

Observed and calculated structure factors for allochalcoselite

# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag

```
#
data_new
_shelx_title ' c2m in C2/m'
_shelx_refl_list_code 4
_shelx_F_calc_maximum 932.89
_exptl_crystal_F_000 1892.00
_reflns_d_resolution_high 0.7511
```

```
loop_
_refln_index_h
_refln_index_k
_refln_index_l
_refln_F_squared_calc
_refln_F_squared_meas
_refln_F_squared_sigma
_refln_observed_status
```

2	0	0	38212.79	33813.00	726.52	o	-3	3	7	53306.57	51367.05	2263.07	o
4	0	0	6401.27	5179.12	205.19	o	-1	3	7	4542.24	4112.59	306.96	o
6	0	0	11185.70	11384.29	475.23	o	1	3	7	4483.38	4130.12	358.18	o
8	0	0	1125.26	1776.74	268.16	o	3	3	7	145.63	462.88	318.99	o
10	0	0	17359.50	17211.78	520.66	o	5	3	7	81407.64	77395.66	3278.21	o
12	0	0	27639.55	27347.16	1317.89	o	7	3	7	36030.95	35681.36	900.08	o
14	0	0	147181.39	155748.61	5502.63	o	9	3	7	1265.23	1055.46	450.20	o
16	0	0	19496.91	21387.02	1220.57	o	11	3	7	1271.38	1447.16	522.12	o
18	0	0	10684.59	12366.05	1118.14	o	13	3	7	5992.87	7239.74	1966.10	o
1	1	0	1217.78	1196.03	81.48	o	-20	4	7	49787.35	46844.56	1721.19	o
3	1	0	9795.29	13102.84	610.68	o	-18	4	7	264.46	-330.71	929.12	o
5	1	0	52498.80	55175.81	939.95	o	-16	4	7	4283.47	4228.02	672.17	o
7	1	0	143427.52	146413.72	3801.20	o	-14	4	7	9976.25	9247.34	742.41	o
9	1	0	51788.88	47930.47	1736.00	o	-12	4	7	391.89	326.04	490.36	o
11	1	0	887.16	1380.09	243.20	o	-10	4	7	27214.99	25503.51	1325.66	o
13	1	0	22608.15	23431.50	583.44	o	-8	4	7	5533.84	5926.62	490.66	o
15	1	0	24127.14	24723.46	722.56	o	-6	4	7	2718.75	3284.71	424.78	o
17	1	0	321.78	251.04	568.27	o	-4	4	7	1931.25	2490.21	491.94	o
19	1	0	181.42	-213.61	976.81	o	-2	4	7	6575.77	7128.45	426.44	o
21	1	0	16774.65	16251.52	1508.04	o	0	4	7	11093.38	10934.51	481.57	o
0	2	0	853560.88	1023363.19	31328.24	o	2	4	7	17251.41	16546.31	1048.77	o
2	2	0	70279.50	69417.55	1136.70	o	4	4	7	5524.93	5363.14	449.80	o
4	2	0	17664.34	16308.10	255.08	o	6	4	7	3803.46	3147.41	461.30	o
6	2	0	8697.23	8578.04	372.39	o	8	4	7	37827.93	38105.52	1385.54	o
8	2	0	88790.13	94944.36	3300.49	o	10	4	7	3146.93	3716.91	750.33	o
10	2	0	11461.66	11661.18	359.80	o	12	4	7	11540.97	9903.35	959.09	o
12	2	0	65588.71	64965.34	891.63	o	-17	5	7	10075.79	10959.26	1280.94	o
14	2	0	100317.54	101212.71	2292.33	o	-15	5	7	4735.72	4881.30	737.49	o
16	2	0	11133.54	11709.35	796.29	o	-13	5	7	4685.54	5058.15	709.78	o
18	2	0	10813.27	10846.19	868.82	o	-11	5	7	39034.83	39124.67	1284.74	o
20	2	0	19325.00	20894.60	1599.35	o	-9	5	7	82.03	404.51	484.37	o
1	3	0	69.16	361.75	167.10	o	-7	5	7	54910.62	56112.23	1676.84	o
3	3	0	13298.84	13922.64	265.21	o	-5	5	7	2529.45	2825.93	561.26	o
5	3	0	29616.84	28027.12	521.23	o	-3	5	7	28632.84	29473.79	1008.29	o
7	3	0	81738.77	84044.98	2055.16	o	-1	5	7	2926.65	2849.46	625.68	o
9	3	0	33747.57	32998.73	612.82	o	1	5	7	748.24	1725.41	466.63	o
11	3	0	47.17	-114.06	373.30	o	3	5	7	499.29	371.20	425.14	o
13	3	0	23495.91	23542.75	787.15	o	5	5	7	37855.54	34222.05	1158.95	o
15	3	0	19491.23	19617.75	801.44	o	7	5	7	30489.02	29956.03	961.16	o
