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## The Crystal Structure of Pyridinium $\mu$ -salicylato-tetrachloro- $\mu$ - -oxo- $\mu$ -ethoxo-dioxodimolibdate(V)\*

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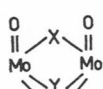
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The crystal structure of the title complex has been determined from diffractometer X-ray intensity data by means of Patterson and Fourier methods and refined by the full matrix least-squares technique to an  $R$  index of 0.060 ( $R_w = 0.064$ ). The crystals are built up of  $\text{pyH}^+$  cations and  $[\text{Mo}_2\text{O}_3\text{Cl}_4(\text{C}_2\text{H}_5\text{O})(\text{HOOC}_6\text{H}_4\text{CO}_2)]^{2-}$  anions. Each molybdenum atom of the binuclear anion is octahedrally coordinated, being bonded to two oxo-oxygen atoms, one terminal (1.669 and 1.670 Å) and one bridging (1.908 and 1.916 Å), one bridging ethoxo-oxygen atom (1.963 and 1.964 Å), one salicylato-oxygen atom (2.295 and 2.317 Å) and two chlorine atoms (from 2.399 to 2.432 Å). The terminal oxo-oxygens occupy a *cis*-position with respect to the  $\text{Mo}_2\text{O}_2$  bridge. The dihedral angle between the two  $\text{MoO}_2$  planes within the bridge amounts to  $164.9^\circ$ . The Mo—Mo bond lengths is 2.646 Å.

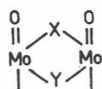
### INTRODUCTION

The study of triply bridged binuclear dioxomolybdenum(V) complexes are of interest because of possible interconversion of mono-, di- and tri-bridged structures in biological systems.<sup>1</sup> They usually contain well established moiety (I) with  $X = Y = Z = \text{O}$  or  $\text{S}$  as in the  $\text{Mo}_2\text{O}_3(\mu - (\text{S},\text{O}) - \text{SCH}_2\text{CH}_2\text{O})$  (oxine)<sub>2</sub><sup>2</sup> or in  $\text{Mo}_2\text{O}_3(\mu - \text{SPh})_2(\text{S}_2\text{CNEt}_2)_2$ .<sup>3</sup> The chlorine or nitrogen atoms may also be included in these triple bridges as has been found in the structures of the complex cation  $[\text{Mo}_2\text{O}_2\text{Cl}(\mu - \text{SPh})_2(\text{S}_2\text{CNEt}_2)_2]^+$  or anion  $[\text{Mo}_2\text{O}_2(\mu - \text{N}_3)\{\text{S}(\text{CH}_2)_3\text{S}\}_3]^-$ .<sup>4,5</sup> Another type (II) of a triple bridge is encountered when the  $\text{Mo}_2\text{O}_2\text{XY}^{2+}$  ( $X = Y = \text{O}$ ) species are in addition bridged by one bidentate ligand such as formate in the structure of the anion  $[\text{Mo}_2\text{O}_4(\text{HCO}_2)(\text{NCS})_4]^{3-}$ , acetate in  $[\text{Mo}_2\text{O}_4(\text{MeCO}_2)(\text{NCS})_4]^{3-}$  or malonate in the tetrameric complex anion of  $[\{\text{Mo}_2\text{O}_4(\text{mal})_2\}_2(\text{mal})]^{6-}$ .<sup>6-8</sup> In contrast to these structures in which the bonds between molybdenum and supplementary bridging atoms are relatively strong (Mo—O 2.230 to 2.336 Å) there are examples in which the supplementary bridging bonds are rather weak (III, IV and V with  $X = Y = \text{O}$  or  $\text{S}$ ). In  $[\text{Mo}_2\text{S}_2\text{O}_2(\text{edta})]^{2-}$  anion<sup>9</sup> the Mo...N bond length amounts to 2.448 Å, in  $\text{Mo}_2\text{O}_3\text{S}(\text{S}_2\text{P}(\text{OPr}^i)_2)_2$  (pyridazine) 2.588 Å (mean value), while in  $\text{Mo}_2\text{O}_3\text{S}(\text{S}_2\text{P}(\text{OPr}^i)_2)_2$  (pyridine) even 2.949 Å (mean value).<sup>10</sup> To describe such weak interactions the authors use the term »crevice coordination«.

