one S_8 molecule, is depicted in Fig. 1 where the atom-numbering scheme is also defined. A unit-cell diagram is shown in Fig. 2.

Ewens & Lister (1938) studied tungsten hexachloride in the vapor phase by electron diffraction. They concluded that in the vapor, WCl_6 exists as regular octahedra with a W—Cl distance of 2·26 (2) Å. The single-crystal X-ray structure of WCl_6 was determined in 1942 and was shown to comprise a distorted hexagonal close-packed array of Cl atoms with W atoms in the octahedral holes. The W atoms are surrounded by a nearly regular octahedron of Cl atoms with an average W—Cl distance of 2·24 Å.

In the compound we report here, the W atom is in the center of a nearly regular octahedron of Cl atoms with an averge W—Cl distance of 2·276 (2) Å. The greatest deviation from regular octahedral angles is 90·8 (1)° for the Cl(2)—W(1)—Cl(5) angle. The S_8 unit assumes the crown ring structure. the average S—S—S angle is 107·9 (1)° and the average S—S bond length is 2·044 (1) Å. These values compare well with those found in naturally occurring orthorhombic sulfur (Caron & Donohue, 1965). The three-dimensional structure is composed of alternating layers of WC_6 and S_8 molecules which are parallel to the *ab* plane.

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Note added in proof: A prior example of S_8 molecules in a crystal of another substance recently came to our attention [A. Müller, M. Römer, H. Bögge, E. Krickemayer & M. Zimmermann (1986). *Z. Anorg. Allg. Chem.* **534**, 69–76].

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trans-(Dimethyl sulfoxide-*O*)(dimethyl sulfoxide-*S*)bis(trifluoroacetato)palladium(II); Alternative Ligation Modes of an Ambidentate Ligand

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Abstract. $[Pd(C_2F_3O_2)_2(C_2H_6OS)_2]$, $M_r = 488{\cdot}69$, monoclinic, $P2_1/c$, $a = 20{\cdot}159\ (3)$, $b = 7{\cdot}498\ (8)$, $c = 23{\cdot}926\ (8)$ Å, $\beta = 101{\cdot}64\ (7)°$, $V = 3542\ (2)$ Å^3, $Z = 8$, $D_x = 1{\cdot}833$ g cm^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 13{\cdot}36$ cm^{-1}, $F(000) = 1920$, $T = 293$ K, $R = 0{\cdot}0582$ for 2836 observed reflections. The two crystallographically independent molecules are substantially identical. Each square complex has a *trans* structure with one S-bonded and one O-bonded dimethyl sulfoxide molecule. Mean dimensions for the S-bonded ligands: Pd—S = 2·205 (4), C—S = 1·78 (1), S—O = 1·45 (1) Å. Mean dimensions for the O-bonded ligands: Pd—O = 2·06 (3), C—S = 1·81 (1), S—O = 1·54 (2) Å. The average of the four Pd—O(CF_3CO_2) distances is 2·011 (9) Å.

Introduction. Dimethyl sulfoxide (dmso), like sulfoxides generally, is an ambidentate ligand, as first discussed nearly thirty years ago (Cotton, Francis & Horrocks, 1960). The factors that determine which way an ambidentate ligand will be found are both steric (not easily evaluated) and electronic (subject to debate). Perhaps the most interesting problem is posed by those rare cases in which two of the same ligand occupy what could be identical sites, sterically and electronically, but adopt opposite modes of attachment. Relatively few are known and only with sulfoxides have they previously been supported by crystallographic proof. We report here one that we encountered recently by chance, *viz.*, $[Pd(OCOCF_3)_2\{Me_2(O)S\}(Me_2SO)]$.

Experimental. The compound was prepared by a modification of the method of Stephenson,

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Morehouse, Powell, Heffer & Wilkinson (1965). Trifluoroacetic acid (45 ml) was added to $Pd_3(CH_3CO_2)_6$ (1·0 g, 1·15 mmol) and the mixture was heated to reflux temperature (346 K). A nearly quantitative amount of a gray-brown solid formed as the mixture was heated. The solid was isolated by filtration, washed with trifluoroacetic acid (*ca* 10 ml) and dried in vacuo. A sample of the brown solid (*ca* 0·4 g) was dissolved in warm acetone (*ca* 20 ml) and 1 ml of dmso was added with stirring. Crystals of composition $[Pd(CF_3CO_2)_2(dmso)_2]$ were formed upon slow evaporation of this solution.

