

```
#
# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag
#
data_camp8
_shelx_title ' CaMnSi2O6 data collection in DAC by Xcaliber-I at VT'
_shelx_refl_list_code 4
_shelx_F_calc_maximum 201.39
_exptl_crystal_F_000 484.00
_reflns_d_resolution_high 0.7107
```

```
loop_
_symmetry_equiv_pos_as_xyz
'x, y, z'
'-x, y, -z+1/2'
'x+1/2, y+1/2, z'
'-x+1/2, y+1/2, -z+1/2'
'-x, -y, -z'
'x, -y, z-1/2'
'-x+1/2, -y+1/2, -z'
'x+1/2, -y+1/2, z-1/2'
```

```
_cell_length_a 9.7491
_cell_length_b 8.8957
_cell_length_c 5.1607
_cell_angle_alpha 90.000
_cell_angle_beta 103.931
_cell_angle_gamma 90.000

_shelx_F_squared_multiplier 1.000
```

```
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
1 1 0 1196.44 1142.01 126.09 o
3 1 0 12532.48 11219.39 1014.82 o
2 2 0 2345.00 2480.86 159.09 o
1 3 0 126.42 133.01 14.15 o
3 3 0 3693.66 3653.02 327.06 o
5 3 0 2000.31 1802.07 206.35 o
2 4 0 86.25 133.37 15.81 o
4 4 0 6918.96 6938.37 458.60 o
6 4 0 26.84 14.02 22.05 o
3 5 0 10103.69 10460.66 653.27 o
5 5 0 247.47 224.64 20.58 o
7 5 0 20010.56 17787.34 1231.47 o
2 6 0 207.25 176.38 28.52 o
4 6 0 823.54 829.87 130.15 o
6 6 0 295.29 378.10 21.41 o
```

8	6	0	765.87	827.00	67.06 o
5	7	0	659.67	643.21	35.08 o
7	7	0	1182.48	1034.60	165.87 o
9	7	0	116.30	100.11	36.21 o
6	8	0	362.27	353.56	53.06 o
10	8	0	872.15	804.69	108.64 o
5	9	0	128.50	112.80	39.09 o
7	9	0	1203.75	1437.92	204.11 o
6	10	0	1243.30	1329.89	129.84 o
8	10	0	1235.54	1246.97	114.34 o
-3	1	1	4048.49	4012.78	750.39 o
-1	1	1	135.86	98.73	5.26 o
1	1	1	30.07	19.12	4.05 o
3	1	1	2936.17	2836.17	138.88 o
-4	2	1	10787.88	10751.82	2217.77 o
-2	2	1	33890.32	33277.39	4195.23 o
2	2	1	25720.90	25091.01	2051.01 o
4	2	1	4472.17	4203.98	217.13 o
-5	3	1	17279.27	16446.09	3593.94 o
-3	3	1	16200.40	17152.97	2307.76 o
-1	3	1	16702.23	18094.95	975.42 o
3	3	1	4583.56	4716.40	264.05 o
5	3	1	33905.99	32235.70	1297.35 o
-4	4	1	24.33	34.07	8.94 o
-2	4	1	891.53	918.25	55.09 o
2	4	1	2556.08	2496.63	208.63 o
4	4	1	646.27	706.11	43.42 o
6	4	1	145.31	96.65	17.76 o
-7	5	1	481.32	419.49	29.85 o
-5	5	1	262.00	263.34	29.27 o
-3	5	1	5.82	35.06	15.25 o
1	5	1	733.52	894.89	137.03 o
5	5	1	831.22	954.46	173.34 o
7	5	1	148.88	133.28	30.45 o
-6	6	1	641.82	639.82	71.57 o
-4	6	1	761.74	858.47	54.63 o
-2	6	1	710.29	795.00	136.32 o
