Anhang

A1 Die Bestimmung der Verzerrung eines Tetraeders

Ein TO_4-Tetraeder besitzt insgesamt sechs O-T-O-Winkel. Im idealen Tetraeder betragen diese Winkel 109,47°, in einem verzerrten Tetraeder weichen die Winkel vom Idealwert ab. Während ein abgeflachtes Tetraeder jeweils vier O-T-O-Winkel <109,47° und zwei >109,47° aufweist, ist es in einem gestreckten genau umgekehrt (die Summe über alle Tetraederwinkel beträgt dabei stets 6×109,47° = 656,82°).

Um ein Maß für die Verzerrung zu erhalten, kann man die drei Kantenabstände, also die Höhen eines Tetraeders, miteinander in Beziehung setzten. Speziell im Falle der Eigensymmetrie $\bar{4}$ bzw. $\bar{4}$m2 sind von den drei Höhen zwei jeweils gleich groß. Nennt man die jeweils gleichen Höhen "m" und die dritte Höhe "n", so stellt das Verhältnis n/m ein Maß für die Verzerrung dar. Im Falle eines abgeflachten Tetraeders ist dann n/m <1, im Falle eines gestreckten ist n/m > 1.

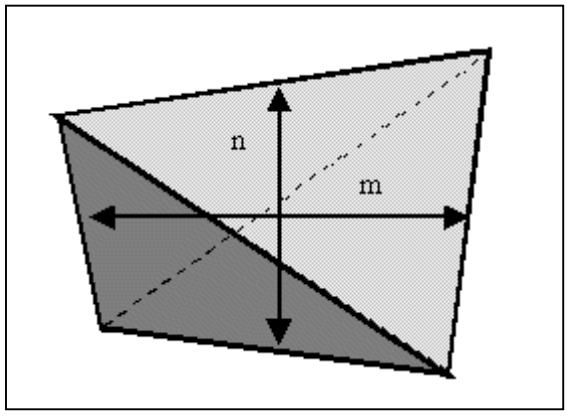

Bild A-1: Tetraedergeometrie

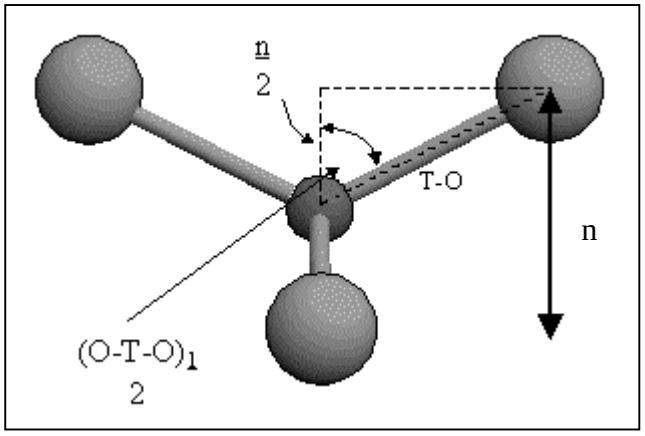

Bild A-2: Berechnung von n im Tetraeder

Wie in Bild A-2 zu erkennen ist, erhält man den Wert n (bzw. m) über den Cosinus des halben Winkels O-T-O und den Abstand T-O. Es gilt:

$$\cos\frac{(O-T-O)_1}{2} = \frac{\frac{n}{2}}{T-O}$$

$$\Leftrightarrow n = 2\times(T-O)\times\cos\frac{(O-T-O)_1}{2}$$

wobei $(O\text{-}T\text{-}O)_1$ der Wert der zwei gleich großen Winkel ist. Auf dieselbe Weise erhält man auch den Wert m. Setzt man nun n und m miteinander in Beziehung, so kürzen sich die Abstände T-O, die gleich groß sind, heraus, und man erhält die einfache Formel:

$$\frac{n}{m} = \frac{\cos\frac{(O-T-O)_1}{2}}{\cos\frac{(O-T-O)_2}{2}}$$

A2 Strukturdaten

Auf den folgenden Seiten sind alle aus den Hochtemperatur-Rietveldverfeinerungen gewonnen Daten tabelliert:

Tabelle A-0: Überblick über die Verfeinerungsparameter aller Rietveldverfeinerungen

Tabelle A-1: Struktur- und Profilparameter für die Rietveldverfeinerungen der Åkermanit-Verbindungen bei Raumtemperatur

Tabelle A-2: Struktur- und Profilparameter für die Hochtemperatur-Rietveldverfeinerungen von $Sr_2CuSi_2O_7$ zwischen 20° und 900°C

Tabelle A3-a: Struktur- und Profilparameter für die Rietveldverfeinerungen von $CuRh_2O_4$, heizend zwischen 20° und 800°C

Tabelle A3-b: Struktur- und Profilparameter für die Rietveldverfeinerungen von $CuRh_2O_4$, kühlend zwischen 800° und 20°C

Tabelle A4-a: Struktur- und Profilparameter für die Rietveldverfeinerungen von $CuCr_2O_4$, heizend zwischen 20° und 800°C

Tabelle A4-b: Struktur- und Profilparameter für die Rietveldverfeinerungen von $CuCr_2O_4$, kühlend zwischen 800° und 20°C

Tabelle A5: Struktur- und Profilparameter für die Hochtemperatur-Rietveldverfeinerungen von $CaCuGe_2O_6$, heizend zwischen 20° und 800°C

Tabelle A-0 Überblick über die Verfeinerungsparameter aller Rietveldverfeinerungen

Verbindung	Temperatur	Globale Parameter	Profilparameter	Intensitätsabhängige Parameter	Anzahl der Reflexe	2θ-Bereich
$Sr_2CuSi_2O_7$	20°C	7	8	16	216	20-140°2θ
$Sr_2CuGe_2O_7$	20°C	8	10	16	231	14-140°2θ
$Sr_2ZnSi_2O_7$	20°C	7	9	16	219	15-140°2θ
$CuRh_2O_4$	20°C	7	8	5	89	17-137°2θ
	650°C	7	8	4	41	17-137°2θ
$CuCr_2O_4$	20°C	1	8	5	82	17-137°2θ
	650°C	1	8	4	39	17-137°2θ
$CaCuGe_2O_6$	20°C	7	13	41	772	16-137°2θ
	500°C	7	11	21	390	16-137°2θ

Tabelle A-1: Struktur- und Profilparameter für die Rietveldverfeinerungen der Åkermanit-Verbindungen bei Raumtemperatur

		$Sr_2CuSi_2O_7$	$Sr_2CuGe_2O_7$	$Sr_2CuZn_2O_7$
a		8.09688 (11)	8.21978 (13)	8.00551 (6)
c		5.07845 (8)	5.24930 (9)	5.17122 (5)
Sr	x	0.33397(8)	0.33476(12)	0.33443(10)
	y	0.16603(8)	0.16524(12)	0.16557(10)
	z	-0.00523(30)	-0.00638(43)	-0.00717(31)
	B	0.668(18)	1.483(35)	0.390(22)
Cu/Zn	x	0	0	0
	y	0	0	0
	z	0.5	0.5	0.5
	B	0.583(40)	1.360(68)	0.439(44)
Si/Ge	x	0.13644(23)	0.13937(13)	0.13791(29)
	y	0.36356(23)	0.36063(13)	0.36209(29)
	z	0.54164(61)	0.52274(46)	0.55300(65)
	B	0.407(62)	1.048(45)	0.137(66)
O1	x	0	0	0
	y	0.5	0.5	0.5
	z	0.65207(181)	0.65790(319)	0.65604(212)
	B	0.983(243)	4.503(542)	0.679(257)
O2	x	0.13661(65)	0.13666(88)	0.13959(77)
	y	0.36339(65)	0.36334(88)	0.36041(77)
	z	0.22001(113)	0.19388(162)	0.24767(137)
	B	0.925(160)	1.423(233)	0.832(194)
O3	x	0.08125(58)	0.08105(109)	0.08133(69)
	y	0.19607(58)	0.18716(126)	0.19433(66)
	z	0.67561(101)	0.67342(213)	0.69901(118)
	B	0.988(116)	6.819(324)	0.583(130)
zero		0.0760	-0.0334	-0.0096
u		0.04541	0.01093	0.01171
w		0.01409	0.01473	0.00741
eta		0.64593	0.25382	0.16524
x		0	0.00608	0.00368
Asym1		0.05483	0.01678	-0.09400
Asym2		0.02715	0.04903	0
R_p		12.7	18.5	18.3
R_{wp}		15.9	20.1	19.7
R_{exp}		13.00	16.79	16.75
Chi2		1.49	1.43	1.39
D-W		1.3809	1.5392	1.5631
R_{Bragg}		4.47	5.94	4.53

Tabelle A-2: Struktur- und Profilparameter für die Hochtemperatur-Rietveldverfeinerungen von $Sr_2CuSi_2O_7$ zwischen 20° und 900°C

