

DIVALENT TRANSITION METALS AND MAGNESIUM IN STRUCTURES THAT CONTAIN THE AUTUNITE-TYPE SHEET: ERRATA

ANDREW J. LOCOCK[§]

Mineralogy, Department of Natural History, Royal Ontario Museum, 100 Queen's Park, Toronto, Ontario M5S 2C6, Canada

PETER C. BURNS

*Department of Civil Engineering and Geological Sciences, University of Notre Dame,
156 Fitzpatrick Hall, Notre Dame, Indiana 46556, U.S.A.*

THEODORE M. FLYNN

Department of Geology, University of Illinois, Urbana-Champaign, Illinois 61801, U.S.A.

Owing to incomplete transfer of certain tables from a PC-based system to the typographer's Mac-based system, fractions expressing atom coordinates in Tables 5, 6, 7, 8, 9, 10, 11 and 13 of the above article (*Can. Mineral.* **42**, 1699-1718, 2004) disappeared. The correct tables are reproduced here, with apologies to the authors and readers.

TABLE 5. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS (\AA^2) FOR *MnUAs12*

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
U(1)	0.2325(1)	0.7301(1)	0.0793(1)	0.013(1)
As(1)	0.7491(1)	0.7545(1)	0.0011(1)	0.013(1)
Mn(1)	½	½	½	0.030(1)
O(1)	0.5475(5)	0.6950(5)	0.0935(4)	0.021(1)
O(2)	0.9152(5)	0.7765(5)	0.0883(3)	0.020(1)
O(3)	0.7273(5)	0.9558(4)	-0.0909(4)	0.021(1)
O(4)	0.8084(5)	0.5869(4)	-0.0854(3)	0.021(1)
O(5)	0.2723(5)	0.7682(5)	-0.0784(4)	0.024(1)
O(6)	0.1889(5)	0.6874(5)	0.2380(4)	0.024(1)
O(7)W	-0.2884(7)	0.7053(6)	0.5258(5)	0.041(1)
O(8)W	0.3030(8)	0.7250(6)	0.4527(4)	0.045(1)
O(9)W	-0.0307(6)	0.2901(6)	0.3035(4)	0.040(1)
O(10)W	0.5765(7)	-0.0576(6)	0.6893(4)	0.039(1)
O(11)W	0.6313(7)	0.5003(7)	0.3161(4)	0.041(1)
O(12)W	-0.1988(7)	0.9405(6)	0.3135(5)	0.042(1)

*U*_{eq} is defined as one third of the orthogonalized *U*_{ij} tensor.

TABLE 6. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS (\AA^2) FOR *CoUAs12*

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
U(1)	0.2303(1)	0.7325(1)	0.0800(1)	0.013(1)
As(1)	0.7462(1)	0.7511(1)	-0.0018(1)	0.014(1)
Co(1)	0	0	½	0.027(1)
O(1)	0.5439(8)	0.7736(8)	0.0918(6)	0.020(1)
O(2)	0.9138(8)	0.6921(8)	0.0854(6)	0.021(1)
O(3)	0.8082(8)	0.9535(8)	-0.0961(6)	0.020(1)
O(4)	0.7233(8)	0.5849(8)	-0.0891(6)	0.022(1)
O(5)	0.2718(7)	0.7767(7)	-0.0804(5)	0.017(1)
O(6)	0.1866(8)	0.6878(8)	0.2412(6)	0.023(1)
O(7)W	-0.1942(10)	0.7926(10)	0.4744(7)	0.035(2)
O(8)W	0.2179(10)	0.8124(10)	0.4548(7)	0.038(2)
O(9)W	0.5592(10)	0.9241(10)	0.3134(7)	0.038(2)
O(10)W	0.5606(11)	-0.3020(11)	0.6825(8)	0.042(2)
O(11)W	0.7930(10)	0.4656(10)	0.3068(7)	0.041(2)
O(12)W	0.0022(10)	0.1310(10)	0.3218(7)	0.038(2)

*U*_{eq} is defined as one third of the orthogonalized *U*_{ij} tensor.

[§] E-mail address: andrewl@rom.on.ca

TABLE 7. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS (\AA^2) FOR *MgUAs12*

	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
U(1)	0.7322(1)	0.2300(1)	0.0798(1)	0.012(1)
As(1)	0.7509(1)	0.7457(1)	-0.0015(1)	0.012(1)
Mg(1)	0	0	½	0.028(1)
O(1)	0.7759(6)	0.2688(6)	-0.0797(4)	0.011(1)
O(2)	0.6863(7)	0.1871(7)	0.2401(5)	0.021(1)
O(3)	0.7726(7)	0.5427(7)	0.0922(5)	0.019(1)
O(4)	0.6926(7)	0.9131(7)	0.0864(5)	0.021(1)
O(5)	0.5854(7)	0.7254(7)	-0.0894(5)	0.020(1)
O(6)	0.9546(7)	0.8049(7)	-0.0959(5)	0.019(1)
O(7)W	0.8013(8)	-0.1966(8)	0.4748(6)	0.034(1)
O(8)W	0.1286(9)	0.0028(9)	0.3236(6)	0.039(2)
O(9)W	0.8163(9)	0.2132(9)	0.4508(6)	0.039(2)
O(10)W	0.4675(9)	0.7906(9)	0.3071(6)	0.040(2)
O(11)W	0.0789(9)	0.4415(9)	0.6868(6)	0.039(2)
O(12)W	0.3002(9)	0.4404(9)	0.3149(6)	0.041(2)

U_{eq} is defined as one third of the orthogonalized U_{ij} tensor.

