JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1997, 119(33), 7901-7902, DOI:10.1021/ja971667x

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at http://pubs.acs.org/page/copyright/permissions.html

ACS Publications
MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1997 American Chemical Society

Table 1: Calculated and Observed X-ray Powder diffraction Pattern for $Na_4Cu_2(UO_2)S_4$ (Cu radiation)

h	k	l	d_{calc}/(Å)	d_{obs}/(Å)	I/I_{max} obs (%)
0	0	2	6.80	6.72	3.87
1	0	0	6.63	6.57	100.00
0	1	2	5.73	5.70	18.43
1	1	0	5.63	5.60	16.20
1	1	-1	5.43	5.39	5.42
0	2	0	5.33	5.29	4.14
1	0	-2	5.11	5.08	2.59
0	2	1	4.961	4.942	5.69
1	1	-2	4.605	4.577	5.88
1	2	0	4.153	4.132	3.44
1	1	2	4.109	4.091	2.77
1	2	-1	4.070	4.052	4.03
1	2	-2	3.686	3.671	5.03
1	2	2	3.417		
0	0	4	3.399	3.387	7.47
2	1	0	3.166		
0	3	2	3.148	3.143	11.35
1	1	-4	3.071	3.054	9.02
1	2	3	2.940	2.905	8.95
1	3	-2	2.916		
2	2	-1	2.822	2.809	46.01
1	1	4	2.772	2.760	3.15
2	2	-2	2.714	2.700	13.73
1	3	-3	2.660	2.646	6.09
1	2	4	2.527	2.515	11.74
2	2	2	2.501		
2	1	-4	2.483	2.487	9.13
1	4	-1	2.454		
2	3	0	2.424	2.411	3.57
1	4	-2	2.362		

Table 1: (cont.)

h	k	l	d_{calc}/(Å)	d_{obs}/(Å)	I/I_{max} obs (%)
0	4	3	2.297	2.288	5.05
2	2	3	2.276		
0	1	6	2.216	2.200	11.92
1	1	-6	2.191		
1	2	5	2.191		
3	2	-2	2.027	2.026	4.50
1	5	1	1.9947	1.9776	3.71
3	1	2	1.9872		
2	4	-3	1.9518	1.9393	8.45
3	1	-4	1.9467		
0	1	7	1.9106		
0	4	5	1.9029	1.9034	3.92
2	3	4	1.8867		
3	0	-6	1.7020		
3	4	0	1.7010		
1	3	-7	1.7000		
0	0	8	1.6993	1.6953	3.68
2	2	-7	1.6924		
4	0	0	1.6577	1.6525	23.27
3	4	-3	1.6503	1.6473	13.08
2	1	-8	1.5854	1.5807	4.81

Table 2: Crystallographic Data for $Na_4Cu_2(UO_2)S_4$

	$Na_4Cu_2(UO_2)S_4$
a, Å	6.693(4)
b, Å	10.656(7)
c, Å	13.722(6)
α, °	
β, °	97.81(4)
γ, °	
V, $Å^3$	969.7(9)
space group	$P2_1/c$
Z	4
F.W., g/mol	617.32
d_{calc}, g/cm^3	4.228
μ, cm^{-1}	60.7
transmission factors	0.63-0.83
crystal dimensions, mm^3	0.012 x 0.20 x 0.20
radiation	Mo Kα
2θ max.	60°
data collection temp., °C	23
# data collected	3199
# unique data	2821
# $F_o^2>3\sigma$	1980
# of variables	118
R/Rw, %	3.5/4.0
final Dif. map max. peak, $e^-/Å^3$	1.72

[a] $R= \Sigma(|Fo|-|Fc|)/\Sigma|Fo|$ $Rw=\{\Sigma w(|Fo|-|Fc|)^2/\Sigma w|Fo|^2\}^{1/2}$

Table 3 Fractional Atomic Coordinates and B_{eq}[a] values for $Na_4Cu_2(UO_2)S_4$ with Estimated Standard Deviations in Parentheses

atom	x	y	z	B_{eq}
U	0.12525(6)	0.21546(4)	0.37179(2)	0.53(1)
Cu(1)	0.0528(3)	0.3923(2)	0.5464(1)	1.81(6)
Cu(2)	0.1700(2)	0.0188(1)	0.2132(1)	1.31(5)
S(1)	0.3471(4)	0.2860(3)	0.5423(2)	1.13(9)
S(2)	-0.1772(4)	0.3787(3)	0.4090(2)	0.92(9)
S(3)	0.4041(4)	0.0346(3)	0.3443(2)	1.02(9)
S(4)	0.0913(4)	0.1597(3)	0.1959(2)	1.3(1)
Na(1)	0.4429(7)	-0.2371(5)	0.2550(3)	1.9(2)
Na(2)	0.549(1)	0.4951(5)	0.6091(4)	2.8(2)
Na(3)	0.154(1)	0.0890(6)	0.6396(4)	2.7(2)
Na(4)	0.3182(8)	-0.1499(6)	0.4927(4)	2.2(2)
O(1)	0.264(1)	0.3323(8)	0.3049(5)	1.1(3)
O(2)	-0.018(1)	0.0998(8)	0.4353(5)	1.3(3)

[a] B values for anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameters defined as $B_{eq} = (4/3)[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)$.