T [°C]		20	100	200	300	400
a		8.09342 (15)	8.09653 (15)	8.10048 (16)	8.10477 (19)	8.10985 (20)
c		5.07577 (11)	5.08153 (11)	5.08850 (12)	5.09543 (14)	5.10256 (14)
Sr	x	0.33427 (10)	0.33418 (10)	0.33397 (11)	0.33389 (11)	0.33357 (12)
	y	0.16573 (10)	0.16582 (10)	0.16604 (11)	0.16612 (11)	0.16644 (12)
	z	-0.00678 (38)	-0.00711 (39)	-0.00738 (41)	-0.00705 (43)	-0.00731 (44)
	B	0.756 (25)	0.891 (27)	1.142 (30)	1.361 (32)	1.601 (33)
Cu	x	0	0	0	0	0
	y	0	0	0	0	0
	z	0.5	0.5	0.5	0.5	0.5
	B	0.849 (50)	1.052 (53)	1.217 (58)	1.505 (63)	1.665 (66)
Si	x	0.13608 (27)	0.13555 (28)	0.13584 (30)	0.13489 (30)	0.13606 (32)
	y	0.36392 (27)	0.36445 (28)	0.36416 (30)	0.36511 (30)	0.36394 (32)
	z	0.53924 (76)	0.53718 (83)	0.53663 (91)	0.53611 (94)	0.53306 (106)
	B	0.575 (78)	0.775 (82)	1.047 (90)	1.107 (93)	1.490 (99)
O1	x	0	0	0	0	0
	y	0.5	0.5	0.5	0.5	0.5
	z	0.64506 (200)	0.64662 (211)	0.64110 (229)	0.64619 (231)	0.64268 (244)
	B	0.853 (276)	1.455 (302)	2.048 (338)	2.314 (353)	3.032 (388)
O2	x	0.13754 (86)	0.13829 (93)	0.13778 (94)	0.13638 (96)	0.13765 (101)
	y	0.36246 (86)	0.36171 (93)	0.36222 (94)	0.36362 (96)	0.36235 (101)
	z	0.22558 (130)	0.22832 (137)	0.22637 (138)	0.22974 (142)	0.22612 (146)
	B	1.209 (189)	1.971 (208)	1.803 (213)	2.130 (226)	2.661 (242)
O3	x	0.08160 (62)	0.08101 (64)	0.08009 (65)	0.08150 (66)	0.08043 (67)
	y	0.19720 (68)	0.19818 (70)	0.19723 (73)	0.19905 (76)	0.19871 (79)
	z	0.67521 (113)	0.67436 (116)	0.67351 (120)	0.67239 (125)	0.67441 (129)
	B	1.091 (143)	1.413 (151)	1.444 (157)	1.878 (172)	2.100 (178)
zero		-0.0391	-0.0330	-0.0343	-0.0359	-0.0343
u		0.03535	0.03204	0.03302	0.02835	0.02539
w		0.01577	0.01539	0.01533	0.01512	0.01495
eta		0.36309	0.36357	0.35273	0.36224	0.34771
x		0.00562	0.00548	0.00595	0.00599	0.00662
R_p		11.9	12.2	12.9	13.2	13.6
R_{wp}		15.1	15.3	15.8	15.9	16.1
R_{exp}		13.00	12.77	13.05	13.35	13.50
Chi2		1.16	1.20	1.20	1.19	1.20
D-W		1.4888	1.4146	1.4872	1.4173	1.4165
R_{Bragg}		4.03	4.23	4.94	4.78	5.12

Tabelle A2 (Fortsetzung)

T [°C]		500	600	700	800	900
a		8.11383 (23)	8.11891 (25)	8.12436 (29)	8.12913 (31)	8.13431 (27)
c		5.10904 (15)	5.11609 (17)	5.12348 (19)	5.13035 (21)	5.13717 (19)
Sr	x	0.33372 (12)	0.33340 (13)	0.33351 (14)	0.33328 (14)	0.33306 (14)
	y	0.16627 (12)	0.16659 (13)	0.16648 (14)	0.16671 (14)	0.16693 (14)
	z	-0.00713 (45)	-0.00791 (47)	-0.00725 (50)	-0.00708 (50)	-0.00750 (51)
	B	1.773 (37)	1.906 (39)	2.128 (43)	2.254 (45)	2.422 (46)
Cu	x	0	0	0	0	0
	y	0	0	0	0	0
	z	0.5	0.5	0.5	0.5	0.5
	B	1.914 (73)	1.939 (78)	2.117 (84)	2.392 (91)	2.643 (95)
Si	x	0.13517 (33)	0.13486 (35)	0.13498 (36)	0.13482 (36)	0.13437 (37)
	y	0.36483 (33)	0.36514 (35)	0.36502 (36)	0.36518 (36)	0.36563 (37)
	z	0.53565 (104)	0.53220 (120)	0.53266 (124)	0.53181 (126)	0.53215 (130)
	B	1.422 (103)	1.818 (113)	1.781 (117)	1.812 (119)	1.990 (123)
O1	x	0	0	0	0	0
	y	0.5	0.5	0.5	0.5	0.5
	z	0.64219 (258)	0.64401 (263)	0.64058 (288)	0.64337 (275)	0.64386 (299)
	B	3.321 (416)	3.176 (423)	4.050 (482)	3.299 (453)	4.550 (520)
O2	x	0.13736 (104)	0.13724 (108)	0.13582 (111)	0.13580 (112)	0.13610 (120)
	y	0.36264 (104)	0.36276 (108)	0.36418 (111)	0.36420 (112)	0.36390 (120)
	z	0.22796 (152)	0.22769 (160)	0.22908 (163)	0.22742 (166)	0.22884 (178)
	B	2.789 (252)	3.157 (272)	3.075 (284)	3.328 (293)	4.303 (322)
O3	x	0.08087 (69)	0.08132 (69)	0.08045 (74)	0.08087 (74)	0.07965 (75)
	y	0.19898 (81)	0.20046 (84)	0.20063 (92)	0.20119 (93)	0.20169 (96)
	z	0.67390 (133)	0.67066 (136)	0.67362 (153)	0.67206 (158)	0.67348 (163)
	B	2.022 (183)	1.975 (190)	2.778 (218)	2.932 (225)	2.866 (222)
zero		-0.0378	-0.0352	-0.0347	-0.0355	-0.0408
u		0.02819	0.02538	0.02891	0.03097	0.02360
w		0.01432	0.01441	0.01417	0.01399	0.01401
eta		0.37995	0.32106	0.33350	0.30030	0.26346
x		0.00557	0.00716	0.00673	0.00679	0.00588
R_p		14.3	15.0	15.4	15.8	16.5
R_{wp}		16.6	16.9	17.3	17.3	17.7
R_{exp}		13.82	14.15	14.28	14.51	14.64
Chi2		1.20	1.20	1.21	1.19	1.20
D-W		1.4274	1.3739	1.4304	1.4457	1.3623
R_{Bragg}		5.62	5.44	6.19	6.10	6.43

Tabelle A3-a: Struktur- und Profilparameter für die Rietveldverfeinerungen von $CuRh_2O_4$, heizend zwischen 20° und 800°C

T [°C]		20	100	150	200	250
a		6.17409 (13)	6.17546 (13)	6.17664 (13)	6.17732 (13)	6.17797 (13)
c		7.90865 (22)	7.92207 (22)	7.93167 (22)	7.94114 (23)	7.95090 (24)
Cu	x	0	0	0	0	0
	y	0.75	0.75	0.75	0.75	0.75
	z	0.125	0.125	0.125	0.125	0.125
	B	1.125(86)	1.245(86)	1.350(87)	1.483(93)	1.534(100)
Rh	x	0	0	0	0	0
	y	0	0	0	0	0
	z	0.5	0.5	0.5	0.5	0.5
	B	0.400(34)	0.510(33)	0.590(32)	0.613(36)	0.567(38)
O	x	0	0	0	0	0
	y	0.03076(102)	0.03100(97)	0.03095(97)	0.03178(98)	0.03185(100)
	z	0.24775(85)	0.24640(81)	0.24704(83)	0.24535(84)	0.24552(87)
	B	1.496(160)	1.293(155)	1.574(165)	1.545(177)	1.289(186)
zero		-0.0028	0.0062	0.0128	0.0155	0.0192
u		0.07060	0.06558	0.06753	0.06302	0.06376
w		0.01759	0.01679	0.01588	0.01657	0.01559
eta		0.89143	0.87105	0.88152	0.83096	0.80610
x		0.05871	0.06066	0.05172	0.07456	0.07944
Asym		0.01151	0.01139	0.00882	0.00994	0.00918
R_p		19.3	19.2	18.9	19.3	19.9
R_{wp}		22.0	21.3	21.1	21.5	22.2
R_{exp}		13.61	12.53	12.61	12.80	12.86
Chi2		2.61	2.90	2.79	2.82	2.97
D-W		0.9103	0.8241	0.7803	0.8243	0.7773
R_{Bragg}		5.19	5.07	4.74	5.06	5.35

Tabelle A3-a (Fortsetzung)

T [°C]		300	350	400	450	500
a		6.17830 (13)	6.17796 (13)	6.17775 (14)	6.17612 (15)	6.17345 (17)
c		6.17830 (24)	7.97653 (25)	7.98982 (25)	8.00953 (27)	8.03955 (30)
Cu	x	0	0	0	0	0
	y	0.75	0.75	0.75	0.75	0.75
	z	0.125	0.125	0.125	0.125	0.125
	B	1.619(100)	1.674(105)	1.775(116)	2.332(123)	2.622(147)

Tabelle A3-a (Fortsetzung)

T [°C]		300	350	400	450	500
Rh	x	0	0	0	0	0
	y	0	0	0	0	0
	z	0.5	0.5	0.5	0.5	0.5
	B	0.654(37)c	0.582(42)	0.657(51)	0.802(47)	0.709(62)
O	x	0	0	0	0	0
	y	0.03060(98)	0.02989(97)	0.03038(104)	0.02715(107)	0.02351(125)
	z	0.24405(85)	0.24460(86)	0.24354(90)	0.24463(90)	0.24879(103)
	B	1.175(190)	1.047(197)	1.082(203)	1.283(189)	2.147(223)
zero		0.0243	0.0302	0.0350	0.0344	0.0556
u		0.07603	0.06100	0.04144	0.05568	0.05684
w		0.01503	0.01617	0.01641	0.01484	0.01386
eta		0.84392	0.75451	0.68931	0.77276	0.72713
x		0.06942	0.09915	0.11485	0.08481	0.10219
Asym		0.01074	0.01052	0.01038	0.01047	0.00504
R_p		19.7	19.6	21.7	22.1	24.1
R_{wp}		21.6	21.7	23.4	23.9	25.8
R_{exp}		12.96	12.96	13.12	13.13	13.14
Chi2		2.79	2.81	3.19	3.31	3.85
D-W		0.7887	0.7958	0.7493	0.6671	0.6234
R_{Bragg}		5.27	5.55	6.11	6.54	7.80

