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(Dimethyl sulfoxide-κO)[3-hydroxy-2-hydroxymethyl-2-(3-methoxy-2-oxidobenzylideneamino-κ^2O^2,N)propanolato-κO]dioxomolybdenum(VI). Corrigendum

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Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.022; wR factor = 0.064; data-to-parameter ratio = 12.7.

The crystal structure of the title compound in the paper by Sui, Fang, Luo, Chen & Zhou [*Acta Cryst.* (2006), E**62**, m1994–m1996] has been rerefined to allow for identification of a disordered dimethyl sulfoxide ligand.

The structure reported by Sui *et al.* (2006) has been rerefined. The compound was originally determined by Rao *et al.* [*J. Chem. Soc. Dalton Trans.* (1998), 2383] and has been redetermined here to a significantly higher precision of the lattice parameters [a = 14.3130 (7) Å, b = 9.2596 (5) Å and c = 14.8563 (7) Å here *versus* a = 14.305 (3) Å, b = 9.249 (2) Å and c = 14.860 (3) Å reported by Rao *et al.*], bond lengths and s.u. values [*e.g.* Mo1—O6 = 1.6937 (17) Å here *versus* Mo1—O6 1.697 (4) Å reported by Rao *et al.*; R = 0.022 here *versus* R = 0.050 reported by Rao *et al.*]. The results of the current redetermination allow the identification of a disordered dimethyl sulfoxide ligand and a clarification of the nature of the intra- and intermolecular hydrogen bonding.

Experimental

Crystal data

$[Mo(C_{12}H_{15}NO_5)O_2(C_2H_6OS)]$
M_r = 459.32
Monoclinic, $P2_1/n$
a = 14.3130 (7) Å
b = 9.2596 (5) Å
c = 14.8563 (7) Å
β = 115.324 (1)°
V = 1779.74 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.90 mm^{-1}
T = 295 K
0.56 × 0.39 × 0.35 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.632, T_{max} = 0.746
10668 measured reflections
3278 independent reflections
3056 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.064
S = 1.07
3278 reflections
259 parameters
40 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O5	0.93	2.22	2.874 (3)	127
C14—H14E···O7^{i}	0.96	2.45	3.343 (4)	154
C8—H8A···O6^{ii}	0.96	2.54	3.475 (4)	164
C11—H11A···O7^{iii}	0.97	2.57	3.534 (3)	170
O5—H5A···O1^{iii}	0.82	2.02	2.834 (2)	175
O5—H5A···O2^{iii}	0.82	2.53	2.970 (2)	115
O4—H4···O3^{iv}	0.82	1.99	2.801 (2)	171

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{5}{2}$; (ii) $x, y-1, z$; (iii) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (iv) $-x+1, -y+2, -z+2$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* (Bruker, 2004); data reduction: *APEX2* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXL97* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG9064).

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