17	3	0	283.37	1086.42	675.98	o	9	5	7	358.66	451.76	618.62	o
19	3	0	104.12	-97.52	769.18	o	-16	6	7	2655.21	2879.85	1352.78	o
0	4	0	870284.56	970421.50	41523.86	o	-14	6	7	148.78	126.62	740.81	o
2	4	0	6146.93	5438.92	278.08	o	-12	6	7	6417.62	7734.97	781.37	o
4	4	0	3963.86	4031.86	252.81	o	-10	6	7	1216.13	1430.91	646.38	o
6	4	0	12583.48	12454.38	612.55	o	-8	6	7	14932.28	16275.84	1051.50	o
8	4	0	162.09	236.74	299.97	o	-6	6	7	263.90	343.19	726.92	o
10	4	0	8450.42	9427.14	553.17	o	-4	6	7	1093.20	633.01	625.31	o
12	4	0	15911.23	17274.85	733.11	o	-2	6	7	1745.33	2224.01	561.04	o
14	4	0	72339.67	70647.65	3832.66	o	0	6	7	14230.88	16711.66	951.54	o
16	4	0	8451.43	9253.49	783.98	o	2	6	7	1416.45	763.38	848.43	o
18	4	0	6980.32	7182.86	931.85	o	4	6	7	13530.81	12668.59	1490.82	o
1	5	0	711.03	590.57	330.26	o	6	6	7	1045.52	1258.04	756.03	o
3	5	0	3428.80	2606.89	378.95	o	8	6	7	2300.14	2441.84	940.87	o
5	5	0	18909.19	19739.80	632.12	o	-11	7	7	15444.13	16099.11	1304.37	o
7	5	0	39710.60	41338.33	878.36	o	-9	7	7	172.42	-66.30	933.50	o
9	5	0	19341.29	20256.51	744.58	o	-7	7	7	35351.31	37052.38	1456.98	o
11	5	0	1051.49	1818.24	508.35	o	-5	7	7	1127.79	421.35	810.52	o
13	5	0	8782.98	9486.61	707.37	o	-3	7	7	4943.95	5959.50	1224.70	o
15	5	0	9749.36	10319.95	837.30	o	-1	7	7	48.52	323.52	978.85	o
17	5	0	546.39	145.18	1547.22	o	1	7	7	1600.46	1552.26	917.94	o
0	6	0	132966.81	131174.73	2716.61	o	3	7	7	251.61	1116.46	821.73	o
2	6	0	20525.61	20931.91	907.50	o	-22	0	8	17589.26	17370.98	2012.19	o
4	6	0	9874.34	9720.60	1220.79	o	-20	0	8	3872.23	3611.37	1481.91	o
6	6	0	1203.26	1451.80	484.22	o	-18	0	8	2264.01	1676.52	1286.44	o
8	6	0	12479.47	12648.29	879.18	o	-16	0	8	21049.97	17999.84	1644.88	o
10	6	0	803.22	1187.42	686.87	o	-14	0	8	42616.98	35535.55	1905.30	o























-19	1	7	243.30	101.54	779.22	o	-10	2	17	7236.95	6653.71	1419.49	o
-17	1	7	38112.13	39978.04	2961.17	o	-8	2	17	4038.80	3028.12	963.02	o
-15	1	7	7481.49	8383.65	1108.50	o	-6	2	17	4901.88	4272.00	1098.10	o
-13	1	7	7291.98	7328.13	594.63	o	-4	2	17	6413.08	6668.94	1104.62	o
-11	1	7	145934.80	140094.77	13205.85	o	-2	2	17	7995.29	6820.32	956.20	o
-9	1	7	1099.86	1379.89	1224.06	o	0	2	17	17325.38	18256.41	1851.44	o
-7	1	7	205650.73	216110.80	14242.35	o	-17	3	17	302.27	-569.31	813.71	o
-5	1	7	960.05	1601.15	286.48	o	-15	3	17	15473.34	15362.95	992.28	o
-3	1	7	127491.88	132963.84	2033.96	o	-13	3	17	1831.60	1681.99	814.64	o
-1	1	7	16136.40	17535.50	499.53	o	-11	3	17	18484.81	20234.19	1526.50	o
1	1	7	1951.26	2380.20	186.65	o	-9	3	17	81.46	623.04	918.72	o
3	1	7	1054.13	1533.65	269.34	o	-7	3	17	589.46	703.11	1007.99	o
5	1	7	111330.89	108946.90	6729.41	o	-5	3	17	239.70	756.98	1010.00	o
7	1	7	60651.02	58924.71	1333.19	o	-3	3	17	25699.22	23406.08	1700.14	o
9	1	7	1103.21	1592.75	426.43	o	-12	4	17	6186.88	6397.34	1942.24	o
11	1	7	1869.83	1840.92	433.91	o	-10	4	17	9534.91	10173.94	1011.15	o
13	1	7	9008.06	9808.76	824.68	o	-8	4	17	2220.62	3597.46	1201.23	o
15	1	7	157.81	347.18	710.41	o	-18	0	18	2893.06	1908.94	1639.20	o
-22	2	7	24783.08	27986.14	1461.03	o	-16	0	18	11487.35	12848.27	1754.12	o