Tabelle A3-a (Fortsetzung)

T [°C]		550	560	570	580
a		6.16679 (19)	6.16412 (21)	6.16234 (23)	6.15839 (26)
c		8.08145 (33)	8.09304 (36)	8.10774 (39)	8.12041 (44)
Cu	x	0	0	0	0
	y	0.75	0.75	0.75	0.75
	z	0.125	0.125	0.125	0.125
	B	3.154(176)	2.947(192)	2.980(210)	2.962(236)
Rh	x	0	0	0	0
	y	0	0	0	0
	z	0.5	0.5	0.5	0.5
	B	0.848(73)	0.784(83)	0.706(96)	0.617(119)
O	x	0	0	0	0
	y	0.02201(142)	0.01856(158)	0.01524(168)	0.01704(180)
	z	0.25305(114)	0.25703(129)	0.25839(135)	0.25980(143)
	B	2.614(246)	2.985(276)	2.980(294)	2.682(317)
zero		0.0679	0.0605	0.0749	0.0654
u		0.05390	0.05902	0.06010	0.06267
w		0.01394	0.01351	0.01306	0.01292
eta		0.72480	0.70417	0.67325	0.63625

Tabelle A3-a (Fortsetzung)

T [°C]	550	560	570	580
x	0.09547	0.10295	0.10956	0.11845
Asym	0.00735	0.00743	0.00275	0.00347
R_p	27.1	28.2	30.0	31.6
R_{wp}	29.0	30.7	32.3	34.6
R_{exp}	13.22	13.24	13.27	13.34
Chi2	4.80	5.37	5.92	6.72
D-W	0.4878	0.4305	0.3905	0.3377
R_{Bragg}	9.58	10.3	11.3	12.6

Tabelle A3-a (Fortsetzung)

T [°C]	590	600	610	620
a_t	6.15711 (34)	6.15256 (31)	6.14568 (28)	6.14103 (24)
c_t	8.14184 (56)	8.15769 (54)	8.17931 (58)	8.20139 (64)
a_c	8.53879 (45)	8.53717 (22)	8.536996	8.53895 (12)

Tabelle A3-a (Fortsetzung)

T [°C]		650	700	750	800
a		8.54356 (12)	8.54805 (11)	8.55372 (11)	8.55791 (10)
Cu	x, y, z	0.125	0.125	0.125	0.125
	B	3.046(155)	3.203(170)	3.281(175)	3.372(176)
Rh	x, y, z	0.5	0.5	0.5	0.5
	B	1.235(65)	1.273(69)	1.316(70)	1.250(69)
O	x, y, z	0.25909(75)	0.25899(82)	0.25866(82)	0.25840(80)
	B	2.390(234)	2.574(254)	2.840(265)	2.699(257)
zero		0.1176	0.1297	0.1488	0.1678
u		0.01177	0.00820	0.00874	0.00772
w		0.00799	0.00766	0.00742	0.00745
eta		0.66664	0.66460	0.71676	0.70935
x		0.58967	0.62355	0.66992	0.68702
y		-0.09235	-0.09879	-0.10697	-0.10842
Asym 1		0.08173	0.09297	0.05736	0.06458
Asym 2		0.02917	0.03116	0.02836	0.03095
R_p		22.3	22.2	23.8	22.6
R_{wp}		21.6	22.0	22.6	22.1
R_{exp}		13.52	13.31	13.38	13.41
Chi2		2.56	2.72	2.84	2.71
D-W		0.8542	0.8442	0.8243	0.8467
R_{Bragg}		3.79	3.93	3.82	4.09

Tabelle A3-b: Struktur- und Profilparameter für die Rietveldverfeinerungen von $CuRh_2O_4$, kühlend zwischen 800° und 20°C

T [°C]		800	700	640	610
a		8.56143 (12)	8.54607 (10)	8.54249 (11)	8.53796 (11)
Cu	x, y, z	0.125	0.125	0.125	0.125
	B	3.449(194)	3.268(172)	3.036(162)	2.927(159)
Rh	x, y, z	0.5	0.5	0.5	0.5
	B	1.390(80)	1.305(66)	1.206(64)	1.181(64)
O	x, y, z	0.25978(87)	0.25931(81)	0.26043(81)	0.26103(82)
	B	2.721(288)	2.722(259)	2.439(252)	2.282(251)
zero		0.1897	0.0805	0.1044	0.0683
u		0.00764	0.00954	0.01039	0.01040
w		0.00791	0.00760	0.00780	0.00807
eta		0.49868	1.09310	0.92821	0.83010
x		0.83186	0.41164	0.48758	0.55040
y		-0.12801	-0.07216	-0.08355	-0.09342
Asym 1		0.09269	0.05740	0.08764	0.01598
Asym 2		0.03839	0.03940	0.03380	0.02629
R_p		25.2	22.8	22.5	22.4
R_{wp}		24.1	22.6	22.2	22.1
R_{exp}		14.58	14.50	14.32	14.30
Chi2		2.74	2.43	2.41	2.39
D-W		0.7883	0.9295	0.9111	0.9333
R_{Bragg}		3.91	4.10	3.64	3.75

Tabelle A3-b (Fortsetzung)

T [°C]	600	590	580
a_c	8.53532 (10)	8.53529 (11)	8.53449 (38)
a_t	6.15684 (43)	6.15295 (27)	6.15484 (30)
c_t	8.17932 (111)	8.14604 (68)	8.12609 (59)

Tabelle A3-b (Fortsetzung)

T [°C]		570	560	550	500
a		6.16087 (24)	6.16353 (24)	6.16495 (23)	6.17280 (18)
c		8.10839 (41)	8.09545 (42)	8.08221 (40)	8.04013 (32)
Cu	x	0	0	0	0
	y	0.75	0.75	0.75	0.75
	z	0.125	0.125	0.125	0.125
	B	2.709(218)	2.571(220)	2.911(214)	2.675(148)
Rh	x	0	0	0	0
	y	0	0	0	0
	z	0.5	0.5	0.5	0.5
	B	0.476(103)	0.383(127)	0.420(121)	0.721(61)
O	x	0	0	0	0
	y	0.01689(182)	0.01780(162)	0.02117(154)	0.02452(123)

Tabelle A3-b (Fortsetzung)

	z	0.25873(146)	0.25540(131)	0.25477(125)	0.24650(101)
	B	2.961(314)	2.404(294)	2.411(285)	1.787(217)
zero		0.0452	0.0424	0.0335	0.0188
u		0.06010	0.06574	0.06791	0.06791
w		0.01306	0.01400	0.01449	0.01449
eta		0.67330	0.56424	0.56276	0.75001
x		0.10960	0.14628	0.15940	0.09309
Asym		0.00497	0.00518	0.00567	0.00718
R_p		32.3	29.1	28.7	24.5
R_{wp}		35.4	31.8	31.1	26.3
R_{exp}		14.60	14.44	14.47	14.42
Chi2		5.87	4.86	4.61	3.32
D-W		0.3968	0.4477	0.4897	0.6614
R_{Bragg}		11.3	10.5	10.2	7.67

Tabelle A3-b (Fortsetzung)

T [°C]		400	300	200	100
a		6.17690 (14)	6.17770 (13)	6.17655 (13)	6.17480 (12)
c		7.99003 (26)	7.96380 (25)	7.94082 (23)	7.92217 (21)
Cu	x	0	0	0	0
	y	0.75	0.75	0.75	0.75
	z	0.125	0.125	0.125	0.125
	B	1.691(116)	1.735(98)	1.458(93)	1.351(85)
Rh	x	0	0	0	0
	y	0	0	0	0
	z	0.5	0.5	0.5	0.5
	B	0.560(55)	0.670(33)	0.507(39)	0.479(31)
O	x	0	0	0	0
	y	0.03150(100)	0.03135(95)	0.03313(92)	0.03231(94)
	z	0.24448(87)	0.24348(82)	0.24523(79)	0.24611(79)
	B	0.711(192)	0.878(179)	1.109(165)	1.333(154)
zero		-0.0043	-0.0079	-0.0180	-0.0237
u		0.04685	0.09368	0.06944	0.07472
w		0.01799	0.01440	0.01810	0.01730
eta		0.66932	0.91803	0.77950	0.91140
x		0.12693	0.04354	0.10141	0.05140
Asym		0.01406	0.01041	0.01181	0.01182
R_p		21.6	19.4	19.0	18.8
R_{wp}		23.3	21.4	21.0	20.9
R_{exp}		14.52	14.29	14.07	14.00
Chi2		2.58	2.24	2.23	2.23
D-W		0.8042	0.9609	0.9605	0.9587
R_{Bragg}		6.28	5.04	4.91	5.09

Tabelle A4-a: Struktur- und Profilparameter für die Rietveldverfeinerungen von $CuCr_2O_4$, heizend zwischen 20° und 800°C