2	6	1	383.93	436.06	26.24 o
4	6	1	148.61	193.73	21.00 o
8	6	1	453.55	410.60	57.72 o
-9	7	1	2134.78	1806.40	115.59 o
-7	7	1	173.63	125.38	28.86 o
-5	7	1	13884.36	14642.70	1122.20 o
-3	7	1	407.23	411.36	31.74 o
3	7	1	1050.84	1345.11	89.89 o
5	7	1	5490.38	6440.77	430.24 o
7	7	1	692.91	664.18	34.54 o
9	7	1	4651.24	4153.32	436.42 o
-10	8	1	265.10	235.60	43.31 o
-8	8	1	2932.50	2572.75	142.28 o
-6	8	1	869.71	928.09	64.13 o
-4	8	1	1278.44	1314.01	95.65 o
4	8	1	1781.88	1766.40	260.73 o
6	8	1	4590.29	5161.60	863.38 o

8	8	1	667.04	648.03	59.99 o
-9	9	1	183.00	251.37	46.68 o
-7	9	1	2084.79	2087.88	308.89 o
-5	9	1	2469.73	2763.93	274.18 o
5	9	1	1383.74	1912.06	246.90 o
7	9	1	774.43	786.41	92.07 o
-8	10	1	906.50	1007.56	94.01 o
-6	10	1	178.68	248.75	49.34 o
6	10	1	914.89	967.43	112.68 o
-2	0	2	22.61	53.97	8.59 o
0	0	2	40556.42	40763.68	760.76 o
2	0	2	18131.91	17278.87	3527.47 o
-3	1	2	650.77	481.15	97.93 o
-1	1	2	1269.49	1331.31	66.29 o
1	1	2	7450.98	7691.77	439.19 o
3	1	2	1998.85	1712.37	97.40 o
-6	2	2	1590.53	1436.55	145.64 o
-4	2	2	766.60	1045.83	103.25 o
0	2	2	1247.47	1608.38	145.65 o
2	2	2	1209.13	1384.92	86.66 o
4	2	2	1699.83	1489.27	89.10 o
-7	3	2	689.68	659.76	116.55 o
-5	3	2	1013.20	1007.41	129.99 o
-1	3	2	3986.45	4149.05	320.49 o
1	3	2	1456.39	1497.74	110.86 o
3	3	2	39.70	39.14	15.73 o
5	3	2	1389.16	1241.68	108.91 o
-8	4	2	461.31	417.17	71.86 o
-6	4	2	1097.75	952.24	168.00 o
-4	4	2	523.43	520.45	61.09 o
-2	4	2	12.74	26.03	8.87 o
0	4	2	9097.84	9825.20	528.37 o
2	4	2	510.94	541.74	30.14 o
4	4	2	2950.42	2429.48	263.88 o
6	4	2	388.34	347.46	34.63 o
-9	5	2	1037.11	938.35	55.07 o
-7	5	2	14889.54	14217.45	2109.36 o
-5	5	2	1591.11	1429.31	80.10 o
-3	5	2	15752.86	16286.10	799.75 o
1	5	2	11489.22	11068.62	1085.83 o
3	5	2	17875.81	18036.97	1354.09 o
5	5	2	192.10	252.65	30.23 o
7	5	2	7407.14	6405.27	314.22 o
-6	6	2	3939.11	4047.89	194.41 o
-4	6	2	650.25	724.44	55.85 o
-2	6	2	2397.48	2535.61	396.08 o
4	6	2	1193.08	1142.51	81.28 o
6	6	2	26.85	75.18	29.25 o
8	6	2	656.48	522.22	40.10 o
-7	7	2	677.65	628.76	38.51 o
-3	7	2	694.96	716.35	43.36 o
3	7	2	757.02	816.79	117.52 o
5	7	2	429.57	412.73	32.41 o
-10	8	2	789.21	704.92	146.51 o

-8	8	2	737.44	715.81	36.27 o
-4	8	2	815.37	906.76	54.51 o
4	8	2	1167.15	1391.22	124.22 o
