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## Key indicators

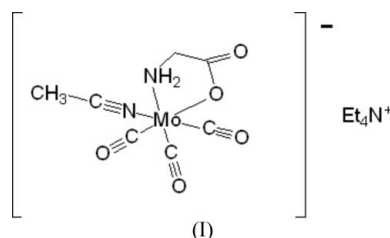
Single-crystal X-ray study  
T = 110 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$   
R factor = 0.023  
wR factor = 0.057  
Data-to-parameter ratio = 20.9For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Tetraethylammonium acetonitriletricarboxyl-  
(glycinato- $\kappa^2\text{N},\text{O}$ )molybdenum(0)

In the title compound,  $(\text{C}_8\text{H}_{20}\text{N})[\text{Mo}(\text{O}_2\text{CCH}_2\text{NH}_2)(\text{NCCH}_3)(\text{CO})_3]$ , obtained from the ligand substitution reaction of  $[\text{Et}_4\text{N}]_3[\text{Mo}_3(\text{CO})_9(\text{OMe})_3]$  with glycine in the solvent acetonitrile the Mo center is in an approximately octahedral geometry.

Received 24 October 2006  
Accepted 9 November 2006

## Comment

Previously we have presented the results of the ligand exchange of the anion of  $[\text{Et}_4\text{N}]_3[\text{Mo}_3(\text{CO})_9(\text{OMe})_3]$  with functionalized aryl alcohols (Adrian *et al.*, 2004). In each of these cases the aryl alcohol caused a break-up of the trimeric unit into a triply bridged dimeric unit. In this study we present the results of the reaction with the amino acid glycine, which shows complete break-up of the trimeric unit into a discrete monomeric complex, (I).



The Mo center is in an approximately octahedral geometry, with three of the coordination sites consisting of three carbonyls with all Mo—C bond lengths in the expected ranges. The glycine ligand chelates to the Mo center through the amine N and one of the carboxylate O atoms. The sixth coordination site is occupied by an acetonitrile solvent molecule. Hydrogen bonding links one of the amine H atoms to the distal O atom of an adjacent molecule.

One tetraethylammonium cation is present to balance the charge of the anion.

Selected geometric parameters are presented in Table 1. All other bond lengths and angles are within expected ranges.

## Experimental

Complex (I) was obtained by the ligand exchange reaction of  $[\text{Et}_4\text{N}]_3[\text{Mo}_3(\text{CO})_9(\text{OMe})_3]$  with 3 equivalents of glycine. In a typical experiment 0.100 g of  $[\text{Et}_4\text{N}]_3[\text{Mo}_3(\text{CO})_9(\text{OMe})_3]$  were dissolved in 20 ml of  $\text{CH}_3\text{CN}$  and 3 equiv. of glycine in 15 ml of  $\text{CH}_3\text{CN}$  were added. This solution was stirred overnight at room temperature. The solvent was then removed at reduced pressure to about 4 ml and the complex was precipitated from the solution by addition of 60 ml diethyl ether, resulting in a yellow solid. Diffraction quality crystals of

(I) were obtained by vapor diffusion of diethyl ether into a concentrated acetonitrile solution.

#### Crystal data

(C<sub>8</sub>H<sub>20</sub>N)[Mo(C<sub>2</sub>H<sub>4</sub>NO<sub>2</sub>)-  
(C<sub>2</sub>H<sub>3</sub>N)(CO)<sub>3</sub>]  
*M<sub>r</sub>* = 425.34  
Monoclinic, *C*2/*c*  
*a* = 12.0407 (8) Å  
*b* = 12.8897 (8) Å  
*c* = 23.4746 (14) Å  
*β* = 97.177 (1)°

*V* = 3614.7 (4) Å<sup>3</sup>  
*Z* = 8  
*D<sub>x</sub>* = 1.563 Mg m<sup>-3</sup>  
Mo *Kα* radiation  
*μ* = 0.76 mm<sup>-1</sup>  
*T* = 110 (2) K  
Block, yellow  
0.18 × 0.14 × 0.10 mm

#### Data collection

Bruker X8 APEX diffractometer  
*φ* and *ω* scans  
Absorption correction: multi-scan  
(*SADABS*; Bruker, 2002)  
*T<sub>min</sub>* = 0.877, *T<sub>max</sub>* = 0.928

24788 measured reflections  
4538 independent reflections  
3956 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.036  
*θ<sub>max</sub>* = 28.5°

#### Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.023  
*wR* (*F*<sup>2</sup>) = 0.057  
*S* = 1.04  
4538 reflections  
217 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0281P)^2 + 3.1028P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
(Δ/σ)<sub>max</sub> = 0.004  
Δρ<sub>max</sub> = 0.40 e Å<sup>-3</sup>  
Δρ<sub>min</sub> = -0.38 e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

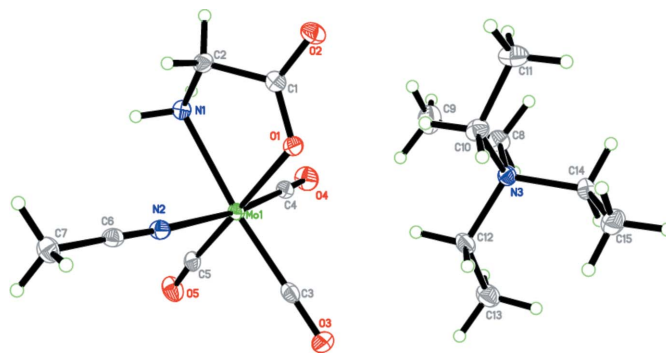
Mo1—O1	2.2195 (11)	Mo1—N1	2.3066 (13)
Mo1—N2	2.2637 (14)		
O1—Mo1—N2	83.82 (4)	N2—Mo1—N1	80.39 (5)
O1—Mo1—N1	74.59 (4)		

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1A...O2 <sup>i</sup>	0.92	2.10	2.9849 (17)	161

Symmetry code: (i)  $-x + 1, -y + 2, -z + 1$ .



**Figure 1**

The molecular structure of (I) with the atom-labeling scheme; displacement ellipsoids are drawn at the 50% probability level

All H atoms were included in calculated positions [N—H = 0.92 Å and C—H = 0.98 (CH<sub>3</sub>) and 0.99 (CH<sub>2</sub>)Å]; isotropic displacement parameters were fixed [*U*<sub>iso</sub>(H) = 1.2*U*<sub>iso</sub>(CH<sub>2</sub>, NH<sub>2</sub>) and 1.5*U*<sub>iso</sub>(CH<sub>3</sub>)].

Data collection: *APEX2* (Bruker, 2003); cell refinement: *APEX2*; data reduction: *SAINT-Plus* (Bruker, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

The Bruker X8 APEX diffractometer was purchased with funds received from the National Science Foundation Major Research Instrumentation Program Grant CHE-0321214. KK thanks the Robert A. Welch Foundation for support (AA-1508).

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