T [°C]		20	100	200	300	400
a		6.03130 (8)	6.03121 (7)	6.03082 (8)	6.02981 (8)	6.02682 (9)
c		7.77784 (12)	7.79786 (12)	7.82258 (12)	7.85096 (13)	7.88556 (13)
Cu	x	0	0	0	0	0
	y	0.75	0.75	0.75	0.75	0.75
	z	0.125	0.125	0.125	0.125	0.125
	B	1.136(64)	1.347(58)	1.793(63)	1.896(68)	2.316(73)
Cr	x	0	0	0	0	0
	y	0	0	0	0	0
	z	0.5	0.5	0.5	0.5	0.5
	B	0.712(46)	0.906(42)	1.150(44)	1.113(47)	1.449(50)
O	x	0	0	0	0	0
	y	0.03229(76)	0.03370(68)	0.03432(67)	0.03339(68)	0.03314(68)
	z	0.24692(60)	0.24734(54)	0.24752(52)	0.24983(53)	0.24940(52)
	B	1.053(144)	1.266(126)	1.771(117)	1.936(117)	2.175(115)
zero		-0.0223	-0.0206	-0.0188	-0.0166	-0.0133
u		0.01097	0.01191	0.01034	0.01209	0.01332
v		-0.00355	-0.00981	-0.00700	-0.00904	-0.00942
w		0.00780	0.01240	0.01197	0.01285	0.01249
eta		0.38324	0.37540	0.30064	0.27858	0.41390
x		0.00250	0.00285	0.00328	0.00332	0.00119
Asym		0.16436	0.05734	-0.00872	-0.06914	-0.06487
R_p		28.4	26.3	28.0	29.8	29.4
R_{wp}		23.9	21.1	21.5	22.4	22.8
R_{exp}		19.60	17.76	17.49	17.73	17.47
Chi2		1.48	1.41	1.51	1.60	1.70
D-W		1.4783	1.5107	1.4278	1.3619	1.2512
R_{Bragg}		3.10	3.95	4.75	5.41	4.46

Tabelle A4-a (Fortsetzung)

T [°C]		500	530	550	570	590
a		6.02075 (10)	6.01630 (10)	6.01226 (10)	6.00711 (11)	5.99824 (11)
c		7.94119 (14)	7.96557 (15)	7.98372 (15)	8.00896 (16)	8.04387 (17)
Cu	x	0	0	0	0	0
	y	0.75	0.75	0.75	0.75	0.75
	z	0.125	0.125	0.125	0.125	0.125
	B	2.411(73)	2.527(77)	2.725(79)	2.603(80)	2.919(95)
Cr	x	0	0	0	0	0
	y	0	0	0	0	0
	z	0.5	0.5	0.5	0.5	0.5

Tabelle A4-a (Fortsetzung)

	B	1.514(51)	1.526(53)	1.669(55)	1.599(56)	1.909(66)
O	x	0	0	0	0	0
	y	0.03237(65)	0.03115(68)	0.03049(68)	0.03051(70)	0.02761(87)
	z	0.25215(49)	0.25295(51)	0.25343(51)	0.25425(52)	0.25398(62)
	B	2.189(111)	2.457(116)	2.483(116)	2.391(120)	3.301(150)
zero		0.0304	0.0297	0.0317	0.0452	0.0421
u		0.01443	0.01493	0.01142	0.01208	0.01282
v		-0.01173	-0.01052	-0.00651	-0.00831	-0.00072
w		0.01344	0.01291	0.01201	0.01354	0.01062
eta		0.28708	0.36488	0.44642	0.26245	0.47689
x		0.00365	0.00229	0.00103	0.00495	-0.00073
Asym		0.08216	0.05076	0.09678	0.09665	0.02132
R_p		29.8	31.5	31.9	31.6	33.2
R_{wp}		22.1	22.6	22.7	23.6	25.3
R_{exp}		17.92	17.85	17.73	17.89	18.61
Chi2		1.52	1.61	1.65	1.73	1.84
D-W		1.3976	1.3619	1.3563	1.2619	1.2079
R_{Bragg}		4.46	6.00	5.72	5.23	5.97

Tabelle A4-a (Fortsetzung)

T [°C]		610	630	650	800
a		8.34755 (10)	8.34926 (9)	8.35052 (9)	
Cu	x, y, z	0.125	0.125	0.125	
	B	2.975(70)	3.239(65)	3.376(68)	
Cr	x, y, z	0.5	0.5	0.5	
	B	1.960(47)	2.093(44)	2.089(45)	
O	x, y, z	0.26121(34)	0.26140(32)	0.26160(33)	
	B	2.402(115)	2.765(111)	2.775(114)	
zero		0.0464	0.0542	0.0572	
u		0.01074	0.00979	0.00817	s Tabelle A4-b
w		0.01046	0.01088	0.01118	
eta		0.47451	0.43671	0.42745	
R_p		31.7	29.9	30.7	
R_{wp}		21.9	21.2	21.8	
R_{exp}		18.22	17.83	18.56	
Chi2		1.44	1.42	1.38	
D-W		1.4710	1.4898	1.5257	
R_{Bragg}		2.92	2.72	2.77	

Tabelle A4-b: Struktur- und Profilparameter für die Rietveldverfeinerungen von $CuCr_2O_4$, kühlend zwischen 800° und 20°C

T [°C]		800	700	640	600	590
a		8.36321 (8)	8.35445 (8)	8.34951 (9)	8.34639 (9)	8.34571 (9)
Cu	x, y, z	0.125	0.125	0.125	0.125	0.125
	B	2.970(62)	2.889(60)	2.860(59)	2.782(59)	2.617(61)
Cr	x, y, z	0.5	0.5	0.5	0.5	0.5
	B	1.751(40)	1.788(39)	1.884(40)	1.852(40)	1.685(40)
O	x, y, z	0.26154(30)	0.26193(30)	0.26185(29)	0.26146(30)	0.26142(32)
	B	2.350(103)	2.489(103)	2.644(103)	2.439(102)	2.383(106)
zero		0.1306	0.0676	0.0392	0.0266	0.0272
u		0.00768	0.00819	0.01006	0.00981	0.00959
w		0.01311	0.01305	0.01294	0.01302	0.01301
eta		0.32079	0.33306	0.35155	0.35480	0.35539
R_p		30.2	28.6	28.3	28.1	29.2
R_{wp}		19.9	19.8	19.7	19.6	20.5
R_{exp}		18.10	17.76	17.58	17.46	17.59
Chi2		1.20	1.24	1.26	1.26	1.36
D-W		1.7296	1.6866	1.6547	1.6163	1.4923
R_{Bragg}		2.50	2.61	3.19	2.71	2.44

Tabelle A4-b (Fortsetzung)

T [°C]	580	570	560	550
$a_{kubisch}$	8.34505 (9)	8.34414 (9)	8.34369 (12)	8.34392 (21)
$c_{tetragonal}$	6.00516 (40)	6.00903 (21)	6.01057 (11)	6.01342 (9)
$a_{tetragonal}$	7.99596 (96)	7.99628 (54)	7.99005 (24)	7.97992 (20)

Tabelle A4-b (Fortsetzung)

T [°C]		540	530	450	350	250
a		6.01549 (13)	6.01721 (13)	6.02533 (11)	6.02923 (11)	6.03101 (10)
c		7.97110 (19)	7.96237 (19)	7.90968 (17)	7.86679 (15)	7.83653 (15)
Cu	x	0	0	0	0	0
	y	0.75	0.75	0.75	0.75	0.75
	z	0.125	0.125	0.125	0.125	0.125
	B	2.764(91)	2.724(91)	2.464(77)	2.087(69)	1.918(66)
Cr	x	0	0	0	0	0
	y	0	0	0	0	0
	z	0.5	0.5	0.5	0.5	0.5
	B	1.521(60)	1.564(61)	1.339(51)	1.134(46)	1.076(45)
O	x	0	0	0	0	0
	y	0.03053(80)	0.03144(77)	0.03169(68)	0.03136(66)	0.03246(66)
	z	0.25296(58)	0.25362(56)	0.25230(51)	0.25026(50)	0.24878(50)
	B	2.353(130)	2.266(129)	1.764(113)	1.714(108)	1.472(111)

zero	0.0246	0.0288	0.0017	-0.0154	-0.0142
u	0.01339	0.01525	0.01102	0.01251	0.01074
v	-0.00580	-0.00867	-0.01011	-0.01043	-0.00918
w	0.01629	0.01715	0.01751	0.01681	0.01655
eta	0.35260	0.39213	0.28379	0.26621	0.18369
x	0.00123	-0.00019	0.00253	0.00284	0.00468
Asym	0.02745	0.06682	-0.04372	-0.02007	-0.00426
R_p	35.1	35.5	31.2	29.0	28.0
R_{wp}	25.9	25.5	23.0	21.4	21.3
R_{exp}	19.71	19.91	19.01	18.79	18.54
Chi2	1.73	1.63	1.46	1.30	1.32
D-W	1.2349	1.3455	1.5088	1.5836	1.6429
R_{Bragg}	5.42	4.55	5.73	4.62	3.88

Tabelle A4-b (Fortsetzung)

T [°C]		150	50
a		6.03143 (10)	6.03153 (9)
c		7.81111 (15)	7.78537 (15)
Cu	x	0	0
	y	0.75	0.75
	z	0.125	0.125
	B	1.561(62)	1.316(60)
Cr	x	0	0
	y	0	0
	z	0.5	0.5
	B	0.988(43)	0.825(42)
O	x	0	0
	y	0.03476(67)	0.03467(72)
	z	0.24729(52)	0.24719(57)
	B	1.123(115)	1.027(140)
zero		-0.0180	-0.0295
u		0.01310	0.00992
v		-0.01078	-0.00774
w		0.01616	0.01554
eta		0.30360	0.23951
x		0.00281	0.00403
Asym		0.00250	-0.01158
R_p		27.0	26.2
R_{wp}		21.1	21.2
R_{exp}		18.40	18.57
Chi2		1.32	1.30
D-W		1.6335	1.7445
R_{Bragg}		4.17	2.85

