 (3)	−0.2906 (3)	4.0 (3)	4.3 (3)	4.4 (3)	1.0 (3)	−0.9 (3)	−0.1 (2)
C(24)	−0.3047 (7)	−0.0508 (3)	−0.3266 (3)	3.8 (3)	6.3 (3)	5.3 (3)	2.5 (3)	−0.9 (3)	−0.1 (3)
C(25)	−0.1937 (7)	−0.0328 (3)	−0.3553 (3)	5.3 (4)	4.4 (3)	4.8 (3)	2.0 (3)	−0.9 (3)	0.9 (3)
C(26)	−0.2940 (7)	−0.0642 (3)	−0.1564 (3)	5.1 (4)	3.2 (2)	5.1 (3)	0.8 (3)	0.4 (3)	0.1 (2)
C(27)	−0.4244 (7)	−0.0699 (3)	−0.1451 (3)	3.8 (3)	5.1 (3)	6.5 (4)	2.0 (3)	0.5 (3)	−0.0 (3)
C(28)	−0.4420 (7)	−0.1336 (3)	−0.1342 (3)	3.3 (3)	5.5 (3)	6.2 (4)	0.5 (3)	0.9 (3)	0.5 (3)
C(29)	0.1549 (7)	−0.2658 (3)	−0.1096 (3)	4.7 (4)	5.5 (3)	4.3 (3)	1.2 (3)	−0.2 (3)	1.6 (3)
C(30)	0.2556 (9)	−0.2746 (4)	−0.0697 (4)	5.9 (4)	8.4 (4)	7.3 (4)	2.6 (4)	−0.1 (4)	3.2 (3)
C(31)	0.2792 (8)	−0.2172 (4)	−0.0466 (3)	3.7 (4)	11.2 (5)	5.6 (4)	0.3 (4)	−1.6 (3)	3.1 (4)
C(32)	0.0357 (7)	−0.0167 (3)	−0.1774 (3)	5.9 (4)	3.1 (2)	3.6 (3)	−0.8 (3)	0.3 (3)	−0.2 (2)
C(33)	0.1126 (9)	0.0303 (3)	−0.1545 (3)	10.7 (6)	5.1 (3)	5.2 (4)	−3.3 (4)	1.3 (4)	0.3 (3)
C(34)	0.1796 (9)	0.0026 (4)	−0.1069 (3)	11.3 (5)	7.2 (4)	5.2 (4)	−6.3 (3)	−1.3 (4)	−0.2 (3)
B(1)	−0.0505 (8)	−0.3224 (3)	−0.2855 (3)	4.4 (4)	2.6 (3)	4.5 (3)	0.1 (3)	−1.0 (3)	−0.7 (2)
B(3)	−0.2846 (8)	−0.2344 (3)	−0.1184 (3)	5.2 (4)	4.9 (3)	7.3 (4)	−0.4 (3)	−0.0 (4)	0.7 (3)
B(2)	0.0472 (8)	−0.0776 (3)	−0.3672 (3)	3.4 (4)	4.3 (3)	3.3 (3)	0.3 (3)	−0.6 (3)	0.0 (3)
B(4)	0.1613 (9)	−0.1041 (4)	−0.0465 (3)	5.2 (5)	7.1 (4)	3.7 (3)	−2.3 (4)	−1.1 (3)	0.7 (3)