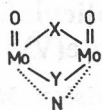
\* Dedicated to Professor D. Grdenić on occasion of his 65th birthday.



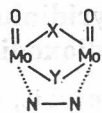
(I)



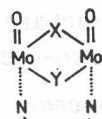
(II)



(III)



(IV)



(V)

In this paper we report another example for the type (II) bridging in which a triple bridge between two molybdenum atoms is realized by the oxo- and ethoxo-oxygen atoms and supplemented by the bidentate salicylato ligand. The complex was described fifty years ago and wrongly formulated as  $(C_5H_6N)_2 [Mo(OH)_5Cl_5OC_6H_4CO_2]$ .<sup>11</sup> Its actual formula is  $(C_5H_6N)_2 [Mo_2O_3Cl_4(C_2H_5O)(HOC_6H_4CO_2)]$ .

#### EXPERIMENTAL

##### Preparation and Crystal Data

The crystals were prepared from salicylic acid, molybdenum(V) chloride and pyridine in ethanolic solution as described by Rosenheim and Nernst.<sup>11</sup>

From oscillation and Weissenberg photographs and single crystal diffractometry,  $CuK\alpha$ ,  $\lambda = 1.5418 \text{ \AA}$ :  $a = 13.643(4)$ ,  $b = 19.340(11)$ ,  $c = 11.146(3)$ ,  $\text{\AA}$ ,  $\beta = 114.07(2)^\circ$ ,  $V = 2685.4 \text{ \AA}^3$ ,  $Z = 4$ ,  $D_{obs} = 1.70 \text{ Mg} \cdot \text{cm}^{-3}$ ,  $D_{calc} = 1.79 \text{ Mg} \cdot \text{cm}^{-3}$ ,  $F(000) = 1432$ ,  $\mu(CuK\alpha) = 120.3 \text{ cm}^{-1}$ , space group  $P2_1/n$ .

##### Intensity Data, Structure Determination and Refinement

The integrated intensities of 1972 independent reflexions from a specimen of dimensions  $0.24 \times 0.03 \times 0.06 \text{ mm}^3$  were collected within the interval  $3^\circ < \theta < 36^\circ$  on a computer controlled automatic diffractometer Philips PW 1100 (graphite monochromatized  $CuK\alpha$  radiation,  $\omega - 2\theta$  scan technique, scan range  $1.6^\circ$ , scan rate  $0.04^\circ \text{ s}^{-1}$ ). Intensities of three standard reflexions 202, 322 and 311, each measured every 120 minutes, showed no significant crystal decomposition. The 1711 reflexions with  $I > 3\sigma(I)$  were used in the structure analysis. The data were corrected for Lorentz and polarization factors but not for absorption and extinction.

The structure was solved by means of three-dimensional Fourier synthesis based upon two molybdenum atom coordinates obtained from Patterson synthesis. The structure was then refined by full matrix least-squares method assigning anisotropic temperature factors to all non-hydrogen atoms. Hydrogens were located either in the difference Fourier maps or generated at fixed positions. Their coordinates and temperature factors were not refined. The final values of the reliability indices  $R$  and  $R_w$  were 0.060 and 0.064 respectively. The function minimized was  $\sum w(|F_o| - |F_c|)^2$  with  $w = 1/\sigma^2(F_o)$ . The atomic scattering factors were taken from International Tables for X-ray Crystallography.<sup>12</sup> Corrections for anomalous scattering were applied for molybdenum atoms only.<sup>13</sup> Final values of atomic coordinates are given in Table I. A list of observed and calculated structure factors can be obtained from the authors on request.

All calculations were carried out on the UNIVAC 1110 computer of the University Computing Centre.