U values for TS_NACCUUOS1/A4229D/NACUUO2S2

6

atom	U11	U22	U33	U12	U13	U23
U(1)	0.0067(2)	0.0063(2)	0.0071(1)	-0.0010(2)	0.0013(1)	-0.0003(2)
Cu(1)	0.0199(8)	0.030(1)	0.0173(6)	0.0094(7)	-0.0038(6)	-0.0097(6)
Cu(2)	0.0186(7)	0.0170(7)	0.0136(6)	0.0014(6)	0.0002(5)	-0.0040(5)
S(1)	0.011(1)	0.017(1)	0.014(1)	0.001(1)	-0.0013(9)	-0.002(1)
S(3)	0.012(1)	0.011(1)	0.014(1)	0.005(1)	-0.002(1)	-0.003(1)
S(2)	0.012(1)	0.011(1)	0.012(1)	-0.000(1)	0.000(1)	0.001(1)
S(4)	0.011(1)	0.024(2)	0.014(1)	0.003(1)	0.000(1)	-0.008(1)
Na(1)	0.013(2)	0.033(3)	0.025(2)	-0.004(2)	0.003(2)	0.007(2)
Na(2)	0.034(3)	0.017(3)	0.049(3)	0.003(3)	-0.010(3)	-0.000(3)
Na(3)	0.038(4)	0.038(4)	0.026(3)	-0.017(3)	0.003(2)	-0.005(2)
Na(4)	0.020(3)	0.031(3)	0.033(3)	0.005(3)	0.011(2)	0.007(2)
O(1)	0.016(4)	0.015(4)	0.013(3)	-0.001(3)	0.009(3)	-0.007(3)
O(2)	0.019(4)	0.016(4)	0.018(3)	-0.003(4)	0.011(3)	0.003(3)

Table 4: Selected Bond Distances (Å) and Angles (°) for $Na_4Cu_2(UO_2)S_6$ with standard deviations in parentheses

U-S(1)	2.702(3)	Cu(1)-S(1)	2.280(3)
U-S(2)	2.769(3)	Cu(1)-S(2)	2.271(3)
U-S(3)	2.745(3)	Cu(1)-S(2)'	2.624(4)
U-S(4)	2.707(3)	Cu(1)-S(4)	2.446(3)
U-O(1)	1.869(8)	Cu(2)-S(2)	2.251(3)
U-O(2)	1.849(8)	Cu(2)-S(3)	2.22693)
U-Cu(1)	3.137(2)	Cu(2)-S(4)	2.293(4)
U-Cu(2)	3.065(2)	Cu(1)-Cu(2)	2.503(2)
		Cu(1)-Cu(1)'	2.674(4)
S(1)-U-S(2)	89.73(9)	S(2)-Cu(1)-S(2)'	114.2(1)
S(1)-U-S(3)	90.60(9)	S(2)-Cu(1)-S(4)	112.5(1)
S(1)-U-S(4)	176.2(1)	S(2)'-Cu(1)-S(4)	99.4(1)
S(1)-U-O(1)	89.3(2)	S(3)-Cu(2)-S(2)'	124.6(1)
S(1)-U-O(2)	92.1(3)	S(3)-Cu(2)-S(4)	118.5(1)
S(2)-U-S(3)	174.01(9)	S(2)'-Cu(2)-S(4)	116.8(1)
S(2)-U-S(4)	89.19(9)	U-S(1)-Cu(1)	77.55(9)
S(2)-U-O(1)	95.6(3)	U-S(2)-Cu(1)	114.2(1)
S(2)-U-O(2)	83.9(3)	U-S(2)-Cu(2)	100.9(1)
S(3)-U-S(4)	90.86(9)	Cu(1)-S(2)-Cu(1)	65.8(1)
S(3)-U-O(1)	90.4(3)	Cu(1)-S(2)-Cu(2)	119.7(1)
S(3)-U-O(2)	90.1(3)	Cu(1)-S(2)-Cu(2)	61.22(9)
S(4)-U-O(1)	87.19(9)	U-S(3)-Cu(2)	75.33(9)
S(4)-U-O(2)	91.5(3)	U-S(4)-Cu(1)'	125.0(1)
S(1)-Cu(1)-S(2)	116.0(1)	U-S(4)-Cu(2)	75.10(9)
S(1)-Cu(1)-S(2)'	102.7(1)	Cu(1)-S(4)-Cu(2)	63.67(9)
S(1)-Cu(1)-S(4)	110.4(1)		