atom	*x*	*y*	*z*	*B*, Å^2	atom	*x*	*y*	*z*	*B*, Å^2
N(S1)	0.3714 (8)	0.2410 (3)	0.3257 (3)	7.9 (2)	H(11A)	−0.1647 (0)	−0.2129 (0)	−0.0456 (0)	5.0000 (0)
N(S2)	0.4786 (12)	0.0571 (5)	0.5906 (5)	15.8 (4)	H(11B)	−0.2350 (0)	−0.2780 (0)	−0.0388 (0)	5.0000 (0)
C1(S1)	0.4717 (9)	0.2278 (4)	0.3442 (4)	6.7 (2)	H(12A)	−0.3016 (0)	−0.2095 (0)	0.0283 (0)	5.0000 (0)
C1(S2)	0.4791 (14)	0.0804 (6)	0.5447 (6)	12.7 (4)	H(12B)	−0.3482 (0)	−0.1624 (0)	−0.0203 (0)	5.0000 (0)
C2(S1	0.6053 (10)	0.2124 (5)	0.3681 (4)	8.8 (3)	H(12C)	−0.4185 (0)	−0.2275 (0)	−0.0135 (0)	5.0000 (0)
C2(S2)	0.4684 (14)	0.1150 (6)	0.4918 (6)	12.9 (4)	H(13A)	−0.0415 (0)	−0.1211 (0)	−0.0409 (0)	5.0000 (0)
HO(1)	−0.2094 (0)	−0.2560 (0)	−0.2675 (0)	5.0000 (0)	H(13B)	0.0046 (0)	−0.0661 (0)	0.0001 (0)	5.0000 (0)
H(1A)	−0.1306 (0)	−0.3288 (0)	−0.3711 (0)	5.0000 (0)	H(14A)	−0.0588 (0)	−0.1528 (0)	0.0560 (0)	5.0000 (0)
H(1B)	−0.0019 (0)	−0.2892 (0)	−0.3688 (0)	5.0000 (0)	H(14B)	0.0441 (0)	−0.1954 (0)	0.0260 (0)	5.0000 (0)
HO(2)	−0.1329 (0)	−0.2846 (0)	−0.1662 (0)	5.0000 (0)	H(14C)	0.0901 (0)	−0.1403 (0)	0.0670 (0)	5.0000 (0)
H(2A)	0.0312 (0)	−0.3827 (0)	−0.4193 (0)	5.0000 (0)	H(15A)	0.3553 (0)	−0.0631 (0)	−0.0376 (0)	5.0000 (0)
H(2B)	0.1199 (0)	−0.3823 (0)	−0.3630 (0)	5.0000 (0)	H(15B)	0.3326 (0)	−0.1134 (0)	0.0107 (0)	5.0000 (0)
H(2C)	−0.0089 (0)	−0.4219 (0)	−0.3652 (0)	5.0000 (0)	H(16A)	0.3430 (0)	−0.0187 (0)	0.0469 (0)	5.0000 (0)
H(3A)	−0.2844 (0)	−0.4266 (0)	−0.3016 (0)	5.0000 (0)	H(16B)	0.2271 (0)	0.0024 (0)	0.0058 (0)	5.0000 (0)
H(3B)	−0.3363 (0)	−0.3801 (0)	−0.2549 (0)	5.0000 (0)	H(16C)	0.2044 (0)	−0.0480 (0)	0.0541 (0)	5.0000 (0)
H(4A)	−0.0992 (0)	−0.4119 (0)	−0.2226 (0)	5.0000 (0)	H(17)	0.3301 (0)	−0.2274 (0)	−0.2244 (0)	5.0000 (0)
H(4B)	−0.0618 (0)	−0.3866 (0)	−0.2835 (0)	5.0000 (0)	H(18)	0.3868 (0)	−0.3424 (0)	−0.2253 (0)	5.0000 (0)
H(4C)	−0.1137 (0)	−0.3400 (0)	−0.2369 (0)	5.0000 (0)	H(19)	0.1790 (0)	−0.4006 (0)	−0.2517 (0)	5.0000 (0)
H(5A)	0.1329 (0)	−0.1511 (0)	−0.4158 (0)	5.0000 (0)	H(20)	0.2903 (0)	−0.1130 (0)	−0.2000 (0)	5.0000 (0)
H(5B)	0.0534 (0)	−0.1779 (0)	−0.3645 (0)	5.0000 (0)	H(21)	0.4186 (0)	−0.0300 (0)	−0.2516 (0)	5.0000 (0)
H(6A)	−0.0506 (0)	−0.2044 (0)	−0.4523 (0)	5.0000 (0)	H(22)	0.2879 (0)	−0.0040 (0)	−0.3425 (0)	5.0000 (0)
H(6B)	−0.1408 (0)	−0.1596 (0)	−0.4174 (0)	5.0000 (0)	H(23)	−0.2652 (0)	−0.1323 (0)	−0.2624 (0)	5.0000 (0)

