After R ($R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, observed reflections only) had been reduced to 0·085 by refinement of the parameters of the non-hydrogen atoms, all hydrogen atoms were located on a difference Fourier synthesis, and were assigned fixed values, $B = 3·3$, for their isotropic thermal parameters. Two final cycles of refinement of all parameters (except the thermal parameters of the hydrogen atoms) gave a final value of $R = 0·062$. The final list of observed and calculated structure factors may be obtained from the authors.

The final positions for all atoms and the final thermal parameters for the non-hydrogen atoms are given in Table 1 and the bond lengths and angles are in Table 2.

Table 2. *Bond lengths and angles*

Mn –O(1)	2·142 (8) Å	C(1)–C(2)	1·515 (16) Å
Mn –O(2)	2·123 (8)	C(2)–C(3)	1·387 (16)
Mn –O(3)	2·257 (8)	C(3)–C(4)	1·406 (16)
O(1)–C(2)	1·284 (11)	C(4)–C(5)	1·493 (16)
O(2)–C(4)	1·291 (11)	O(1)–O(2)	2·907 (10)
O(1)–Mn–O(2)	85·9 (3)°	O(1)–C(2)–C(3)	125·6 (7)°
O(1)–Mn–O(3)	91·2 (3)	O(2)–C(4)–C(3)	124·8 (7)
O(2)–Mn–O(3)	87·8 (3)	O(1)–C(2)–C(1)	115·4 (7)
Mn–O(1)–C(2)	124·7 (5) Å	O(2)–C(4)–C(5)	115·7 (7)
Mn–O(2)–C(4)	124·0 (5)	C(2)–C(3)–C(4)	127·4 (9)
C(5)–C(4)–C(3)	119·5 (9)°		
C(1)–C(2)–C(3)	119·0 (9)		

The structure is essentially identical with that previously reported for the cobalt (Bullen, 1959), nickel (Montgomery & Lingafelter, 1964) and magnesium (Morosin, 1967) compounds. The average Mn–O(acetylacetonate) distance is 2·13 Å, while the Mn–O(water) distance is considerably longer, 2·26 Å. The water molecule is hydrogen-bonded to two oxygen atoms of an adjacent molecule with O···O distances 2·87 and 2·90 Å. The chelate ring O–C–C–C–O is planar with the manganese atom 0·58 Å out of the least-squares plane. One of the methyl carbon atoms is displaced significantly (0·13 Å) from this plane, while the displacement of the other methyl carbon atom (0·06 Å) is probably not significant.

This investigation was supported in part by Grant 9510-31 from the Defence Research Board of Canada and in part by the U.S. National Science Foundation.

References

Bullen, G. J. (1959). *Acta Cryst.* **12**, 703.

Charles, R. G. (1960). *Inorg. Synth.* Vol. VI, p. 164. New York: McGraw Hill.

International Tables for X-ray Crystallography (1962). Vol. III, p. 202. Birmingham: Kynoch Press.

Montgomery, H. & Lingafelter, E. C. (1963). *Acta Cryst.* **16**, 748.

Montgomery, H. & Lingafelter, E. C. (1964). *Acta Cryst.* **17**, 1481.

Morosin, B. (1967). *Acta Cryst.* **22**, 315.

Stewart, J. M. (1964). *Crystal Structure Calculations System X-Ray-63*. Univ. of Maryland TR-64-6.

Stewart, R. F., Davidson, E. R. & Simpson, W. T. (1965). *J. Chem. Phys.* **42**, 3175.

Acta Cryst. (1968). B**24**, 1128

The crystal structure of α-glycylglycine: Correction.

By Edward W. Hughes, *Gates and Crellin Laboratories of Chemistry, California Institute of Technology, Pasadena, California* 91109, *U.S.A.*

(*Received* 19 *April* 1968)

Corrections to lattice constants given in *Acta Cryst.* (1968), B**24**, 40.

The paper of the above title (Biswas, Hughes, Sharma & Wilson, 1968) unfortunately gives lattice constants which are in error by amounts considerably larger than the error estimates listed. The exploratory examination of the α crystals was made in 1939 but the investigation was soon abandoned in favor of that of the β crystals (Hughes & Moore, 1949) and both problems were delayed by World War II. When the research was reinstigated many years later the first rough estimates of the lattice constants were inadvertently substituted for the more accurate values. This error is entirely the fault of the present author and should not reflect on his later colleagues in the structure determination and refinement.

The errors were called to my attention by Dr Hans C. Freeman, who has kindly supplied me with lattice constants determined in his laboratory by a least-squares adjustment based on numerous scattering angle measurements made on a goniometer with Cu $K\alpha$ radiation in the wide range ($\theta > 45°$).