Tabelle A5: Struktur- und Profilparameter für die Hochtemperatur-Rietveldverfeinerungen von $CaCuGe_2O_6$, heizend zwischen 20° und 800°C

20°C:

```
Name    x     sx       y     sy       z      sz      B   sB  occ.  socc.
 CA    0.71734(  44)  0.54476(  39)  0.19220( 102)  1.822( 94)  4.000(  0)
 CU    0.77250(  27)  0.16120(  33)  0.24272(  59)  1.509( 68)  4.000(  0)
 GE    0.04882(  22)  0.34956(  30)  0.20855(  49)  1.342( 53)  4.000(  0)
 GE    0.49010(  21)  0.35002(  29)  0.40041(  45)  1.414( 55)  4.000(  0)
 O1    0.87216( 117)  0.35785( 154)  0.11159( 243)  2.527(315)  4.000(  0)
 O2    0.14250( 110)  0.47992( 144)  0.37581( 250)  2.171(309)  4.000(  0)
 O3    0.10159( 102)  0.19194( 125)  0.42186( 225)  1.458(295)  4.000(  0)
 O4    0.65925( 123)  0.32517( 148)  0.37347( 268)  3.262(357)  4.000(  0)
 O5    0.43129( 125)  0.52225( 130)  0.24430( 252)  3.276(334)  4.000(  0)
 O6    0.39537( 105)  0.25436( 119)  0.59143( 259)  1.722(307)  4.000(  0)

=> Cell parameters      :    10.19249   0.00014
                              9.20694   0.00012
                              5.21000   0.00008
                             90.00000   0.00000
                            105.70013   0.00071
                             90.00000   0.00000
 => overall scale factor :    0.000020764   0.000000112
 => Eta(p-v) or m(p-vii) :    0.69874   0.00943
 => Overall tem. factor  :    0.00000   0.00000
 => Halfwidth parameters :    0.00777   0.00038
                              0.00000   0.00000
                              0.00574   0.00010
 => Preferred orientation:    1.11425   0.00338
                              0.00000   0.00000
 => Asymmetry parameters :    0.04220   0.00912
 => Zero-point:  -0.0070  0.0012
 => Rp: 15.0     Rwp: 17.4     Rexp:   11.84 Chi2:  2.16
 => DW-Stat.:    1.1278     DW-exp:     1.9375
 => Bragg R-factor:  5.57
```

100°C:

```
Name    x     sx       y     sy       z      sz      B   sB  occ.  socc.
 CA    0.71785(  46)  0.54576(  40)  0.19316( 109)  2.512(106)  4.000(  0)
 CU    0.77180(  28)  0.16167(  33)  0.24386(  60)  1.766( 70)  4.000(  0)
 GE    0.04912(  22)  0.34979(  30)  0.21037(  49)  1.395( 54)  4.000(  0)
 GE    0.48967(  22)  0.35054(  29)  0.39747(  45)  1.590( 57)  4.000(  0)
 O1    0.87191( 102)  0.35314( 142)  0.10819( 222)  1.537(265)  4.000(  0)
 O2    0.13913( 121)  0.47978( 155)  0.35954( 276)  3.561(358)  4.000(  0)
 O3    0.10018( 101)  0.19031( 123)  0.41616( 224)  1.690(301)  4.000(  0)
 O4    0.66271( 116)  0.32802( 139)  0.37517( 253)  2.866(327)  4.000(  0)
 O5    0.42807( 123)  0.52271( 134)  0.24659( 261)  3.907(354)  4.000(  0)
 O6    0.39945( 104)  0.25151( 118)  0.58718( 267)  1.858(312)  4.000(  0)

 => Cell parameters      :   10.19833   0.00015
                              9.21671   0.00013
                              5.21638   0.00008
                             90.00000   0.00000
                            105.74365   0.00073
                             90.00000   0.00000
 => overall scale factor :    0.000021325   0.000000113
 => Eta(p-v) or m(p-vii) :    0.66120   0.00912
 => Overall tem. factor  :    0.00000   0.00000
 => Halfwidth parameters :    0.00853   0.00041
                              0.00000   0.00000
                              0.00615   0.00010
 => Preferred orientation:    1.12183   0.00336
                              0.00000   0.00000
 => Asymmetry parameters :    0.02874   0.00934
 => Zero-point:  -0.0024  0.0013
 => Rp: 15.0     Rwp: 17.2     Rexp:   11.85 Chi2:  2.12
 => DW-Stat.:    1.0717     DW-exp:     1.9375
 => Bragg R-factor:  6.21
```

200°C:

```
 Name    x     sx       y     sy       z      sz      B   sB  occ.  socc.
 CA    0.71755(  50)  0.54539(  43)  0.19507( 115)  2.926(118)  4.000(  0)
 CU    0.77161(  29)  0.16055(  35)  0.24500(  64)  1.950( 75)  4.000(  0)
 GE    0.04861(  23)  0.34989(  31)  0.20993(  50)  1.518( 58)  4.000(  0)
 GE    0.48914(  23)  0.35031(  31)  0.39407(  48)  1.792( 62)  4.000(  0)
 O1    0.87002( 105)  0.35129( 147)  0.11347( 233)  1.566(275)  4.000(  0)
 O2    0.13905( 127)  0.48300( 164)  0.36165( 287)  3.763(391)  4.000(  0)
 O3    0.10006( 104)  0.19096( 125)  0.41484( 233)  1.625(313)  4.000(  0)
 O4    0.66145( 124)  0.32649( 145)  0.37435( 267)  3.199(353)  4.000(  0)
 O5    0.42728( 133)  0.52128( 145)  0.24549( 275)  4.647(394)  4.000(  0)
 O6    0.40013( 105)  0.25253( 121)  0.58842( 270)  1.545(304)  4.000(  0)

 => Cell parameters      :   10.20676   0.00016
                              9.23093   0.00014
                              5.22690   0.00009
```

```
                            90.00000   0.00000
                           105.80697   0.00075
                            90.00000   0.00000
 => overall scale factor :    0.000021256   0.000000118
 => Eta(p-v) or m(p-vii) :    0.64925   0.00915
 => Overall tem. factor  :    0.00000   0.00000
 => Halfwidth parameters :    0.00889   0.00045
                              0.00000   0.00000
                              0.00610   0.00010
 => Preferred orientation:    1.12779   0.00350
                              0.00000   0.00000
 => Asymmetry parameters :    0.02970   0.00975
 => Zero-point:   0.0082  0.0013
 => Conventional Rietveld R-factors:
 => Rp: 15.7     Rwp: 17.7     Rexp:   12.03 Chi2:  2.17
 => DW-Stat.:    1.0933     DW-exp:     1.9375
 => Bragg R-factor:  6.77
```

300°C:

```
Name    x     sx       y     sy       z      sz      B   sB  occ.  socc.
 CA    0.71838(  56)  0.54596(  50)  0.19689( 128)  3.158(133)  4.000(  0)
 CU    0.77134(  34)  0.15991(  38)  0.24593(  73)  2.302( 89)  4.000(  0)
 GE    0.04816(  26)  0.35028(  35)  0.21096(  56)  1.712( 67)  4.000(  0)
 GE    0.48836(  27)  0.34929(  36)  0.38850(  54)  2.049( 73)  4.000(  0)
 O1    0.87192( 114)  0.35210( 158)  0.11431( 249)  1.146(286)  4.000(  0)
 O2    0.13747( 140)  0.48639( 183)  0.36635( 308)  3.553(433)  4.000(  0)
 O3    0.10193( 116)  0.19291( 137)  0.42254( 257)  1.645(354)  4.000(  0)
 O4    0.66157( 145)  0.32863( 164)  0.36953( 297)  3.847(420)  4.000(  0)
 O5    0.42479( 151)  0.52453( 164)  0.24580( 317)  5.480(471)  4.000(  0)
 O6    0.39981( 116)  0.25457( 138)  0.58286( 299)  1.567(331)  4.000(  0)

 => Cell parameters      :   10.21430   0.00018
                              9.24587   0.00015
                              5.24040   0.00010
                             90.00000   0.00000
                            105.88737   0.00083
                             90.00000   0.00000
 => overall scale factor :    0.000021188   0.000000132
 => Eta(p-v) or m(p-vii) :    0.65799   0.01002
 => Overall tem. factor  :    0.00000   0.00000
 => Halfwidth parameters :    0.00862   0.00052
                              0.00000   0.00000
                              0.00599   0.00012
 => Preferred orientation:    1.13209   0.00395
                              0.00000   0.00000
 => Asymmetry parameters :    0.02965   0.01069
 => Zero-point:   0.0170  0.0015
 => Rp: 16.9     Rwp: 19.4     Rexp:   12.25 Chi2:  2.51
 => DW-Stat.:    0.9904     DW-exp:     1.9374
 => Bragg R-factor:  7.70
```