TABLE I

Atomic Coordinates ( $\times 10^4$ , for H atoms  $\times 10^3$ ) and Equivalent Isotropic Thermal Parameters for the non-H atoms with Estimated Standard Deviations in Parentheses

$$B_{\text{eq}} = \frac{4}{3} \sum_i \sum_j b_{ij} a_i a_j$$

Atom	<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	<i>B<sub>eq</sub></i> (Å <sup>2</sup> )
Mo(1)	710(1)	1667(7)	2568(1)	3.87(6)
Mo(2)	551(1)	2912(1)	3457(1)	3.92(6)
Cl(11)	1533(4)	636(3)	3745(5)	5.9(2)
Cl(12)	-386(4)	931(3)	773(5)	6.2(2)
Cl(21)	-725(4)	3864(3)	2785(5)	6.2(2)
Cl(22)	1148(4)	3343(3)	5691(4)	5.4(2)
O(1)	1637(10)	1847(6)	1995(12)	5.7(6)
O(2)	1505(9)	3325(6)	3162(11)	4.8(5)
O(3)	1278(9)	2084(6)	4275(11)	4.4(5)
O(4)	-261(9)	2447(6)	1775(11)	4.6(6)
C(31)	-1266(14)	2576(9)	559(15)	4.9(8)
C(32)	-937(17)	2786(15)	-520(21)	6.3(9)
O(5)	-681(8)	1394(6)	3170(11)	4.6(5)
O(6)	-797(10)	2442(6)	3926(12)	5.1(5)
C(1)	-1038(14)	1820(10)	3789(15)	3.6(7)
C(2)	-1857(14)	1533(10)	4205(16)	4.2(6)
C(3)	-2355(16)	906(11)	3817(18)	4.6(8)
C(4)	-3075(16)	649(11)	4264(21)	6.3(9)
C(5)	-3266(18)	1036(15)	5171(23)	7.4(1)
C(6)	-2734(22)	1679(13)	5640(22)	7.9(1)
C(7)	-1933(20)	2007(14)	5263(23)	10.9(1)
O(7)	-2090(12)	515(9)	2967(16)	9.3(8)
C(11)	806(23)	883(14)	6427(24)	7.6(1)
C(12)	525(24)	634(14)	7321(31)	9.5(2)
C(13)	730(23)	991(19)	8424(29)	8.3(1)
C(14)	1254(27)	1600(18)	8589(26)	9.8(1)
C(15)	1530(22)	1833(14)	7602(29)	9.1(1)
N	1256(14)	1478(13)	6538(17)	6.5(9)
C(21)	2873(23)	28(18)	1585(32)	9.0(2)
C(22)	3416(33)	551(19)	2242(28)	10.6(2)
C(23)	4024(24)	916(13)	1650(35)	10.0(1)
C(24)	4011(21)	716(13)	535(27)	6.7(1)
C(25)	3497(20)	178(15)	-45(21)	7.0(1)
C(26)	2893(18)	-184(11)	470(25)	6.7(10)
HC(31)	-86	286	145	
HC(32)	-115	202	78	
HC(33)	-51	237	-69	
HC(34)	-166	290	-136	
HC(35)	-44	324	-19	
HC(4)	-347	17	392	
HC(5)	-380	86	552	
HC(6)	-303	192	623	
HC(7)	-145	249	573	
HC(11)	63	58	559	
HC(12)	14	16	722	
HC(13)	54	81	917	
HC(14)	146	190	945	
HC(15)	192	231	772	
H(N)	140	167	577	
HC(21)	248	-24	208	
HC(22)	348	76	309	
HC(23)	454	134	215	
HC(24)	440	100	11	
HC(25)	353	2	-90	
HC(26)	250	-62	1	

## DESCRIPTION OF THE STRUCTURE AND DISCUSSION

Selected interatomic distances and bond angles with their standard deviations are given in Table II.