TABLE 8. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS (\AA^2) FOR *NiUAs12*

	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
U(1)	0.2301(1)	0.7327(1)	0.0802(1)	0.013(1)
As(1)	0.7458(1)	0.7511(1)	-0.0018(1)	0.014(1)
Ni(1)	0	0	½	0.025(1)
O(1)	0.5437(4)	0.7756(5)	0.0926(3)	0.022(1)
O(2)	0.9133(4)	0.6899(5)	0.0869(3)	0.023(1)
O(3)	0.8065(4)	0.9530(4)	-0.0956(3)	0.021(1)
O(4)	0.7231(4)	0.5848(4)	-0.0894(3)	0.022(1)
O(5)	0.2711(4)	0.7764(5)	-0.0806(3)	0.028(1)
O(6)	0.1858(4)	0.6878(5)	0.2424(3)	0.024(1)
O(7)W	-0.1892(5)	0.7975(6)	0.4726(3)	0.033(1)
O(8)W	0.2148(5)	0.8173(6)	0.4544(3)	0.035(1)
O(9)W	0.0034(5)	0.1287(6)	0.3253(3)	0.040(1)
O(10)W	0.4404(5)	0.0746(6)	0.6835(4)	0.037(1)
O(11)W	0.7893(6)	0.4653(6)	0.3082(4)	0.040(1)
O(12)W	0.4374(5)	0.3013(6)	0.3187(4)	0.042(1)
H(1)	-0.3020(60)	0.7770(100)	0.4410(60)	0.050
H(2)	-0.1970(90)	0.8940(70)	0.4070(40)	0.050
H(3)	0.2020(90)	0.7560(90)	0.3860(40)	0.050
H(4)	0.3160(60)	0.8980(80)	0.4170(50)	0.050
H(5)	-0.0310(90)	0.2530(40)	0.2970(60)	0.050
H(6)	0.0700(80)	0.1060(100)	0.2500(30)	0.050
H(7)	0.4470(90)	0.1080(100)	0.7600(30)	0.050
H(8)	0.4330(90)	-0.0560(30)	0.7140(60)	0.050
H(9)	0.8360(80)	0.5430(70)	0.2340(30)	0.050
H(10)	0.8100(90)	0.5440(90)	0.3670(50)	0.050
H(11)	0.5580(50)	0.3570(90)	0.3180(60)	0.050
H(12)	0.3470(80)	0.3720(80)	0.2750(50)	0.050

U_{eq} is defined as one third of the orthogonalized U_{ij} tensor.
 U_{eq} of H atoms constrained during refinement.

TABLE 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS (\AA^2) FOR *NiUP12*

	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
U(1)	-0.2646(1)	0.7316(1)	0.0729(1)	0.011(1)
P(1)	0.2493(1)	0.7536(1)	0.0019(1)	0.012(1)
Ni(1)	0	½	½	0.023(1)
O(1)	0.0599(4)	0.7039(5)	0.0866(4)	0.020(1)
O(2)	0.4087(4)	0.7690(5)	0.0827(3)	0.020(1)
O(3)	-0.3056(5)	0.6880(5)	0.2359(3)	0.020(1)
O(4)	0.2311(5)	0.9453(5)	-0.0818(3)	0.019(1)
O(5)	0.2993(5)	0.5939(5)	-0.0789(4)	0.020(1)
O(6)	-0.2246(6)	0.7717(5)	-0.0887(3)	0.028(1)
O(7)W	0.1300(7)	0.5052(7)	0.3234(4)	0.036(1)
O(8)W	-0.2068(7)	0.3103(6)	0.4708(4)	0.032(1)
O(9)W	0.1896(7)	0.2801(6)	0.5438(4)	0.034(1)
O(10)W	0.4728(6)	0.2917(7)	0.3046(5)	0.035(1)
O(11)W	0.9245(6)	0.0609(7)	0.3113(5)	0.035(1)
O(12)W	0.3075(7)	0.9332(7)	0.3185(5)	0.040(1)
H(1)	0.1390(110)	0.1550(60)	0.5740(80)	0.050
H(2)	-0.2730(100)	0.2050(80)	0.5180(70)	0.050
H(3)	0.2560(60)	0.4500(110)	0.3170(90)	0.050
H(4)	0.2650(100)	0.3110(120)	0.6030(60)	0.050
H(5)	0.8680(110)	0.0710(120)	0.2370(40)	0.050
H(6)	-0.1500(110)	0.2480(110)	0.4040(50)	0.050
H(7)	0.5600(90)	0.3280(110)	0.2310(40)	0.050
H(8)	0.3600(110)	0.8850(120)	0.2460(50)	0.050
H(9)	0.0460(60)	0.0370(120)	0.2680(70)	0.050
H(10)	0.5600(100)	0.2830(120)	0.3640(60)	0.050
H(11)	0.3740(100)	0.0530(60)	0.2990(80)	0.050
H(12)	0.0510(100)	0.5470(120)	0.2610(60)	0.050