Table II (*Continued*)

atom	*x*	*y*	*z*	*B*, Å²	atom	*x*	*y*	*z*	*B*, Å²
H(6C)	−0.0613 (0)	−0.1329 (0)	−0.4687 (0)	5.0000 (0)	H(24)	−0.3906 (0)	−0.0334 (0)	−0.3310 (0)	5.0000 (0)
H(7A)	−0.0100 (0)	−0.0164 (0)	−0.4373 (0)	5.0000 (0)	H(25)	−0.1905 (0)	0.0002 (0)	−0.3837 (0)	5.0000 (0)
H(7B)	0.0870 (0)	0.0172 (0)	−0.3937 (0)	5.0000 (0)	H(26)	−0.2519 (0)	−0.0252 (0)	−0.1658 (0)	5.0000 (0)
H(8A)	0.1839 (0)	0.0043 (0)	−0.4820 (0)	5.0000 (0)	H(27)	−0.4887 (0)	−0.0371 (0)	−0.1448 (0)	5.0000 (0)
H(8B)	0.2602 (0)	−0.0352 (0)	−0.4349 (0)	5.0000 (0)	H(28)	−0.5231 (0)	−0.1530 (0)	−0.1248 (0)	5.0000 (0)
H(8C)	0.1632 (0)	−0.0688 (0)	−0.4784 (0)	5.0000 (0)	H(29)	0.1162 (0)	−0.2985 (0)	−0.1330 (0)	5.0000 (0)
H(9A)	−0.4804 (0)	−0.2690 (0)	−0.1289 (0)	5.0000 (0)	H(30)	0.2996 (0)	−0.3133 (0)	−0.0603 (0)	5.0000 (0)
H(9B)	−0.3997 (0)	−0.2820 (0)	−0.1841 (0)	5.0000 (0)	H(31)	0.3445 (0)	−0.2085 (0)	−0.0172 (0)	5.0000 (0)
H(10A)	−0.4480 (0)	−0.3772 (0)	−0.1392 (0)	5.0000 (0)	H(32)	−0.0196 (0)	−0.0128 (0)	−0.2114 (0)	5.0000 (0)
H(10B)	−0.2970 (0)	−0.3670 (0)	−0.1372 (0)	5.0000 (0)	H(33)	0.1194 (0)	0.0730 (0)	−0.1680 (0)	5.0000 (0)
H(10C)	−0.3777 (0)	−0.3540 (0)	−0.820 (0)	5.0000 (0)	H(34)	0.2442 (0)	0.0229 (0)	−0.0827 (0)	5.0000 (0)

[a] The form of the anisotropic thermal parameter is $\exp[-0.25(h^2a^2B(1,1) + k^2b^2B(2,2) + l^2c^2B(3,3) + 2hkabB(1,2) + 2hlacB(1,3) + 2klbcB(2,3)]$ where *a*, *b*, and *c* are reciprocal lattice constants. [b] Estimated standard deviations in the least significant digits are shown in parentheses.

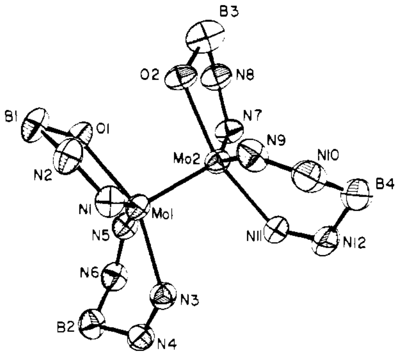


Figure 2. Partial representation of the molecular structure showing only the atoms in the chelate rings and the molybdenum atoms.

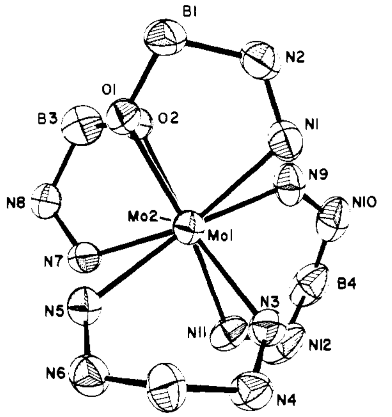


Figure 3. View directly down the Mo–Mo bond of all atoms making up the chelate rings.

the large number of atoms makes it difficult to see the essential features, namely, the Mo_2 unit and the chelate rings, Figure 2 presents another view in which only these 20 atoms are shown. A third view, Figure 3, directly down the Mo–Mo bond, provides an excellent picture of the conformational features of the four ligands. The bond lengths and bond angles are listed in Table III. The torsional angles pertaining to the rotational conformation about the Mo–Mo bond are listed in Table IV.