6	8	2	1134.56	981.21	146.68 o
8	8	2	192.67	117.86	45.28 o
-7	9	2	1477.20	1441.80	103.69 o
7	9	2	653.68	839.80	47.94 o
-8	10	2	1256.62	1265.80	76.83 o
6	10	2	890.83	880.07	52.12 o
-5	1	3	1725.58	1714.61	172.37 o
-3	1	3	2013.02	2132.29	131.47 o
-1	1	3	9.72	34.71	14.09 o
1	1	3	35.95	26.08	9.13 o
3	1	3	357.23	393.75	18.39 o
-6	2	3	1055.55	946.07	60.35 o
-4	2	3	3040.88	2969.47	128.64 o
-2	2	3	25943.99	25629.12	680.32 o
0	2	3	885.76	1001.12	69.30 o
2	2	3	9424.95	9783.73	322.80 o
4	2	3	645.77	633.98	31.28 o
-5	3	3	9182.62	8565.04	601.24 o
-3	3	3	2050.04	2138.00	99.78 o
-1	3	3	20236.64	20899.63	713.16 o
1	3	3	2557.77	2478.44	133.37 o
3	3	3	245.75	271.51	70.27 o
5	3	3	11220.52	10438.14	477.56 o
-8	4	3	678.73	773.91	97.38 o
-6	4	3	724.71	683.48	41.78 o
-4	4	3	252.84	254.98	22.43 o
-2	4	3	3489.47	3467.46	133.97 o
0	4	3	1443.60	1463.12	86.69 o
2	4	3	219.15	218.57	54.15 o
4	4	3	494.03	444.36	22.41 o
6	4	3	575.92	535.91	59.66 o
-5	5	3	2778.74	2677.03	499.99 o
-3	5	3	68.49	76.63	25.09 o
1	5	3	1792.22	1590.04	109.52 o
3	5	3	345.56	264.96	23.90 o
-8	6	3	143.45	51.08	32.44 o
-4	6	3	215.57	219.23	24.23 o
4	6	3	1411.99	1209.84	279.55 o
-9	7	3	4237.93	3944.98	209.30 o
-5	7	3	5757.83	5753.19	817.84 o
-3	7	3	940.05	831.36	77.87 o
3	7	3	905.84	979.56	109.57 o
5	7	3	5370.76	4759.17	726.05 o
-10	8	3	199.11	133.97	46.86 o
-8	8	3	2503.82	2272.00	575.88 o
-6	8	3	961.65	928.23	93.49 o
4	8	3	8.28	39.45	37.75 o
6	8	3	3224.44	3270.15	215.98 o
-7	9	3	880.73	833.46	79.72 o
5	9	3	1969.13	2151.15	457.97 o
-4	0	4	10766.60	11035.12	242.25 o

-2	0	4	488.95	497.94	35.10 o
0	0	4	16262.14	16724.12	1258.80 o
2	0	4	1925.99	1907.06	285.26 o
-3	1	4	7260.66	6890.94	399.84 o
-1	1	4	1213.91	1188.12	82.64 o
1	1	4	854.83	802.06	65.81 o
3	1	4	4653.41	4458.64	435.63 o
-4	2	4	1083.44	1180.84	92.68 o
-2	2	4	94.79	119.08	14.42 o
0	2	4	1174.58	1103.17	137.62 o
2	2	4	2362.48	2417.41	137.16 o
-5	3	4	1108.60	1216.46	82.96 o
-3	3	4	637.46	692.23	84.59 o
-1	3	4	257.18	405.76	82.24 o
1	3	4	233.36	239.70	19.43 o
3	3	4	739.21	763.89	42.57 o
5	3	4	301.97	401.32	65.59 o
-6	4	4	686.62	666.09	26.27 o
-4	4	4	1488.03	1664.75	91.75 o
0	4	4	1752.42	1738.93	153.55 o
4	4	4	3042.73	2924.18	158.80 o
-9	5	4	420.56	347.73	70.53 o
-7	5	4	11183.05	10772.82	803.20 o
-5	5	4	1153.83	1124.00	84.65 o