500°C:

```
Name    x     sx       y     sy       z      sz      B   sB  occ.  socc.
 CA    0.00000(   0)  0.29951(  54)  0.25000(   0)  3.098(137)  1.000(  0)
 CU    0.00000(   0)  0.90582(  37)  0.25000(   0)  2.586( 84)  1.000(  0)
 GE    0.28375(  17)  0.09746(  18)  0.21416(  41)  1.905( 52)  2.000(  0)
 O1    0.10267(  72)  0.09020(  93)  0.11248( 154)  2.446(199)  2.000(  0)
 O2    0.35797( 100)  0.25646(  95)  0.33952( 188)  4.677(302)  2.000(  0)
 O3    0.35212(  80)  0.03214(  83) -0.03433( 190)  2.333(223)  2.000(  0)

 => Cell parameters      :   10.24595   0.00019
                              9.19230   0.00016
                              5.40415   0.00011
                             90.00000   0.00000
                            107.12151   0.00084
                             90.00000   0.00000
 => overall scale factor :    0.000078503   0.000000489
 => Eta(p-v) or m(p-vii) :    0.53733   0.02544
 => Overall tem. factor  :    0.00000   0.00000
 => Halfwidth parameters :    0.01784   0.00206
                             -0.01109   0.00179
                              0.00823   0.00038
 => Preferred orientation:    1.10440   0.00384
                              0.00000   0.00000
 => Asymmetry parameters :    0.02588   0.01125
 => X and y parameters   :    0.00504   0.00065
 => Zero-point:   0.0465  0.0015
 => Rp: 18.3     Rwp: 19.7     Rexp:   12.70 Chi2:  2.41
 => DW-Stat.:    1.0405     DW-exp:     1.9280
 => Bragg R-factor:  6.56
```

600°C:

```
Name    x     sx       y     sy       z      sz      B   sB  occ.  socc.
 CA    0.00000(   0)  0.30007(  58)  0.25000(   0)  3.142(149)  1.000(  0)
 CU    0.00000(   0)  0.90552(  39)  0.25000(   0)  2.338( 88)  1.000(  0)
 GE    0.28357(  18)  0.09722(  19)  0.21392(  42)  1.731( 55)  2.000(  0)
```

```
 O1    0.10304(  77)  0.09128( 101)  0.11400( 164)  2.718(217)  2.000(  0)
 O2    0.35978( 103)  0.25718(  99)  0.33934( 191)  4.159(299)  2.000(  0)
 O3    0.35536(  89)  0.02857(  94) -0.03583( 209)  3.203(257)  2.000(  0)

 => Cell parameters      :   10.25770   0.00020
                              9.21319   0.00017
                              5.41116   0.00011
                             90.00000   0.00000
                            107.15478   0.00088
                             90.00000   0.00000
 => overall scale factor :    0.000068468   0.000000453
 => Eta(p-v) or m(p-vii) :    0.49248   0.02637
 => Overall tem. factor  :    0.00000   0.00000
 => Halfwidth parameters :    0.02682   0.00249
                             -0.02020   0.00212
                              0.01052   0.00045
 => Preferred orientation:    1.09069   0.00395
                              0.00000   0.00000
 => Asymmetry parameters :    0.03811   0.01110
 => X and y parameters   :    0.00534   0.00067
 => Zero-point:   0.1076  0.0016

 => Rp: 19.1     Rwp: 20.2     Rexp:   13.40 Chi2:  2.27
 => DW-Stat.:    0.9922     DW-exp:     1.9276
 => Bragg R-factor:  7.22
```

700°C:

```
Name    x     sx       y     sy       z      sz      B   sB  occ.  socc.
 CA    0.00000(   0)  0.29932(  62)  0.25000(   0)  3.592(164)  1.000(  0)
 CU    0.00000(   0)  0.90601(  41)  0.25000(   0)  2.978( 96)  1.000(  0)
 GE    0.28325(  18)  0.09748(  20)  0.21305(  45)  2.265( 60)  2.000(  0)
 O1    0.10229(  80)  0.09178( 103)  0.11333( 176)  3.197(236)  2.000(  0)
 O2    0.36066( 111)  0.25997( 107)  0.33438( 201)  5.050(327)  2.000(  0)
 O3    0.35267(  92)  0.02752(  97) -0.03816( 217)  3.479(268)  2.000(  0)

 => Cell parameters      :   10.26752   0.00022
                              9.23181   0.00018
                              5.41671   0.00012
                             90.00000   0.00000
                            107.19489   0.00091
                             90.00000   0.00000
 => overall scale factor :    0.000076642   0.000000557
 => Eta(p-v) or m(p-vii) :    0.42284   0.02862
 => Overall tem. factor  :    0.00000   0.00000
 => Halfwidth parameters :    0.02583   0.00096
                             -0.02020   0.00000
                              0.01015   0.00015
 => Preferred orientation:    1.09861   0.00429
                              0.00000   0.00000
 => Asymmetry parameters :    0.05454   0.01113
 => X and y parameters   :    0.00731   0.00074
 => Zero-point:   0.1483  0.0016
 => Conventional Rietveld R-factors:
 => Rp: 19.6     Rwp: 21.0     Rexp:   13.09 Chi2:  2.58
 => DW-Stat.:    0.9546     DW-exp:     1.9272
 => Bragg R-factor:  7.06
```

800°C:

```
 Name    x     sx       y     sy       z      sz      B   sB  occ.  socc.

 CA    0.00000(   0)  0.29809(  72)  0.25000(   0)  4.202(198)  1.000(  0)
 CU    0.00000(   0)  0.90431(  46)  0.25000(   0)  3.057(109)  1.000(  0)
 GE    0.28329(  20)  0.09749(  22)  0.21231(  50)  2.394( 71)  2.000(  0)
 O1    0.10408(  88)  0.08970( 111)  0.11296( 194)  3.180(263)  2.000(  0)
 O2    0.35854( 122)  0.25991( 119)  0.33584( 219)  5.101(363)  2.000(  0)
 O3    0.35470( 100)  0.02554( 108) -0.03878( 234)  3.378(297)  2.000(  0)

 => Cell parameters      :   10.28050   0.00023
                              9.25355   0.00020
                              5.42384   0.00013
                             90.00000   0.00000
                            107.23234   0.00102
                             90.00000   0.00000

 => overall scale factor :    0.000075245   0.000000716
 => Eta(p-v) or m(p-vii) :    0.21934   0.03115
 => Overall tem. factor  :    0.00000   0.00000
 => Halfwidth parameters :    0.02363   0.00104
                             -0.02020   0.00000
                              0.01092   0.00019
 => Preferred orientation:    1.10445   0.00486
                              0.00000   0.00000
 => Asymmetry parameters :    0.11280   0.00978
 => X and y parameters   :    0.01020   0.00081
 => Zero-point:   0.2215  0.0016
 => Rp: 21.4     Rwp: 23.0     Rexp:   13.25 Chi2:  3.02
 => DW-Stat.:    0.8126     DW-exp:     1.9272
 => Bragg R-factor:  7.55
```

A3 Röntgenpulverdaten

Im Rahmen dieser Arbeit wurden einige neue Verbindungen synthetisiert und die Röntgenpulverdaten dieser Verbindungen in der Datenbank ICDD-PDF2 veröffentlicht. Die entsprechenden Einträge sind auf den folgenden Seiten aufgeführt.

1: $CsFeGe_2O_6$
2: $CsGaGe_2O_6$
3: $CsGaSi_2O_6$
4: $ZnCuTiO_4$
5: $CuRh_2O_4$
6: $Li_2CoTi_3O_8$
7: $Li_2CuTi_3O_8$
8: $Sr_2Al_2GeO_7$
9: $Ba_2Ga_2GeO_7$

---

d | 3.52 | 3.00 | 3.76 I 5.75 I	Formula Cs Fe Ge2 O6																
I/I1 | 100 | 40 | 29 I 2 I	Name Caesium Iron Germanium Oxide																
Rad. | CuKa1	Lambda | 1.5406	Filter Mono. Type: NI	X	Crystal Sys. | Cubic	Space Group | I-43d	S.G. # | 220										
Intensities	d values	a 14.0699(4)	b	c													
Diffractom. X Densitom. Visual Calc.	Diff. X Guinier Debye Calc.	A	B	C													
		A	C														
d value std.	Cut off	I/I cor. | 5.1	D calc. | 4.101	mp													
Internal X External		Z | 16	D exp.	Dia.													
Reference (Powder Data) Tovar M.,Eysel W., Mineraloqisches Institut der Universitaet Heidelberq, FRG, Grant-in-Aid Report, ICDD (1998)																	
Reference (Crystal Data) Ibid.																	
Preparation & Chemistry Stoichiometric mixture of Cs2CO3 (Aldrich 99.9%), Fe2O3 (Fluka 99.5 %) and GeO2 (Heraeus 99.999%) annealed in an open corundum crucible at 850 C for 4 days and at 900 C for 20 days. Vaporization of Cs was compensated for by intermediate addition of 10% Cs2CO3.																	
Additional Comments Pollucite structure type. Color: beige F(30)=113.5(.0073, 36) Si used as internal standard.																	