While the molecule has no crystallographic symmetry, it does have virtual C_2 symmetry, the C_2 axis being a perpendicular bisector of the Mo–Mo bond and of a line that can be drawn between O(1) and O(2). Each pair of ligands is formally gauche with respect to the Mo–Mo bond, but the six Mo–N and two Mo–O bonds which, with the Mo–Mo bond, comprise the coordination spheres of the two molybdenum atoms do not form an exactly eclipsed arrangement. The torsional angles listed in Table IV indicate an average 15.3° twist in a clockwise direction of the coordination sphere of Mo(2) with respect to that of Mo(1). This average includes, however, the low (4.3°) O(1)–Mo(1)–Mo(2)–O(2) angle, which is indicative of the smallest cross Mo–Mo bond steric ligand interaction. Each of the six-membered rings formed by the molybdenum atoms and the pyrazolyl ligands adopts the less sterically demanding boat configuration characteristic of this ligand type.[1] In each case the four nitrogen atoms are virtually coplanar while the molybdenum and boron atoms deviate 0.45 and 0.72 Å from these planes. Despite the staggered arrangement of these bulky ligands, there is also a dihedral angle of 60.2° between the two Mo–N–N–N–N planes. In addition, the boron atoms of the pyrazolylhydroxoborato ligands are distorted, in opposite directions, (by 0.34 and 0.61 Å) out of the approximately coplanar N–N–Mo–O systems, emphasizing the steric demands of this relatively crowded molecule. The MO–Mo–N bond angles and Mo–N bond lengths are typical of those found for chelate ligands in Mo_2^{4+} systems;[1,3] however Mo–O (pyrazolylhydroxoborato) distances of 2.129 (3) and 2.145 (3) Å, which are significantly longer than those found in the (β-ketonato)- and (β-ketoiminato)metal rings (average 2.08 Å),[2,3] yet notably shorter than the Mo–O(CH_3)–(bridging ligand) (average 2.269 Å) bond lengths in $Mo_2(2,6\text{-}(OMe)_2Ph)_4$,[8] give an indication of the differing electronic requirements associated with the various ligand types.

There is another noteworthy pattern in the metal–ligand bonding in this complex. Metal–ligand bond lengths are, when averaged, appreciably longer at Mo(1) than at Mo(2). This is explainable by the evidence for some interaction between solvent molecule S1 and the hydroxo moiety of the pyrazolylhydroxoborato ligand at Mo(1), where N(S1) is only ca. 2.9 Å distant from O(1) and the calculated position for HO(1) is ca. 2.1 Å from Mo(1).

Collins et al.[1] noted that by substituting two acetate groups with two diethylpyrazolylborato ligands in $Mo_2(OOCCH_3)_4$, thereby removing carboxylato π orbitals, which appear extensively involved in metal–metal bonding, a significant increase in Mo–Mo bond length (0.036 Å) is observed. In view of this, it is then not surprising to find that complete substitution of bridging acetate ligands as in the title complex results in a bond length of 2.156 (1) Å, which represents a further increase of 0.027 Å over that in the disubstituted complex $Mo_2(O_2CCH_3)_2(Et_2B(pz)_2)_2\cdot CS_2$.[1] In this light a bond length of approximately 2.165 Å for the slightly more sterically crowded complex $Mo_2(Et_2B(pz)_2)_4$ could be predicted.

As the chemistry of the Mo–Mo quadruple bond has developed, many interesting variations in the Mo–Mo bond lengths have been noted in the Mo_2^{4+} systems. We know, for

---

(8) Cotton, F. A.; Koch, S. A.; Millar, M. *Inorg. Chem.* **1978**, *17*, 2087.