The compound crystallized readily as air-stable orange prisms with well-developed faces. A crystal was mounted with epoxy cement on the end of a glass fiber and examined on an Enraf–Nonius CAD-4 diffractometer. Information pertaining to data collection and refinement is summarized in Table 1. Data of one quadrant ($+h$, $+k$, $\pm l$) were collected up to $(\sin\theta)/\lambda = 0{\cdot}538$ Å^{-1}. Periodically monitored check reflections showed no evidence of decay over the period, 42·6 h, of data collection. The structure was solved by a combination of Patterson analysis and direct methods (*SHELX*86; Sheldrick, 1986) and refinement was carried out by employing the Enraf–Nonius (1979) *Structure Determination Package*. H atoms were omitted from the model and all other atoms were refined with anisotropic displacement parameters using scattering factors from *SHELX*86.

Discussion. The positional parameters and equivalent isotropic thermal parameters are given in Table 2 and two crystallographically independent formula units are depicted in Fig. 1, where the atom-numbering scheme is defined. Table 3 lists the interatomic distances and angles.*

There are two molecules in the asymmetric unit, but they are essentially identical in structure. Palladium displays its usual square coordination and the CF_3CO_2 ligands are in *trans* positions with a mean Pd—O distance of 2·011 (9) Å. The important feature of the structure is that each molecule contains one S-bonded and one O-bonded dmso. The internal dimensions for the two types of dmso ligand are the same within the uncertainties except for the S—O bond lengths, which differ by 0·09 (2) Å, with that in the O-bonded dmso being longer. This difference is qualitatively in accord with expectation (Cotton, Francis & Horrocks, 1960) and quantitatively consistent with previously reported results

Table 1. *Data-collection parameters*

Systematic absences	$h0l$: $l = 2n$; $0k0$: $k = 2n$
Crystal size (mm)	0·3 × 0·5 × 0·15
Data-collection instrument	CAD-4S
Orientation reflections, No., range 2θ(°)	25, 18·38–31·83
Scan method	θ–2θ
Data-collection range 2θ(°)	4–45°
No. of unique data, total	4858
with $F_o^2 > 3\sigma(F_o^2)$	2836
No. of parameters refined	400
Transmission factors, max., min.	0·999, 0·886
R	0·0582
wR*	0·0753
Quality-of-fit indicator	2·084
Largest shift/e.s.d. in final cycle	0·05
Largest peak (e Å^{-3})	1·7

* $w = 1/\sigma^2(|F_o|)$.

Table 2. *Atomic positional parameters and equivalent isotropic displacement parameters* (Å^2) *and their estimated standard deviations for* $[Pd(CF_3COO)_2(Me_2SO)_2]$

The equivalent isotropic displacement factor is $\frac{1}{3}[a^2a^{*2}B_{11} + b^2b^{*2}B_{22} + c^2c^{*2}B_{33} + 2ab(\cos\gamma)a^*b^*B_{12} + 2ac(\cos\beta)a^*c^*B_{13} + 2bc(\cos\alpha)b^*c^*B_{23}]$.