TABLE II

*Selected Interatomic Distances (Å) and Angles (°), with Standard Deviations in Parentheses*

## (a) Distances

Mo(1) — Mo(2)	2.646(2)	O(4) — C(31)	1.51(2)
Mo(1) — Cl(11)	2.399(5)	C(31) — C(32)	1.50(3)
Mo(1) — Cl(12)	2.414(5)	O(5) — C(1)	1.29(2)
Mo(1) — O(1)	1.669(16)	O(6) — C(1)	1.24(2)
Mo(1) — O(3)	1.916(11)	C(1) — C(2)	1.48(3)
Mo(1) — O(4)	1.963(11)	C(2) — C(3)	1.37(3)
Mo(1) — O(5)	2.317(13)	C(2) — C(7)	1.53(3)
Mo(2) — Cl(21)	2.432(6)	C(3) — C(4)	1.36(4)
Mo(2) — Cl(22)	2.430(5)	C(3) — O(7)	1.37(3)
Mo(2) — O(2)	1.670(14)	C(4) — C(5)	1.37(4)
Mo(2) — O(3)	1.908(11)	C(5) — C(6)	1.43(4)
Mo(2) — O(4)	1.964(10)	C(6) — C(7)	1.47(4)
Mo(2) — O(6)	2.295(15)		

## (b) Angles

O(1) — Mo(1) — Cl(11)	97.1(4)	O(2) — Mo(2) — Cl(21)	95.4(4)
O(1) — Mo(1) — Cl(12)	96.6(4)	O(2) — Mo(2) — Cl(22)	94.3(4)
O(1) — Mo(1) — O(3)	103.3(6)	O(2) — Mo(2) — O(3)	101.6(6)
O(1) — Mo(1) — O(4)	98.4(6)	O(2) — Mo(2) — O(4)	102.3(6)
O(1) — Mo(1) — O(5)	174.8(5)	O(2) — Mo(2) — O(6)	174.7(6)
Cl(11) — Mo(1) — Cl(12)	87.5(2)	Cl(21) — Mo(2) — Cl(22)	87.4(2)
Cl(11) — Mo(1) — O(3)	84.1(4)	Cl(21) — Mo(2) — O(3)	161.7(5)
Cl(11) — Mo(1) — O(4)	164.5(5)	Cl(21) — Mo(2) — O(4)	89.9(4)
Cl(11) — Mo(1) — O(5)	84.7(3)	Cl(21) — Mo(2) — O(6)	80.3(3)
Cl(12) — Mo(1) — O(3)	159.2(4)	Cl(22) — Mo(2) — O(3)	84.6(4)
Cl(12) — Mo(1) — O(4)	90.2(3)	Cl(22) — Mo(2) — O(4)	163.4(4)
Cl(12) — Mo(1) — O(5)	78.6(3)	Cl(22) — Mo(2) — O(6)	82.4(3)
O(3) — Mo(1) — O(4)	92.8(5)	O(3) — Mo(2) — O(4)	93.0(5)
O(3) — Mo(1) — O(5)	81.7(5)	O(3) — Mo(2) — O(6)	82.4(5)
O(4) — Mo(1) — O(5)	79.8(5)	O(4) — Mo(2) — O(6)	81.0(5)
Mo(1) — O(3) — Mo(2)	87.6(4)	Mo(2) — O(4) — Mo(1)	84.7(4)
Mo(1) — O(4) — C(31)	137.2(10)	Mo(2) — O(4) — C(31)	137.3(10)
Mo(1) — O(5) — C(1)	122.7(11)	Mo(2) — O(6) — C(1)	123.6(14)
O(5) — C(1) — O(6)	123.2(19)	C(2) — C(3) — O(7)	118.0(21)
O(5) — C(1) — C(2)	115.1(16)	O(4) — C(31) — C(32)	107.8(15)
O(6) — C(1) — C(2)	121.4(19)		

The crystal structure of the title complex is built up of pyridinium cations and  $\mu$ -salicylato-tetrachloro- $\mu$ -oxo- $\mu$ -ethoxo-di-oxodimolibdate(V) anions as shown in Figure 1. The anion (Figure 2.) consists of two molybdenum atoms, each coordinated in a distorted octahedral environment by two oxo-ligands, one terminal and one bridging, one bridging ethoxo-oxygen atom, one salicylato-oxygen atom and two chlorine atoms. Oxygens O(3) and O(4) are shared between two Mo atoms forming a double bridge while the salicylato ligand forms a third supplementary bridge via O(5) and O(6).