Table III. List of Bond Distances (Å) and Bond Angles (Deg) with Esd's

Distances			
Mo(1)-Mo(2)	2.156 (1)	N(12)-B(4)	1.603 (8)
Mo(1)-O(1)	2.145 (3)	C(1)-C(2)	1.516 (8)
Mo(1)-N(1)	2.176 (4)	C(1)-B(1)	1.605 (8)
Mo(1)-N(3)	2.153 (4)	C(3)-C(4)	1.522 (8)
Mo(1)-N(5)	2.181 (4)	C(3)-B(1)	1.635 (8)
Mo(2)-O(2)	2.129 (3)	C(5)-C(6)	1.518 (8)
Mo(2)-N(7)	2.159 (4)	C(5)-B(2)	1.605 (8)
Mo(2)-N(9)	2.140 (4)	C(7)-C(8)	1.506 (9)
Mo(2)-N(11)	2.153 (4)	C(7)-B(2)	1.630 (8)
O(1)-B(1)	1.547 (6)	C(9)-C(10)	1.515 (8)
O(2)-B(3)	1.527 (7)	C(9)-B(3)	1.629 (8)
N(1)-N(2)	1.368 (5)	C(11)-C(12)	1.442 (11)
N(1)-C(17)	1.327 (6)	C(11)-B(3)	1.596 (8)
N(2)-C(19)	1.343 (7)	C(13)-C(14)	1.537 (8)
N(2)-B(1)	1.588 (8)	C(13)-B(4)	1.602 (10)
N(3)-N(4)	1.365 (5)	C(15)-C(16)	1.334 (13)
N(3)-C(20)	1.341 (6)	C(15)-B(4)	1.652 (11)
N(4)-C(22)	1.333 (6)	C(17)-C(18)	1.365 (7)
N(4)-B(2)	1.598 (7)	C(18)-C(19)	1.372 (8)
N(5)-N(6)	1.371 (5)	C(20)-C(21)	1.375 (7)
N(5)-C(23)	1.355 (7)	C(21)-C(22)	1.366 (7)
N(6)-C(25)	1.351 (6)	C(23)-C(24)	1.364 (7)
N(6)-B(2)	1.582 (7)	C(24)-C(25)	1.376 (8)
N(7)-N(8)	1.373 (5)	C(26)-C(27)	1.366 (8)
N(7)-C(26)	1.336 (6)	C(27)-C(28)	1.373 (8)
N(8)-C(28)	1.333 (7)	C(29)-C(30)	1.365 (9)
N(8)-B(3)	1.603 (7)	C(30)-C(31)	1.333 (10)
N(9)-N(10)	1.368 (6)	C(32)-C(33)	1.355 (8)
N(9)-C(29)	1.344 (7)	C(33)-C(34)	1.395 (9)
N(10)-C(31)	1.363 (8)	N(S1)-C1(S1)	1.128 (8)
N(10)-B(4)	1.592 (9)	C(S1)-C2(S1)	1.485 (10)
N(11)-N(12)	1.349 (5)	N(S2)-C1(S2)	1.159 (14)
N(11)-C(32)	1.342 (6)	C1(S2)-C2(S2)	1.412 (14)
N(12)-C(34)	1.335 (7)		
Angles			
Mo(2)-Mo(1)-O(1)	100.0 (1)	C(10)-C(9)-B(3)	114.3 (5)
Mo(2)-Mo(1)-N(1)	102.5 (1)	C(12)-C(11)-B(3)	118.2 (6)
Mo(2)-Mo(1)-N(3)	103.7 (1)	C(14)-C(13)-B(4)	114.5 (6)
Mo(2)-Mo(1)-N(5)	103.3 (1)	C(16)-C(15)-B(4)	110.0 (10)
O(1)-Mo(1)-N(1)	76.9 (1)	N(1)-C(17)-C(18)	110.6 (5)
O(1)-Mo(1)-N(3)	155.1 (1)	C(17)-C(18)-C(19)	105.5 (5)
O(1)-Mo(1)-N(5)	94.1 (1)	N(2)-C(19)-C(18)	108.6 (5)
N(1)-Mo(1)-N(3)	90.6 (2)	N(3)-C(20)-C(21)	110.7 (5)
N(1)-Mo(1)-N(5)	153.8 (1)	C(20)-C(21)-C(22)	104.6 (5)
N(3)-Mo(1)-N(5)	87.8 (2)	N(4)-C(22)-C(21)	109.6 (5)
Mo(1)-Mo(2)-O(2)	96.3 (1)	N(5)-C(23)-C(24)	110.7 (5)
Mo(1)-Mo(2)-N(7)	110.1 (1)	C(23)-C(24)-C(25)	104.7 (5)
Mo(1)-Mo(2)-N(9)	106.6 (1)	N(6)-C(25)-C(24)	110.3 (5)
Mo(1)-Mo(2)-N(11)	101.2 (1)	N(7)-C(26)-C(27)	111.1 (5)
O(2)-Mo(2)-N(7)	78.3 (1)	C(26)-C(27)-C(28)	104.7 (5)
O(2)-Mo(2)-N(9)	91.0 (2)	N(8)-C(28)-C(27)	109.6 (5)
O(2)-Mo(2)-N(11)	161.8 (1)	N(9)-C(29)-C(30)	110.5 (6)
N(7)-Mo(2)-N(9)	142.6 (2)	C(29)-C(30)-C(31)	105.4 (6)
N(7)-Mo(2)-N(11)	90.8 (2)	N(10)-C(31)-C(30)	110.8 (6)
N(9)-Mo(2)-N(11)	88.9 (2)	N(11)-C(32)-C(33)	109.8 (5)
N(2)-N(1)-C(17)	106.9 (4)	C(32)-C(33)-C(34)	105.1 (5)
N(1)-N(2)-C(19)	108.4 (4)	N(12)-C(34)-C(33)	108.7 (5)
N(1)-N(2)-B(1)	121.8 (4)	O(1)-B(1)-N(2)	101.1 (4)
C(19)-N(2)-B(1)	129.0 (4)	O(1)-B(1)-C(1)	108.6 (4)
N(4)-N(3)-C(20)	106.1 (4)	O(1)-B(1)-C(3)	110.6 (5)
N(3)-N(4)-C(22)	108.9 (4)	N(2)-B(1)-C(1)	109.8 (5)
N(3)-N(4)-B(2)	121.2 (4)	N(2)-B(1)-C(3)	108.7 (4)
C(22)-N(4)-B(2)	129.6 (4)	C(1)-B(1)-C(3)	116.8 (4)
N(6)-N(5)-C(23)	107.0 (4)	O(2)-B(3)-N(8)	102.2 (4)
N(5)-N(6)-C(25)	107.3 (5)	O(2)-B(3)-C(9)	110.5 (5)
N(5)-N(6)-B(2)	121.9 (4)	O(2)-B(3)-C(11)	107.0 (5)
C(25)-N(6)-B(2)	128.7 (5)	N(8)-B(3)-C(9)	107.1 (5)
N(8)-N(7)-C(26)	106.3 (4)	N(8)-B(3)-C(11)	110.1 (5)
N(7)-N(8)-C(28)	108.4 (4)	C(9)-B(3)-C(11)	118.8 (5)
N(7)-N(8)-B(3)	119.5 (4)	N(4)-B(2)-N(6)	106.2 (4)
C(28)-N(8)-B(3)	130.7 (5)	N(4)-B(2)-C(5)	110.0 (4)
N(10)-N(9)-C(29)	106.9 (4)	N(4)-B(2)-C(7)	108.3 (4)
N(9)-N(10)-C(31)	106.5 (5)	N(6)-B(2)-C(5)	109.1 (5)
N(9)-N(10)-B(4)	122.6 (5)	N(6)-B(2)-C(7)	110.1 (4)
C(31)-N(10)-B(4)	128.2 (6)	C(5)-B(2)-C(7)	113.0 (5)
N(12)-N(11)-C(32)	108.0 (4)	N(10)-B(4)-N(12)	108.1 (5)
N(11)-N(12)-C(34)	108.3 (5)	N(10)-B(4)-C(13)	109.5 (5)