	x	y	z	B_{eq}
Pd(1)	0·98366 (5)	0·1004 (1)	0·65533 (4)	3·22 (2)
S(1)	0·9576 (2)	0·3331 (5)	0·7028 (1)	3·46 (8)
S(2)	1·0448 (2)	−0·1058 (5)	0·5669 (1)	3·89 (8)
F(1)	0·7992 (8)	−0·234 (2)	0·5480 (9)	20·5 (9)
F(2)	0·7628 (6)	−0·094 (2)	0·6082 (6)	13·7 (6)
F(3)	0·7499 (7)	0·000 (2)	0·5259 (7)	15·8 (6)
F(4)	1·2145 (5)	0·181 (2)	0·7034 (8)	14·7 (6)
F(5)	1·2131 (7)	0·366 (4)	0·6422 (9)	27 (1)
F(6)	1·1951 (6)	0·440 (3)	0·718 (1)	28 (1)
O(1)	1·0846 (4)	0·150 (1)	0·6800 (4)	3·8 (2)
O(2)	1·0105 (4)	−0·131 (1)	0·6175 (4)	4·3 (2)
O(3)	0·8856 (4)	0·030 (1)	0·6333 (4)	4·4 (3)
O(4)	1·0133 (4)	0·409 (1)	0·7432 (4)	5·1 (3)
O(5)	1·0761 (5)	0·406 (1)	0·6302 (5)	6·7 (3)
O(6)	0·8855 (7)	0·077 (2)	0·5420 (5)	9·8 (5)
C(1)	0·8941 (6)	0·270 (2)	0·7409 (6)	4·1 (4)
C(2)	0·9191 (7)	0·504 (2)	0·6556 (6)	4·9 (4)
C(3)	1·1043 (5)	0·292 (2)	0·6606 (6)	4·3 (4)
C(4)	1·1770 (8)	0·314 (2)	0·6804 (8)	11·0 (9)
C(5)	1·1311 (7)	−0·181 (2)	0·5950 (6)	5·1 (4)
C(6)	1·0133 (7)	−0·290 (2)	0·5222 (6)	4·9 (4)
C(7)	0·8622 (6)	0·024 (2)	0·5811 (7)	5·3 (5)
C(8)	0·7959 (7)	−0·069 (2)	0·5662 (7)	9·3 (7)
Pd(2)	0·48347 (5)	0·0920 (1)	0·83906 (4)	3·27 (3)
S(3)	0·4548 (2)	0·3254 (5)	0·7831 (1)	3·99 (9)
S(4)	0·5477 (2)	−0·1079 (5)	0·9484 (1)	4·19 (9)
F(7)	0·2900 (7)	−0·232 (2)	0·08369 (8)	18·5 (8)
F(8)	0·2476 (6)	0·016 (2)	0·0222 (7)	16·0 (7)
F(9)	0·2619 (6)	−0·090 (2)	0·9032 (6)	12·9 (5)
F(10)	0·7028 (5)	0·475 (1)	0·8876 (6)	11·0 (5)
F(11)	0·6939 (6)	0·296 (2)	0·8221 (6)	15·3 (7)
F(12)	0·7182 (5)	0·205 (2)	0·9036 (7)	14·9 (6)
O(7)	0·3867 (4)	0·018 (1)	0·8286 (4)	4·4 (2)
O(8)	0·5112 (5)	−0·134 (1)	0·8854 (4)	4·5 (2)
O(9)	0·5821 (4)	0·145 (1)	0·8464 (4)	4·0 (2)
O(10)	0·5104 (5)	0·408 (1)	0·7620 (4)	5·6 (3)
O(11)	0·3850 (6)	0·056 (2)	0·9208 (5)	9·6 (5)
O(12)	0·5756 (5)	0·401 (1)	0·8947 (5)	6·3 (3)
C(9)	0·3917 (7)	0·258 (2)	0·7233 (5)	4·8 (4)
C(10)	0·4122 (9)	0·490 (2)	0·8154 (7)	7·0 (5)
C(11)	0·3620 (6)	0·010 (2)	0·8733 (7)	4·9 (4)
C(12)	0·2946 (7)	−0·074 (2)	0·8608 (7)	8·7 (7)
C(13)	0·5171 (8)	−0·293 (2)	0·9845 (7)	6·3 (5)
C(14)	0·6332 (7)	−0·183 (2)	0·9502 (6)	5·7 (4)
C(15)	0·6039 (5)	0·290 (2)	0·8724 (6)	4·1 (4)
C(16)	0·6774 (6)	0·318 (2)	0·8728 (7)	6·8 (6)

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51898 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

from crystallographic studies (Davies, 1981). The Pd—S distance, 2·205 (4) Å, is appreciably shorter than that found in [$PdCl_2$(S-dmso)$_2$] (2·298 Å) (Bennett, Cotton, Weaver, Williams & Watson, 1967). This may be attributed to the fact that in the present case the other three ligands are not π-acceptors and so the one S-dmso has maximal access to π-electron density on Pd, whereas in [$PdCl_2$(S-dmso)$_2$], all four ligands are competing.