The angles at Mo(1) and at Mo(2) range from 78.6° to 103.3° and from 80.3° to 102.3°, respectively. The displacement of the molybdenum atoms out of the equatorial Cl, Cl, O, O, planes towards the terminal oxo-oxygen atoms

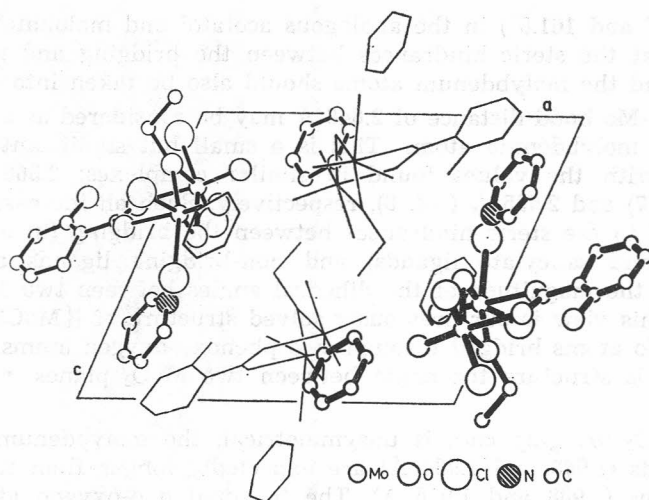


Figure 1. The crystal structure of pyridinium  $\mu$ -salicylato-tetrachloro- $\mu$ -oxo- $\mu$ -ethoxo-dioxodimolybdate(V) projected along the  $b$  axis.

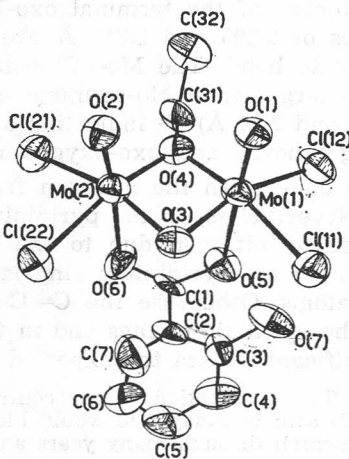


Figure 2. ORTEP drawing of the binuclear  $[\text{Mo}_2\text{O}_3\text{Cl}_4(\text{C}_2\text{H}_5\text{O})(\text{HOC}_6\text{H}_4\text{CO}_2)]^{2-}$  anion, showing the atom numbering scheme. The hydrogen atoms are omitted for clarity.

amounts to 0.330 Å for Mo(1) and 0.318 Å for Mo(2). The  $\text{Mo}_2\text{O}_2$  four-membered ring is folded along the line connecting two bridging oxygen atoms: the dihedral angle between the Mo(1), O(3), O(4) and Mo(2), O(3), O(4) planes is 164.9°, significantly larger than in the other similar complexes containing  $\text{Mo}_2\text{O}_4$  core. It is difficult to say that this can be attributed solely to the small »bite« of the supplementary bridging ligand as has been stated by the authors of the malonato bridged molybdenum(V) complex.<sup>8</sup> It is true that in the double bridged structures the dihedral angles between two  $\text{MoO}_2$  planes have smaller values, e. g. 150.6° in  $[\text{Mo}_2\text{O}_4(\text{oxalato})_2(\text{H}_2\text{O})_2]^{2-}$ , 151° in  $[\text{Mo}_2\text{O}_4(\text{cysteinato})_2]^{2-}$  or 153° in  $[\text{Mo}_2\text{O}_4(\text{NCS})_6]^{4-}$ ,<sup>14-16</sup> but such an angle is of the same value (151.1°) in the triple bridged formate complex<sup>6</sup> and of considerably larger

values (158.1° and 161.0°) in the analogous acetato<sup>7</sup> and malonato<sup>8</sup> complexes. We think that the steric hindrances between the bridging and non-bridging ligands around the molybdenum atoms should also be taken into account.