U_{eq} is defined as one third of the orthogonalized U_{ij} tensor.
 U_{eq} of H atoms constrained during refinement.

TABLE 10. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS (\AA^2) FOR *MnUP10*

	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
U(1)	0	0.2091(1)	½	0.013(1)
P(1)	0	0.2482(1)	0	0.016(1)
Mn(1)	0	0	0	0.042(1)
O(1)	0	0.1209(2)	½	0.024(1)
O(2)	0	0.2966(2)	½	0.027(1)
O(3)	0.0371(5)	0.2035(1)	0.1743(5)	0.023(1)
O(4)	0.3264(5)	0.2075(1)	0.5354(5)	0.023(1)
O(5)W	0.2991(7)	0.4203(3)	0.4268(7)	0.055(1)
O(6)W	0.1116(16)	0	-0.2925(16)	0.087(3)
O(7)W	0.0542(9)	0.4151(4)	0.7897(9)	0.072(2)

U_{eq} is defined as one third of the orthogonalized U_{ij} tensor.

TABLE 11. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS (\AA^2) FOR *CoUP10*

	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
U(1)	0.4503(1)	0.2083(1)	0.9805(1)	0.009(1)
Co(1)	0	½	0	0.023(1)
P(1)	0.9484(3)	0.2515(1)	0.9779(3)	0.011(1)
O(1)W	0.5941(14)	0.0035(4)	0.2187(13)	0.039(2)
O(2)	0.4074(10)	0.2015(4)	0.3070(9)	0.019(1)
O(3)	0.4862(10)	0.2042(4)	0.6538(9)	0.019(1)
O(4)	0.1247(8)	0.2082(4)	-0.0614(10)	0.018(1)
O(5)	0.7790(9)	0.2047(4)	0.0213(10)	0.018(1)
O(6)	0.4545(10)	0.2975(4)	0.9848(9)	0.022(1)
O(7)	0.4463(9)	0.1193(4)	0.9789(9)	0.020(1)
O(8)W	0.2295(12)	0.5714(4)	0.0721(12)	0.031(2)
O(9)W	0.8283(12)	0.5817(4)	0.9404(12)	0.032(2)
O(10)W	0.0229(12)	0.0837(5)	0.7426(13)	0.038(2)
O(11)W	0.9350(18)	0.0739(6)	0.1491(17)	0.066(4)

U_{eq} is defined as one third of the orthogonalized U_{ij} tensor.
The largest residual peak in the difference Fourier map is at x 0.6541, y 0.2084, z 0.0672, height 16.5 $e/\text{\AA}^3$; the nearest atoms are: O(5) 0.93 \AA , U(1) 1.53 \AA , P(1) 2.31 \AA . The next largest peak has height 4.6 $e/\text{\AA}^3$. See text for discussion.

TABLE 13. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS (\AA^2) FOR *MgUAs10*

	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
U(1)	0.0592(1)	0.2044(1)	0.0227(1)	0.015(1)
As(1)	-0.4395(2)	0.2511(1)	0.0263(2)	0.016(1)
Mg(1)	-½	½	0	0.033(2)
O(1)	-0.2585(15)	0.2000(5)	-0.0214(15)	0.018(2)
O(2)	0.0561(17)	0.2922(6)	0.0168(16)	0.026(3)
O(3)	-0.4844(16)	0.3008(6)	-0.1584(14)	0.020(2)
O(4)	-0.6280(20)	0.2020(6)	0.0780(20)	0.034(3)
O(5)	-0.3940(15)	0.3040(6)	0.2065(15)	0.021(2)
O(6)	0.0614(14)	0.1161(5)	0.0261(13)	0.015(2)
O(7)W	-0.3320(20)	0.5798(6)	0.0700(19)	0.035(3)
O(8)W	-0.4100(20)	0.5039(6)	-0.2700(20)	0.041(3)
O(9)W	-0.7218(19)	0.5677(7)	-0.0720(20)	0.040(3)
O(10)W	-0.5240(20)	0.0816(8)	0.2670(20)	0.045(4)
O(11)W	-0.4190(40)	0.0739(11)	-0.1570(30)	0.099(9)

U_{eq} is defined as one third of the orthogonalized U_{ij} tensor.