The crystallographically verified occurrence of one S-bonded and one O-bonded dmso in a molecule where the positions available to the two ambidentate ligands are potentially identical has only two (closely similar) precedents among dmso complexes, and few among ambidentate ligands generally. Of the two mixed-ligand ruthenium(II) complexes (*cf.* Davies, 1981), only one, [$RuCl_2$(S-dmso)$_2$(O-dmso)$_2$], has been accurately characterized as to structure (Mercer & Trotter, 1975), and is found to have a coplanar set of ligands comprising Cl_2(S-dmso)$_2$ with one S-dmso and one O-dmso above and below that plane. No conclusion as to the reason or reasons why one ligand is O-bonded and three S-bonded (steric, electronic, or both) was drawn. In a spectroscopic study of a series of Pd complexes, Price, Schramm & Wayland (1970) found variations ranging from all S-bonded, through mixed species, to all O-bonded species, with the [$Pd(dmso)_4$]$^{2+}$ ion having two of

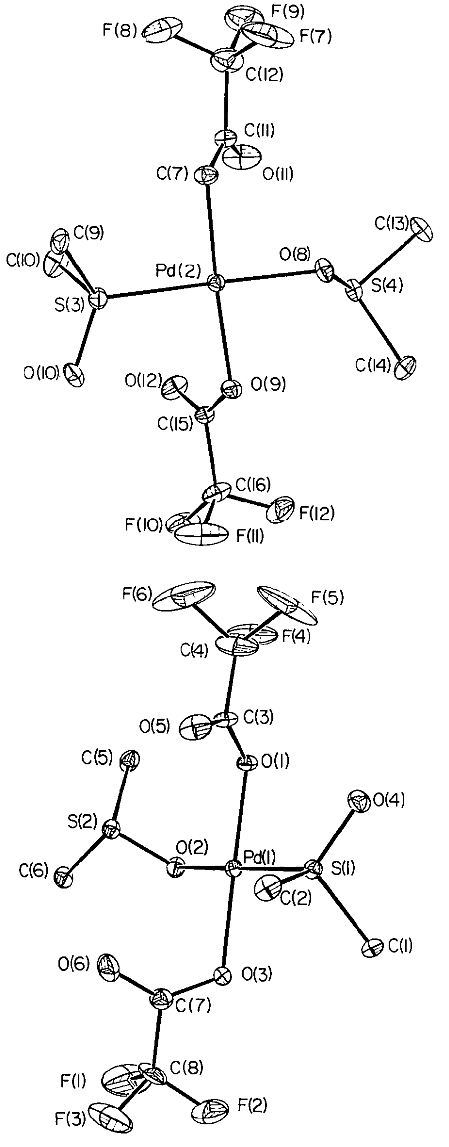

Fig. 1. *ORTEP* (Johnson, 1976) drawings of the two crystallographically distinct molecules. Atoms are represented by their thermal displacement ellipsoids drawn at the 30% probability level.

Table 3. *Bond lengths* (Å) *and angles* (°)

Pd(1)—S(1)	2·203 (4)	Pd(2)—S(3)	2·208 (4)
Pd(1)—O(1)	2·036 (7)	Pd(2)—O(7)	1·995 (9)
Pd(1)—O(2)	2·076 (9)	Pd(2)—O(8)	2·039 (8)
Pd(1)—O(3)	2·011 (8)	Pd(2)—O(9)	2·000 (8)
S(1)—O(4)	1·440 (9)	S(3)—O(10)	1·46 (1)
S(1)—C(1)	1·78 (1)	S(3)—C(9)	1·79 (1)
S(1)—C(2)	1·78 (1)	S(3)—C(10)	1·77 (2)
S(2)—O(2)	1·52 (1)	S(4)—O(8)	1·550 (9)
S(2)—C(5)	1·82 (1)	S(4)—C(13)	1·81 (2)
S(2)—C(6)	1·78 (1)	S(4)—C(14)	1·81 (1)
F(1)—C(8)	1·31 (2)	F(7)—C(12)	1·31 (2)
F(2)—C(8)	1·33 (2)	F(8)—C(12)	1·36 (2)
F(3)—C(8)	1·30 (2)	F(9)—C(12)	1·32 (2)
F(4)—C(4)	1·30 (2)	F(10)—C(16)	1·30 (2)
F(5)—C(4)	1·34 (3)	F(11)—C(16)	1·33 (2)
F(6)—C(4)	1·30 (3)	F(12)—C(16)	1·30 (2)
O(1)—C(3)	1·25 (2)	O(7)—C(11)	1·27 (2)
O(3)—C(7)	1·24 (2)	O(9)—C(15)	1·28 (2)
O(5)—C(3)	1·19 (2)	O(11)—C(11)	1·19 (2)
O(6)—C(7)	1·20 (2)	O(12)—C(15)	1·19 (2)
C(3)—C(4)	1·46 (2)	C(11)—C(12)	1·47 (2)
C(3)—C(4)	1·46 (2)	C(11)—C(12)	1·47 (2)
C(7)—C(8)	1·49 (2)	C(15)—C(16)	1·50 (2)