-20	2	7	10964.23	10141.93	855.09	o	-14	0	18	8798.45	9740.66	1487.38	o
-18	2	7	46423.52	43487.73	4602.16	o	-12	0	18	1780.18	2429.29	1213.61	o
-16	2	7	5950.14	7657.74	1345.47	o	-10	0	18	42391.88	44193.63	2101.37	o
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-12	2	7	18557.31	17117.99	1535.18	o	-6	0	18	9246.53	8575.85	1327.51	o
-10	2	7	1282.54	2233.83	417.68	o	-4	0	18	9.35	-138.95	1184.16	o
-8	2	7	49521.28	47701.46	1671.58	o	-2	0	18	101.52	423.07	1256.76	o
-6	2	7	201.72	382.76	438.76	o	-19	1	18	11702.41	10864.27	1379.24	o
-4	2	7	1789.78	2582.45	323.96	o	-17	1	18	1448.16	2070.70	1130.90	o
-2	2	7	4318.54	3965.72	286.32	o	-15	1	18	1683.74	2398.93	1087.90	o
0	2	7	47502.54	46225.11	1168.09	o	-13	1	18	5110.96	5363.21	761.16	o
2	2	7	1743.03	1815.24	286.62	o	-11	1	18	6268.83	6066.31	849.55	o
4	2	7	50788.84	46139.98	3328.08	o	-9	1	18	557.55	1223.69	1061.91	o
6	2	7	2600.19	2514.53	372.72	o	-7	1	18	28009.51	27579.81	1303.94	o
8	2	7	8255.32	8794.25	676.28	o	-5	1	18	6470.60	6222.61	952.51	o
10	2	7	8665.64	9214.01	1083.39	o	-3	1	18	448.49	-183.03	818.66	o
12	2	7	289.95	33.24	472.13	o	-18	2	18	17908.18	17278.16	1827.74	o
14	2	7	26890.55	26952.25	969.14	o	-16	2	18	94.91	367.54	826.40	o
-21	3	7	5027.22	5932.49	1039.69	o	-14	2	18	59.09	-876.06	876.06	o
-19	3	7	170.45	65.47	677.08	o	-12	2	18	22142.52	21113.59	1146.80	o
-17	3	7	30533.21	28694.33	3923.17	o	-10	2	18	3199.44	2285.81	782.85	o
-15	3	7	3675.09	3457.43	587.77	o	-8	2	18	8792.51	8491.84	1285.82	o
-13	3	7	5952.40	6558.35	581.68	o	-6	2	18	33506.04	31129.44	1894.73	o
-11	3	7	98508.10	93544.98	2322.09	o	-4	2	18	5561.58	3657.78	1162.52	o
-9	3	7	1370.52	1111.93	397.12	o	-2	2	18	6986.67	7176.04	1615.44	o
-7	3	7	166967.19	173459.39	1663.67	o	-17	3	18	714.27	117.70	1258.97	o
-5	3	7	729.44	786.34	429.52	o	-15	3	18	1482.16	990.06	925.72	o
							-13	3	18	5521.16	5356.89	949.13	o
							-11	3	18	3341.43	4801.77	880.13	o
							-9	3	18	340.85	-64.10	767.25	o
							-7	3	18	21477.92	19882.16	1634.29	o
							-18	0	19	1048.76	1852.28	1644.85	o
							-16	0	19	36530.54	38296.29	2344.46	o
							-14	0	19	4830.00	5261.87	1396.94	o
							-10	0	19	59.67	-933.23	1242.24	o
							-8	0	19	7844.39	9277.25	1420.56	o
							-6	0	19	308.70	122.36	1182.15	o
							-4	0	19	23292.65	23048.60	1965.84	o
							-17	1	19	9897.75	11532.91	1355.05	o
							-15	1	19	1828.34	1783.41	1438.68	o
							-13	1	19	1994.36	1828.82	913.40	o
							-11	1	19	547.84	584.88	1194.65	o
							-9	1	19	42439.86	41013.37	2175.76	o
							-7	1	19	15702.04	14444.08	1597.27	o
							-5	1	19	808.02	636.55	1311.89	o
							-16	2	19	14019.27	14062.86	1411.36	o
							-14	2	19	8838.91	9248.69	2723.14	o
							-12	2	19	456.35	1512.56	1190.48	o
							-10	2	19	603.11	752.88	1178.06	o
							-8	2	19	7250.09	5162.30	1283.31	o
							-11	3	19	225.65	2567.50	1327.30	o
							-16	0	20	46204.10	47764.09	2561.22	o
							-8	0	20	82.19	-1267.13	1302.38	o
							-15	1	20	941.40	-29.04	1563.93	o
							-13	1	20	30377.69	29693.58	2020.44	o
							-11	1	20	11871.40	9873.68	1562.83	o
							-9	1	20	289.44	-462.49	1292.06	o