Table III *(Continued)*

Angles			
N(11)-N(12)-B(4)	122.8 (4)	N(10)-B(4)-C(15)	106.0 (6)
C(34)-N(12)-B(4)	127.8 (5)	N(12)-B(5)-C(13)	106.5 (6)
C(2)-C(1)-B(1)	114.9 (5)	N(12)-B(4)-C(15)	107.1 (6)
C(4)-C(3)-B(1)	112.4 (5)	C(13)-B(4)-C(15)	119.3 (6)
C(6)-C(5)-B(2)	113.9 (5)	N(S1)-C1(S1)-C2(S1)	178.3 (8)
C(8)-C(7)-B(2)	116.2 (5)	N(52)-C1(S2)-C2(S2)	172.5 (16)

Table IV. Some Molecular Planes and Torsional Angles

atom	dev, Å	atom	dev, Å
(a)[a] Pyrazolylhydroxoborato Ligand at Mo(1) $0.1796x + 0.1063y - 0.9780c = 5.2711$			
O(1)	0.001	N(1)	0.002
Mo(1)	−0.002	N(2)	−0.002
Other Atom			
B(1)	0.341		
Pyrazolylhydroxoborato Ligand at Mo(2)			
O(2)	0.031	N(7)	0.059
Mo(2)	−0.038	N(8)	−0.052
Other Atom			
B(3)	−0.504		
(b)[b] Pyrazolylborato Ligand at Mo(1)			
N(3)	−0.029	N(5)	0.029
N(4)	0.034	N(6)	−0.034
Other Atoms			
Mo(1)	0.645	B(2)	0.716
Pyrazolylborato Ligand at Mo(2)			
N(9)	0.004	N(11)	−0.004
N(10)	−0.004	N(12)	0.004
Other Atoms			
Mo(2)	−0.454	B(4)	−0.655