The Mo—Mo bond distance of 2.646 Å may be considered as a single bond between two molybdenum atoms. This is a small but significant increase in comparison with the values found in similar complexes: 2.566 Å (ref. 6), 2.560 Å (ref. 7) and 2.555 Å (ref. 8), respectively. Such an increase may again be attributed to the steric hindrances between the bridging (in our structure the ethoxo and salicylato ligands) and non-bridging ligands and directly correlated to the magnitude of the dihedral angles between two MoO<sub>2</sub> planes. Supporting this view is our previously solved structure of  $[\{\text{MoCl}_2(\text{OPh})_3\}]_2$  in which two Mo atoms bridged through two phenoxo-oxygen atoms are 2.801 Å apart.<sup>17</sup> In this structure the angle between two MoO<sub>2</sub> planes was, by symmetry, 180°.

The Mo<sub>2</sub>O<sub>2</sub> bridging core is unsymmetrical, the molybdenum to ethoxo-oxygen bonds (1.963 and 1.964 Å) are expectedly longer than those to oxo-oxygen atoms (1.908 and 1.916 Å). The terminal oxo-oxygen atoms are *cis* with respect to the Mo<sub>2</sub>O<sub>2</sub> bridge and the molybdenum to terminal oxo-oxygen bonds of 1.669 and 1.670 Å are of usual values for such bonds.<sup>18,19</sup>

Due to the *trans* influence of the terminal oxo-ligands the molybdenum to salicylato-oxygen bonds of 2.295 and 2.317 Å are longer than one would expect for the Mo—O single bond. The Mo—Cl bond lengths ranging from 2.399 to 2.432 Å are also larger than Mo-terminal chlorine bond lengths in MoCl<sub>3</sub>O and Mo<sub>2</sub>Cl<sub>10</sub> (2.26 and 2.24 Å)<sup>20,21</sup> indicating a weak but obvious *trans* influence of the bridging ethoxo- and oxo-oxygen ligands.

We were not able to distinguish the nitrogen from carbon atoms within the pyridinium cations. Nevertheless, in the pyridinium ring labelled (1) one atom might be considered as nitrogen due to the possible N(1)—H...O(3) hydrogen bond of 2.793 Å. In the pyridinium ring labelled (2) all ring atoms were treated as carbon atoms. Otherwise the C—C and C—O bond lengths and bond angles within the pyridinium rings and in the salicylato and ethoxo ligands do not differ significantly from the expected values.

*Acknowledgements.* — This publication is our contribution to the celebration of Professor Drago Grdenić's 65th birthday. We would like to say our thank for his teaching, his help in our research through many years and above all for his human relationship.

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#### SAŽETAK

#### Kristalna struktura piridinij- $\mu$ -salicilato-tetrakloro- $\mu$ -okso- $\mu$ -etokso-diksodimolibdata(V)

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Kristalna struktura kompleksa u naslovu određena je na osnovi intenziteta refleksa prikupljenih na automatskomu rendgenskom difraktometru. Struktura je riješena s pomoću Pattersonove i Fourierove sinteze i utočnjena metodom najmanjih kvadrata do faktora  $R = 0,060$ . ( $R_w = 0,064$ ). Kristali su izgrađeni od kationa  $\text{pyH}^+$  i aniona  $[\text{Mo}_2\text{O}_8\text{Cl}_4(\text{C}_2\text{H}_5\text{O})(\text{HOC}_6\text{H}_4\text{CO}_2)]^{2-}$ . Oba atoma molibdena binuklearnog aniona oktaedarski su koordinirana tako, da su vezani sa dva atoma okso-kisika, jedan terminalni (1,669 i 1,670 Å) i jedan premosni (1,908 i 1,916 Å), jedan premosni etokso-kisik (1,963 i 1,964 Å), jedan salicilato-kisik (2,295 i 2,317 Å) i dva atoma klora (od 2,399 do 2,432 Å). Terminalni okso-kisikovi atomi nalaze se u *cis*-položaju prema  $\text{Mo}_2\text{O}_2$ -mostu. Dihedralni kut između dviju  $\text{MoO}_2$ -ploha u mostu iznosi  $164,9^\circ$ . Duljina veze Mo—Mo jest 2,646 Å.