S(1)—Pd(1)—O(1)	91·9 (3)	S(3)—Pd(2)—O(7)	90·9 (3)
S(1)—Pd(1)—O(2)	174·9 (2)	S(3)—Pd(2)—O(8)	175·7 (3)
S(1)—Pd(1)—O(3)	91·2 (3)	S(3)—Pd(2)—O(9)	91·7 (3)
O(1)—Pd(1)—O(2)	86·9 (3)	O(7)—Pd(2)—O(8)	89·5 (4)
O(1)—Pd(1)—O(3)	175·1 (4)	O(7)—Pd(2)—O(9)	174·8 (4)
O(2)—Pd(1)—O(3)	89·6 (4)	O(8)—Pd(2)—O(9)	87·7 (3)
Pd(1)—S(1)—O(4)	115·1 (4)	Pd(2)—S(3)—O(10)	115·0 (4)
Pd(1)—S(1)—C(1)	109·0 (5)	Pd(2)—S(3)—C(9)	108·6 (5)
Pd(1)—S(1)—C(2)	111·2 (5)	Pd(2)—S(3)—C(10)	112·3 (6)
O(4)—S(1)—C(1)	107·8 (6)	O(10)—S(3)—C(9)	108·4 (6)
O(4)—S(1)—C(2)	108·9 (6)	O(10)—S(3)—C(10)	109·3 (7)
C(1)—S(1)—C(2)	104·4 (6)	C(9)—S(3)—C(10)	102·5 (7)
O(2)—S(2)—C(5)	102·8 (6)	O(8)—S(4)—C(13)	103·2 (6)
O(2)—S(2)—C(6)	102·7 (6)	O(8)—S(4)—C(14)	104·3 (6)
C(5)—S(2)—C(6)	100·3 (7)	C(13)—S(4)—C(14)	99·5 (8)
Pd(1)—O(1)—C(3)	114·9 (7)	Pd(2)—O(7)—C(11)	116·5 (7)
Pd(1)—O(2)—S(2)	116·4 (5)	Pd(2)—O(8)—S(4)	116·7 (5)
Pd(1)—O(3)—C(7)	115·3 (9)	Pd(2)—O(9)—C(15)	116·6 (7)
O(1)—C(3)—O(5)	133 (1)	O(7)—C(11)—O(11)	131 (1)
O(1)—C(3)—C(4)	111 (1)	O(7)—C(11)—C(12)	111 (1)
O(5)—C(3)—C(4)	116 (1)	O(11)—C(11)—C(12)	119 (2)
F(4)—C(4)—F(5)	99 (2)	F(7)—C(12)—F(8)	100 (1)
F(4)—C(4)—F(6)	102 (2)	F(7)—C(12)—F(9)	104 (2)
F(4)—C)4)—C(3)	120 (1)	F(7)—C(12)—C(11)	117 (1)
F(5)—C(4)—F(6)	99 (2)	F(8) C(12) F(9)	100 (1)
F(5)—C(4)—C(3)	118 (2)	F(8)—C(12)—C(11)	115 (1)
F(6)—C(4)—C(3)	116 (1)	F(9)—C(12)—C(11)	118 (1)
O(3)—C(7)—O(6)	130 (1)	O(9)—C(15)—O(12)	131 (1)
O(3)—C(7)—C(8)	114 (1)	O(9)—C(15)—C(16)	111 (1)
O(6)—C(7)—C(8)	116 (1)	O(12)—C(15)—C(16)	118 (1)
F(1)—C(8)—F(2)	101 (2)	F(10)—C(16)—F(11)	102 (1)
F(1)—C(8)—F(3)	102 (2)	F(10)—C(16)—F(12)	105 (1)
F(1)—C(8)—C(7)	115 (1)	F(10)—C(16)—C(15)	118 (1)
F(2)—C(8)—F(3)	103 (1)	F(11)—C(16)—F(12)	101 (1)
F(2)—C(8)—C(7)	117 (1)	F(11)—C(16)—C(15)	114 (1)
F(3)—C(8)—C(7)	117 (2)	F(12)—C(16)—C(15)	115 (1)