d A	I/I0	h k l
5.749	2	2 1 1C
4.970	1	2 2 0C
4.450	3	3 1 0C
3.761	29	3 2 1C
3.518	100	4 0 0C
2.999	40	3 3 2C
2.872	7	4 2 2C
2.759	5	5 1 0C
2.569	2	5 2 1C
2.4875	27	4 4 0C
2.4131	5	5 3 0C
2.2824	4	6 1 1C
2.0751	7	6 3 1C
2.0312	4	4 4 4C
1.9901	3	7 1 0C
1.9513	1	6 4 0C
1.8803	2	6 4 2C
1.8467	1	7 3 0C
1.7871	12	6 5 1C
1.7591	2	8 0 0C
1.7320	4	7 4 1C
1.7064	1	8 2 0C
1.6821	1	6 5 3C
1.6581	2	6 6 0C
1.5924	1	7 5 2C
1.5729	2	8 4 0C
1.5351	1	8 4 2C
1.5171	2	7 6 1C
1.4996	1	6 6 4C
1.4831	2	9 3 0C
1.4511	2	9 3 2C
1.4357	1	8 4 4C
1.4208	1	9 4 1C
1.4070	1	8 6 0C
1.3930	3	10 1 1C
1.3796	1	10 2 0C
1.3414	3	10 3 1C
1.3176	2	8 7 1C
1.3069	1	10 4 0C
1.2951	1	9 6 1C

d A	I/I0	h k l
1.2741	1	11 1 0C
1.2534	2	10 5 1C
1.2153	1	9 7 2C
1.1976	1	11 4 1C
1.1645	1	11 5 0C
1.1491	1	10 7 1C

d	3.49	2.97	2.47	I 5.69
I/I1	100	48	29	I 3

Formula
Cs Ga Ge2 O6

Name
Caesium Gallium Germanium Oxide

Rad.	Lambda	Filter Mono.	X
CuKa1	1.5406	Type: NI	

Crystal Sys.	Space Group	S.G. #
Cubic	I-43d	220

a 13.9431(3)b c

A B C

A C

I/I cor.	D calc.	mp
5.3	4.350	

Z	D exp.	Dia.
16		

Intensities	d values
Diffractom. X	Diff. X
Densitom.	Guinier
Visual	Debye
Calc.	Calc.

d value std.	Cut off

Internal X
External

Reference (Powder Data)
Tovar, M., Eysel, W., Mineralogisches Institut der Universitaet Heidelberg, FRG, Grant-in-Aid Report, ICDD (1998)

Reference (Crystal Data)

Ibid.

Preparation & Chemistry
Stoichiometric mixture of CsHCO3 (Heraeus, 99.99%), Ga2O3 (Heraeus 99.99%) and GeO2 (Heraeus, 99.999%) annealed in an open corundum crucible at 900 C for 5 days.

Additional Comments

Pollucite structure type
Tiny unknown peaks at d=3.29, 3.23, 3.19 and 2.82
Color: white
F(30)=109.8(.0080, 34)
Si used as internal standard.

d A	I/I0	h k l
5.686	3	2 1 1C
4.921	1	2 2 0C
4.409	2	3 1 0C
3.726	27	3 2 1C
3.486	100	4 0 0C
3.122	2	4 2 0C
2.973	48	3 3 2C
2.847	8	4 2 2C
2.735	6	5 1 0C
2.547	4	5 2 1C
2.465	29	4 4 0C
2.3916	4	5 3 0C
2.2622	4	6 1 1C
2.0561	9	6 3 1C
2.0126	5	4 4 4C
1.9722	4	7 1 0C
1.9330	2	6 4 0C
1.8975	15	7 2 1C
1.8637	3	6 4 2C
1.7709	16	6 5 1C
1.7430	2	8 0 0C
1.7164	4	7 4 1C
1.6910	1	8 2 0C
1.6665	1	6 5 3C
1.6430	2	6 6 0C
1.6210	4	7 5 0C
1.5785	1	7 5 2C
1.5589	3	8 4 0C
1.5211	1	8 4 2C
1.5035	3	7 6 1C
1.4863	1	6 6 4C
1.4698	3	9 3 0C
1.4382	4	9 3 2C
1.4229	1	8 4 4C
1.4082	1	9 4 1C
1.3944	1	8 6 0C
1.3806	4	10 1 1C
1.3672	1	10 2 0C
1.3294	4	10 3 1C
1.3059	2	8 7 1C

d	3.43	2.93	3.67	I 5.61
I/I1	100	45	29	I 2

Formula
Cs Ga Si2 O6

Name
Cesium Gallium Silicon Oxide

Rad.	Lambda	Filter Mono.	X
CuKa1	1.5406	Type: Ge	

Crystal Sys.	Space Group	S.G. #
Cubic	I-43d	220

a 13.7347 b c

(.0007) ( ) ( )

A B C

A C

I/I cor.	D calc.	mp
3.1	3.638	

Z	D exp.	DIA.
16		

Intensities	d values
Diffractom. X	Diff. X
Densitom.	Guinier
Visual	Debye
Calc.	Calc.

d value std.	Cut off

Internal X
External

Reference (Powder Data)
Tovar, M., Eysel, W., Mineralogisches Institut der Universitaet Heidelberg, FRG, ICDD Grant-in-Aid Report (1998)

Reference (Crystal Data)

Ibid.

Preparation & Chemistry
Stoichiometric mixture of Cs2CO3 (Aldrich, 99.9%), Ga2O3 (Fluka, 99.5%) and SiO2 (Heraeus, 99.999%) annealed in an open corundum crucible at 850 C for 4 days and at 900 C for 20 days.

Additional Comments

Pollucite structure type
Due to high vapor pressure of Cs2O the sample always contains Ga2O3 as second phase, even though excess Cs2CO3 was added during synthesis.
Color: beige
F(30)= 40.4(.0158, 47)
Si used as internal standard.

d A	I/I0	h k l
5.61	2	2 1 1C
4.859	1	2 2 0C
3.671	29	3 2 1C
3.434	100	4 0 0C
3.073	8	4 2 0C
2.930	45	3 3 2C
2.695	5	5 1 0C
2.508	2	5 2 1C
2.428	29	4 4 0C
2.229	9	6 1 1C
2.172	1	6 2 0C
2.025	8	6 3 1C
1.983	4	4 4 4C
1.870	17	7 2 1C
1.837	1	6 4 2C
1.7443	19	6 5 1C
1.7164	4	8 0 0C
1.6900	2	7 4 1C
1.6646	1	8 2 0C
1.6415	2	6 5 3C
1.5962	1	7 5 0C
1.5557	3	7 5 2C
1.5357	5	8 4 0C
1.4814	4	7 6 1C
1.4480	1	9 3 0C
1.4168	4	9 3 2C
1.4022	2	8 4 4C
1.3729	1	8 6 0C
1.3091	6	10 3 1C
1.2638	2	9 6 1C
1.2234	1	10 5 1C
1.1865	3	9 7 2C
1.1215	2	10 7 1C

d A	I/I0	h k l
1.2945	1	10 4 0C
1.2835	1	9 6 1C
1.2625	1	11 1 0C
1.2421	5	10 5 1C
1.2046	1	9 7 2C
1.1868	2	11 4 1C
1.1538	1	11 5 0C
1.1385	1	10 7 1C

d 2.55	2.99	1.49	I 4.88
I/I1 100	38	25	I 6

Formula: Zn Cu Ti O4

Name: Zinc Copper Titanium Oxide

Rad.	Lambda	Filter Mono. X	Crystal Sys.	Space Group	S.G. #
CuKa1	1.5406	Type: NI	Cubic	Fd3m	227

Intensities	d values
Diffractom. X	Diff. X
Densitom.	Guinier
Visual	Debye
Calc.	Calc.

a 8.4471(2) b c

A B C

A C

I/I cor.	D calc.	mp
5.7	5.308	

d value std.	Cut off

Internal X	Z	D exp.	Dia.
External	8		

d A	I/I0	h k l
4.879	6	1 1 1C
2.986	38	2 2 0C
2.5471	100	3 1 1C
2.4381	7	2 2 2C
2.1118	11	4 0 0C
1.7246	9	4 2 2C
1.6256	15	5 1 1C
1.4933	25	4 4 0C
1.3354	2	6 2 0C
1.2881	4	5 3 3C
1.2736	2	6 2 2C
1.2191	1	4 4 4C
1.1290	2	6 4 2C
1.0997	4	7 3 1C

Reference (Powder Data)
Tovar M.,Eysel W. Mineraloqisches Institut der Universitaet
Heidelberq, FRG, ICDD, Grant-in-Aid (1997)

Reference (Crystal Data)

Ibid.

Preparation & Chemistry
Stoichiometric mixture of ZnO (Aldrich, 99.99 %), CuO (Heraeus, 99.99%) and TiO2 (Merck, 99.9%) annealed in an open corundum crucible at 1000 C for 4 days.

Additional Comments

Spinel structure type

Color: black
F(14)=114.7(.0068, 18)
Si used as internal standard.

d: 2.57	4.93	1.51	I 4.93
I/I1: 100	43	35	I 43

Formula: Cu Rh2 O4

Name: Copper Rhodium Oxide

Rad.	Lambda	Filter Mono. X	Crystal Sys.	Space Group	S.G. #
CuKa1	1.5406	Type: Ge	Cubic	Fd3m	227

Intensities	d values
Diffractom. X	Diff. X
Densitom.	Guinier
Visual	Debye
Calc.	Calc.

a 8.5397 b c
(.0002) ( ) ( )

A B C

A C

I/I cor.	D calc.	mp
5.5	7.111	

d value std.	Cut off

Internal X	Z	D exp.	DIA.
External	8		

d A	I/I0	h k l
4.926	43	1 1 1C
3.019	13	2 2 0C
2.5748	100	3 1 1C
2.4650	33	2 2 2C
2.1349	26	4 0 0C
1.9590	6	3 3 1C
1.7429	3	4 2 2C
1.6435	26	5 1 1C
1.5096	35	4 4 0C
1.4437	7	5 3 1C
1.3506	1	6 2 0C
1.3022	8	5 3 3C
1.2874	10	6 2 2C
1.2325	4	4 4 4C
1.1958	7	7 1 1C
1.1409	1	6 4 2C
1.1118	10	7 3 1C
1.0675	3	8 0 0C
1.0433	1	7 3 3C

Reference (Powder Data)
Tovar, M., Eysel, W., Mineraloqisches Institut der Universitaet
Heidelberq, FRG, ICDD Grant-in-Aid Report (1998)

Reference (Crystal Data)
Tovar, M., Molter, F., Neininqer, K., Eysel, W., Powder Diffr.
11.2, 136 (1996)

Preparation & Chemistry
Stoichiometric mixture of CuO (Fluka,99.98%) and Rh2O3 (99.9%)
annealed in an open corundum crucible at 1000 C for 2 weeks.