-3	5	4	10249.90	10889.22	713.69 o
1	5	4	5750.04	5547.67	261.96 o
3	5	4	6238.72	6427.58	308.66 o
5	5	4	1100.93	1090.47	71.00 o
-8	6	4	667.17	612.87	34.87 o
-6	6	4	1756.48	1935.72	160.45 o
-4	6	4	3197.60	3919.97	707.48 o
4	6	4	3881.07	3597.78	199.02 o
6	6	4	397.15	320.38	53.80 o
-9	7	4	140.84	156.14	44.45 o
-7	7	4	671.25	708.86	71.13 o
-5	7	4	224.13	204.50	23.61 o
5	7	4	50.66	66.62	41.05 o
-8	8	4	867.19	802.75	65.86 o
-6	8	4	286.21	209.84	39.99 o
4	8	4	413.25	412.09	33.53 o
-7	9	4	754.42	716.67	117.04 o
-5	1	5	364.01	365.01	67.88 o
-3	1	5	595.87	627.62	35.42 o
1	1	5	177.94	231.53	41.40 o
3	1	5	12.56	33.35	29.04 o
-6	2	5	1300.35	1294.21	128.99 o
-4	2	5	1256.43	1195.11	100.21 o
-2	2	5	5741.40	5866.24	211.04 o
0	2	5	1167.62	1289.25	103.77 o
2	2	5	7908.82	8267.46	464.90 o
-7	3	5	792.78	881.27	83.96 o
-5	3	5	3917.79	3627.32	169.92 o
-1	3	5	11812.81	11976.37	788.07 o
1	3	5	1825.59	1883.48	121.04 o

3	3	5	295.32	396.80	31.05 o
5	3	5	3502.71	3360.08	405.88 o
-8	4	5	402.89	383.86	54.09 o
0	4	5	168.71	119.27	34.16 o
2	4	5	1003.74	917.09	75.71 o
4	4	5	1335.71	1330.38	228.92 o
-9	5	5	324.46	315.18	45.74 o
-5	5	5	308.60	391.53	42.49 o
-3	5	5	336.41	363.46	40.93 o
1	5	5	2.58	45.42	39.27 o
3	5	5	391.47	390.33	44.85 o
5	5	5	350.43	307.38	45.17 o
-6	6	5	702.01	679.92	39.68 o
-4	6	5	310.40	280.77	39.06 o
4	6	5	277.06	255.57	29.87 o
-7	7	5	225.87	183.55	49.03 o
-5	7	5	5665.86	6248.69	542.77 o
3	7	5	1038.44	1180.06	71.25 o
-6	8	5	117.66	43.02	39.83 o
-4	0	6	8572.79	9406.15	334.44 o
-2	0	6	1939.45	2148.74	273.11 o
0	0	6	2864.96	3037.64	176.72 o
2	0	6	523.16	626.16	83.66 o
-5	1	6	200.21	200.41	38.21 o
-3	1	6	2628.35	2763.29	166.77 o
1	1	6	387.77	409.68	28.84 o
-2	2	6	300.37	300.55	28.55 o
0	2	6	6.31	38.46	34.23 o
2	2	6	165.96	128.38	39.61 o
-7	3	6	416.21	514.28	39.67 o
-1	3	6	973.97	1030.74	140.80 o
1	3	6	217.85	256.77	25.26 o
-6	4	6	1031.45	1209.20	70.27 o
0	4	6	2000.93	2207.14	158.38 o
2	4	6	335.96	396.50	51.30 o
-7	5	6	2834.38	2940.61	182.57 o
-5	5	6	767.37	741.59	77.57 o
-3	5	6	9389.10	10620.21	1757.18 o
1	5	6	2294.24	2382.22	157.09 o
-6	6	6	479.24	566.06	117.36 o
-4	6	6	727.79	778.69	49.22 o
-5	1	7	103.31	83.29	41.23 o
-3	1	7	416.37	475.33	43.94 o
-4	2	7	1205.67	1266.21	127.73 o
-2	2	7	1826.70	2033.24	201.28 o
-3	3	7	225.90	253.20	44.90 o