each type. They attributed the variations to steric effects. In the present case we believe that electronic factors are likely to be at work, but it is not clear why a mixed species results. There would appear to be room for the two dmso ligands both to adopt the same bonding mode (S- or O-). The structure of this molecule exposes the inadequacy of our understanding of the behavior of ambidentate ligands.

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Bis(benzenethiolato)nitrosyl[tris(3,5-dimethyl-1-pyrazolyl)hydroborato]-molybdenum(II)

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Abstract. $[Mo(C_{15}H_{22}BN_6)(C_6H_5S)_2(NO)]$, $M_r = 641{\cdot}5$, monoclinic, $P2_1/n$, $a = 10{\cdot}898\,(1)$, $b = 18{\cdot}484\,(2)$, $c = 15{\cdot}989\,(2)$ Å, $\beta = 109{\cdot}81\,(1)°$, $V = 3030{\cdot}2$ Å^3, $Z = 4$, $D_x = 1{\cdot}41$, $D_m = 1{\cdot}41$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 5{\cdot}9$ cm^{-1}, $F(000) = 1320$, $T = 293$ K, $wR = 0{\cdot}047$ for 3997 observed reflections. In each complex, the Mo atom is six-coordinate, ligated by a terminal NO group, a tridentate pyrazolylborate ligand and two benzenethiolate ligands. The structure is compared with that of similar complexes and the Mo—S bonding is discussed.

Introduction. The unusual stability of monomeric $[CpMo(NO)(SC_6H_5)_2]$ has been ascribed to $d\pi$–$p\pi$ bonding interactions between the thiolate lone pairs, primarily S $3p$ in character, and the empty Mo $4d_{xy}$ orbital (Ashby & Enemark, 1986). The extent of this interaction is revealed by the torsion angle ON—Mo—S—C; a torsion angle of 0 or 180° maximizes the d_{xy}–p overlap, whereas a torsion angle near 90° leads to an overlap of filled Mo d_{xz} and d_{yz} orbitals with S p orbitals and should not be favored. In $[CpMo(NO)(SC_6H_5)_2]$, these torsional angles are 12 and −174°. In the oxomolybdenum(V) complex $[\{HB(Me_2pz)_3\}MoO(SC_6H_5)_2]$ (Cleland, Barnhart, Yamanouchi, Collison, Mabbs, Ortega & Enemark, 1987) the d_{xz} and d_{yz} orbitals are empty and the complex adopts a structure with O—Mo—S—C torsional angles of −34 and −110°; similar torsion angles occur in $[\{HB(Me_2pz)_3\}MoO(OC_6H_5)_2]$, −49 and −90° (Kipke, Cleland, Roberts & Enemark, 1989). This conformation minimizes overlap of the S p orbital with the half-filled d_{xy} orbital and allows overlap with the empty d_{xz}, d_{yz} orbitals. It was also noted that the rotational conformations of the thiolate ligands place the S $p\pi$ orbitals in the same orientation as the $p\pi$ orbitals on the respective *trans* pyrazole ring, which raises the possibility that the electronic structure of the polypyrazolylborate ligand may influence the overall stereochemistry of the complex. We report here the structure of $[\{HB(Me_2pz)_3\}Mo(NO)(SC_6H_5)_2]$ and compare it to the previously described structures.

Experimental. The complex was prepared as described elsewhere (McCleverty, Drane, Bailey & Smith, 1983). Crystals were grown by slow evaporation of a dichloromethane–hexane solution of the complex.

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