Additional Comments

Transition tetraqonal-cubic at about 600 C
Pattern taken at 650 C
Additional peaks from Pt sample carrier at d=2.28, 1.97, 1.40, 1.19, 1.14
Color: black
F(19)=138.6(.0069, 20)
Al2O3 (NIST SRM 676) used as internal standard.

d	2.53	4.84	2.09	5.93
I/I1	100	48	42	20

Formula: Li2 Co Ti3 O8

Name: Lithium Cobalt Titanium Oxide

Rad.	Lambda	Filter Mono. / Type:	Crystal Sys.	Space Group	S.G. #
CuKa1	1.5406	NI	Cubic	P4332	212

Intensities: Diffractom. / Densitom. / Visual / Calc.

d values: Diff. / Guinier / Debye / Calc.

a 8.3753(3) b c

A B C

A C

I/I cor.	D calc.	mp
2.7	3.895	

d value std.: Cut off

Z	D exp.	Dia.
4		

Internal / External

Reference (Powder Data)
Tovar M., Eysel W., Mineraloqisches Institut der Universitaet
Heidelberq, FRG, ICDD, Grant-in-Aid Report(1997)

Reference (Crystal Data)

Ibid.

Preparation & Chemistry
Stoichiometric mixture of Li2CO3 (Merck, 99.9%), CoO (Ventron 99.9%) and TiO2 (Merck, 99.99%) annealed in an open corundum crucible at 600 C for 1 day, at 800 C for 2 days and at 900 C for 1 day.

Additional Comments

Spinel structure type
Color: turquoise
F(22)= 54.9(.0082, 49)
Si used as internal standard.

d A	I/I0	h k l
5.926	20	1 1 0C
4.838	48	1 1 1C
3.746	32	2 1 0C
3.419	18	2 1 1C
2.961	27	2 2 0C
2.792	2	2 2 1C
2.650	4	3 1 0C
2.525	100	3 1 1C
2.3227	2	3 2 0C
2.0943	42	4 0 0C
1.8277	4	4 2 1C
1.7098	6	4 2 2C
1.6118	24	5 1 1C
1.5550	2	5 2 0C
1.5291	3	5 2 1C
1.4803	36	4 4 0C
1.4151	3	5 3 1C
1.3239	2	6 2 0C
1.2771	5	5 3 3C
1.2627	2	6 2 2C
1.2089	3	4 4 4C
1.0907	5	7 3 1C

d	4.84	2.09	2.53	4.84
I/I1	100	80	65	100

Formula: Li2 Cu Ti3 O8

Name: Lithium Copper Titanium Oxide

Rad.	Lambda	Filter Mono. / Type:	Crystal Sys.	Space Group	S.G. #
CuKa1	1.5406	NI	Cubic	Fd3m	227

Intensities: Diffractom. / Densitom. / Visual / Calc.

d values: Diff. / Guinier / Debye / Calc.

a 8.3825(3) b c

A B C

A C

I/I cor.	D calc.	mp
1.8	3.937	

d value std.: Cut off

Z	D exp.	Dia.
4		

Internal / External

Reference (Powder Data)
Tovar M., Eysel W., Mineraloqisches Institut der Universitaet
Heidelberq, FRG, ICDD Grant-in-Aid Report (1997)

Reference (Crystal Data)

Ibid.

Preparation & Chemistry
Stoichiometric mixture of Li2CO3 (Merck, 99.99 %), CuO (Heraeus 99.99%) and TiO2 (Merck, 99.9%) decarbonized at 600 C annealed in an open corundum crucible at 1000 C for 2 days.

Additional Comments

Spinel structure type
Color: black
F(15)= 96.0(.0087, 18)
Si used as internal standard.

d A	I/I0	h k l
4.835	100	1 1 1C
2.963	15	2 2 0C
2.528	65	3 1 1C
2.421	6	2 2 2C
2.0952	80	4 0 0C
1.9227	5	3 3 1C
1.7111	1	4 2 2C
1.6130	28	5 1 1C
1.4816	10	4 4 0C
1.4168	4	5 3 1C
1.2782	2	5 3 3C
1.2636	1	6 2 2C
1.2100	1	4 4 4C
1.1739	1	5 5 1C
1.0914	3	7 3 1C

d	2.951	3.180	2.504	I 5.598 I
I/I1	100	15	15	I 12 I

Formula: Sr2 Al2 Ge O7

Name: Strontium Aluminium Germanium Oxide

Rad.	Lambda	Filter Mono. X Type: NI	Crystal Sys.	Space Group	S.G. #
CuKa1	1.5406		Tetragonal	P-421m	113

a 7.9209(1) b c 5.3375(1)

A B C

A C .67385

I/I cor.	D calc.	mp
7.0	4.104	

Z: 2 | D exp. | Dia.

Intensities | d values | Diffractom. X | Densitom. | Visual | Calc. | Diff. X | Guinier | Debye | Calc. | d value std. | Cut off | Internal X | External

Reference (Powder Data)
Tovar M.,Eysel W. Mineraloqisches Institut der Universitaet
Heidelberq, FRG, ICDD, Grant-in-Aid (1997)

Reference (Crystal Data)

Ibid.

Preparation & Chemistry
Stoichiometric mixture of SrCO3 (Heraeus 99.999%), Al2O3 (Ventron 99.99%) and GeO2 (Heraeus 99.999%) annealed in an open corundum crucible at 1000 C for 10 days and at 1200 C for 17 days.

Additional Comments

Gehlenite structure type

Color: white
F(30)= 78.6(.0075, 51)
Si used as internal standard.

d A	I/I0	h k l
5.598	12	1 1 0C
3.962	6	2 0 0C
3.866	9	1 1 1C
3.180	15	2 0 1C
2.951	100	2 1 1C
2.800	3	2 2 0C
2.669	10	0 0 2C
2.529	4	1 0 2C
2.504	15	3 1 0C
2.4793	2	2 2 1C
2.4094	2	1 1 2C
2.3660	2	3 0 1C
2.2668	1	3 1 1C
2.2130	2	2 0 2C
2.1312	6	2 1 2C
2.0312	1	3 2 1C
1.9799	5	4 0 0C
1.9312	1	2 2 2C
1.9197	2	4 1 0C
1.8667	7	3 3 0C
1.8261	11	3 1 2C
1.8074	6	4 1 1C
1.7714	2	4 2 0C
1.7621	2	3 3 1C
1.6962	2	3 2 2C
1.5900	8	2 1 3C
1.5299	2	3 3 2C
1.4757	1	4 2 2C
1.4181	6	5 2 1C
1.4002	1	4 4 0C
1.3208	1	6 0 0C
1.3058	2	4 1 3C
1.2040	1	2 2 4C
1.1330	1	5 2 3C

d	3.08	3.33	1.91	I 5.82 I
I/I1	100	22	18	I 4 I

Formula: Ba2 Ga2 Ge O7

Name: Barium Gallium Germanium Oxide

Rad.	Lambda	Filter Mono. X Type: NI	Crystal Sys.	Space Group	S.G. #
CuKa1	1.5406		Tetragonal	P-421m	113

a 8.2212(4) b c 5.6579(3)

A B C

A C .68821

I/I cor.	D calc.	mp
7.1	5.199	

Z: 2 | D exp. | Dia.

Intensities | d values | Diffractom. X | Densitom. | Visual | Calc. | Diff. X | Guinier | Debye | Calc. | d value std. | Cut off | Internal X | External

Reference (Powder Data)
Tovar M.,Eysel W., Mineraloqisches Institut der Universitaet
Heidelberq, FRG, ICDD, Grant-in-Aid (1997)

Reference (Crystal Data)

Ibid.

Preparation & Chemistry
Stoichiometric mixture of BaCO3 (Aldrich 99.999%), Ga2O3 (Heraeus 99.99%) and GeO2 (Heraeus 99.999%) annealed in an open corundum crucible at 1100 C for 13 days.

Additional Comments

Weak peak of BaGa2O4 at d=3.1782

Gehlenite structure type

Color: white
F(30)= 94.1(.0061, 52)
Si used as internal standard.

d A	I/I0	h k l
5.817	4	1 1 0C
5.665	2	0 0 1C
4.110	3	2 0 0C
4.055	12	1 1 1C
3.676	3	2 1 0C
3.325	20	2 0 1C
3.082	100	2 1 1C
2.906	4	2 2 0C
2.829	22	0 0 2C
2.6755	3	1 0 2C
2.5990	18	3 1 0C
2.5441	2	1 1 2C
2.4656	1	3 0 1C
2.3300	2	2 0 2C
2.2415	6	2 1 2C
2.1155	1	3 2 1C
2.0553	3	4 0 0C
2.0275	2	2 2 2C
1.9940	3	4 1 0C
1.9375	5	3 3 0C
1.9142	18	3 1 2C
1.8806	7	4 1 1C
1.8338	5	3 3 1C
1.7938	2	1 1 3C
1.7141	1	2 0 3C
1.6781	9	2 1 3C
1.6623	1	4 0 2C
1.5985	3	3 3 2C
1.4739	6	5 2 1C
1.4533	2	3 2 3C
1.4144	1	0 0 4C
1.3702	4	6 0 0C
1.2427	2	3 1 4C
1.2331	1	6 0 2C
1.1865	2	5 2 3C
1.1076	1	7 2 1C