atom 1	atom 2	atom 3	atom 4	angle, deg
O(1)	Mo(1)	Mo(2)	O(2)	4.3
O(1)	Mo(1)	Mo(2)	N(9)	97.3
O(1)	Mo(1)	Mo(2)	N(11)	−170.6
O(1)	Mo(1)	Mo(2)	N(7)	−75.6
N(1)	Mo(1)	Mo(2)	N(9)	18.6
N(1)	Mo(1)	Mo(2)	N(11)	110.8
N(1)	Mo(1)	Mo(2)	N(7)	−154.2
N(1)	Mo(1)	Mo(2)	O(2)	−74.3
N(3)	Mo(1)	Mo(2)	N(11)	17.1
N(3)	Mo(1)	Mo(2)	N(7)	112.1
N(3)	Mo(1)	Mo(2)	O(2)	−168.1
N(3)	Mo(1)	Mo(2)	N(9)	−75.1
N(5)	Mo(1)	Mo(2)	N(7)	21.1
N(5)	Mo(1)	Mo(2)	O(2)	100.9
N(5)	Mo(1)	Mo(2)	N(9)	−166.1
N(5)	Mo(1)	Mo(2)	N(11)	−73.9

[a] Dihedral angle between planes is 21.7°. [b] Dihedral angle between planes is 60.2°.

example, that when only bridging ligands are present and the molecule is devoid of axial interactions, as the "bite" of the ligand decreases, the metal–metal bond length decreases to a present lower limit of 2.037 (3) Å.[9] In contrast and despite the relatively narrow range of bond lengths observed for the Mo_2^{4+} system, complexes containing only terminal ligands in general exhibit significantly longer bond lengths; these range between 2.134 (1) Å for $(enH_2)_2(Mo_2Cl_8)\cdot 2H_2O$[10] and 2.177 (1) Å for $(NH_4)_4Mo_2(NCS)_8\cdot 6H_2O$.[6] In the compound reported here we have been provided with the first example of a complex containing four chelating ligands, and it gives indications of possible structural trends with this new type of complex. For example, in the present case it is evident that introduction of relatively bulky chelate rings has increased the ligand–ligand repulsive forces, resulting in a relatively long bond length. The δ–δ bond is doubtless weakened, and while the four ligands are staggered with respect to one another, a significant twisting of the usually eclipsed coordination spheres has occurred. It is important to note that Mo–Mo bond lengths in the two known diacetate bis(chelating ligand) complexes $Mo_2(O_2CCH_3)_2(C_6H_5NC(CH_3)C(H)C(CH_3)O)_2$, 2.131 (1) Å,[3] and $Mo_2(O_2CCH_3)_2(C_5H_7O_2)_2$, 2.129 (1) Å,[2] suggests that tetrakischelate coordination with these ligands would result in Mo–Mo bond lengths of ca. 2.16 Å not unlike that in the title complex. In view of the unsuccessful attempts at preparation of $Mo_2(C_6H_5NC(CH_3)C(H)C(CH_3)O)_4$ and $Mo_2(C_5H_7O_2)_4$, both of which should be less sterically crowded molecules, particularly if the partly staggered ligand conformation present in the title complex is duplicated, it is likely that these latter complexes are then simply electronically unfavorable. We intend to continue our studies in this new and important direction with a view to increasing our understanding the versatility of the Mo_2^{4+} unit in accommodating widely differing ligands.

Acknowledgment. We thank the National Science Foundation for financial support. B.W.S.K. is the recipient of a NATO Postdoctoral Fellowship from the National Sciences and Engineering Research Council of Canada.

Registry No. $Mo_2[Et_2B(pz)_2]_2[Et_2B(OH)pz]_2\cdot 2CH_3CN$, 78804-44-1; $Mo_2(O_2CCH_3)_4$, 14221-06-8.

Supplementary Material Available: A table of observed and calculated structure factors (21 pages). Ordering information is given on any current masthead page.

---

(9) Cotton, F. A.; Ilsley, W. H.; Kaim, W. *Inorg. Chem.* **1979**, *18*, 2717.

(10) Brencic, J. V.; Cotton, F. A. *Inorg. Chem.* **1969**, *8*, 2698.