Table 1 gives the old (erroneous) and new (Freeman) values and also the corresponding values for the perdeuteroglycylglycine (Freeman, Paul & Sabine, 1967). Our better

Table 1. *Values for unit-cell dimensions of α-glycylglycine*

	Old	New	Perdeutero
a	7·70 ± 0·02 Å	7·812 ± 0·0024 Å	7·8271 ± 0·0003 Å
b	9·57 ± 0·03	9·566 ± 0·0030	9·5586 ± 0·0006
c	9·48 ± 0·03	9·410 ± 0·0029	9·4251 ± 0·0002
β	124°35′ ± 20′	124°36′ ± 1·0′	124°51′ ± 0·1′
ϱ calc.	1·516 g.cm^{-3}	1·512 g.cm^{-3}	

Table 2. *Bond lengths and angles*

	Old	New		Old	New
N(1)–C(2)	1·497 Å	1·491 Å	C(7)–O(8)	1·262 Å	1·260 Å
C(2)–C(3)	1·528	1·519	C(7)–O(9)	1·239	1·232
C(3)–O(4)	1·249	1·249	N(1)···O(8)	2·712	2·747
C(3)–N(5)	1·328	1·319	N(1)···O(9)	2·729	2·728
N(5)–C(6)	1·462	1·451	N(1)···O(8)	2·782	2·790
C(6)–C(7)	1·516	1·514	N(5)···O(4)	2·966	2·963
Standard deviation	±0·007 Å				
N(1)–C(2)–C(3)	110·3°	109·5°	N(5)–C(6)–C(7)	112·7°	112·4°
C(2)–C(3)–O(4)	120·1	120·4	C(6)–C(7)–O(8)	117·6	117·9
C(2)–C(3)–N(5)	116·8	116·3	C(6)–C(7)–O(9)	115·6	115·5
O(4)–C(3)–N(5)	123·1	123·3	O(8)–C(7)–C(9)	126·7	126·5
C(3)–N(5)–C(6)	121·6	121·2			
Standard deviation	±0·4°				

earlier measurements agree with the new values within their own much larger standard deviations. The differences between the hydrogen and deuterium compounds, although perhaps significant, are now quite small and the earlier remarks (Biswas, Hughes, Sharma & Wilson, 1968 p.50) regarding these discrepancies should be largely disregarded.

Because the chief error is in the length of *a* and because the molecular plane is nearly parallel to (100), the errors have only a small effect on the intramolecular bond lengths and angles. The maximum error is 0·011 Å and the r.m.s. error is ±0·007 Å. Table 2 shows the new values of the bond lengths. The maximum error in an H-bond length is 0·035 Å, for the N(1)···O(8) bond, which is nearly parallel to **a**. Other H-bond lengths (Table 2) and van der Waals contacts have in general much smaller errors, the r.m.s. value being well under 0·01 Å. With the exception of the comments on the perdeutero compound the other arguments given in the original paper still stand. In particular, the old estimates of standard deviations apply to the newly calculated bond lengths and angles given in Table 2.

I am indebted to Dr Freeman for prepublication use of his lattice constants and for the newly calculated bond lengths, which are based on our parameters and the new lattice constants.

References

Biswas, A. B., Hughes, E. W., Sharma, B. D. & Wilson, J. N. (1968). *Acta Cryst.* B**24**, 40.

Freeman, H. C., Paul, G. L. & Sabine, T. M. (1967). Private communication.

Hughes, E. W. & Moore, W. J. (1949). *J. Amer. Chem. Soc.* **71**, 2618.

Acta Cryst. (1968). B**24**, 1129

Crystal data for $UO_2(OAc)_2 . 2Ph_3AsO$ and $[UO_2 (OAc)_2 . Ph_3AsO]_2$.

By Giuliano Bandoli, Rodolfo Graziani and Bruno Zarli, *Centro Chimica delle Radiazioni e dei Radioelementi and Centro Strutturistica Chimica C.N.R. Padova, via Loredan 4, Italy.*

(*Received* 26 *March* 1968)

Crystal data are reported for $UO_2(OAc)_2.2Ph_3AsO$ and $[UO_2(OAc)_2.Ph_3AsO]_2$, which are crystallographically isomorphous with their respective triphenylphosphine analogues.

Four uranyl acetate complexes with triphenylphosphine and triphenylarsine oxides were recently prepared (Volponi, Zarli & Panattoni, 1967). They are $[UO_2(OAc)_2.Ph_3PO]_2$ and $UO_2(OAc)_2.2Ph_3PO$, for which the crystal data were obtained from precession and Weissenberg photographs and have been reported elsewhere (Graziani, Zarli & Bandoli, 1967), and $[UO_2(OAc)_2.Ph_3AsO]_2$ and $UO_2(OAc)_2.2Ph_3AsO$.

From oscillation and precession photographs taken with Cu *Kα* radiation, $[UO_2(OAc)_2.Ph_3AsO]_2$ was shown to be isomorphous with $[UO_2(OAc)_2.Ph_3PO]_2$, the structure of which has been successfully determined (Panattoni, Bandoli, Graziani & Croatto, 1968). The presence of dimers was recognized for both compounds by molecular weight measurements.

X-ray powder diffraction photographs were taken for $UO_2(OAc)_2.2Ph_3AsO$ and $UO_2(OAc)_2.2Ph_3PO$ with Cu *Kα* radiation on a 114·6 mm camera using sodium fluoride as internal standard, and by comparison the compounds were found to be isomorphous. Densities were measured by the flotation method with the use of mixtures of *sym*-tetrabromoethane and *sym*-dichloroethane. The cell di-