

```
#
# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag
#
data_camp0
_shelx_title ' CaMnSi2O6 data collection i n DAC by Xcaliber-I at VT'
_shelx_refln_list_code      4
_shelx_F_calc_maximum      204.40
_exptl_crystal_F_000       484.00
_reflns_d_resolution_high  0.7095
```

```
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    9.9227
_cell_length_b    9.1416
_cell_length_c    5.2745
_cell_angle_alpha 90.000
_cell_angle_beta  105.087
_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   1274.67   1283.79   119.74 o
  3  1  0   13329.38   12747.81   497.78 o
  5  1  0   1307.83   1352.10    59.88 o
  2  2  0   3489.81   3597.85   193.32 o
  4  2  0    61.06    68.99    9.30 o
  6  2  0    33.50    39.15    5.98 o
  3  3  0   3076.18   3254.84   112.24 o
  5  3  0   1044.72    941.48   101.53 o
  7  3  0    92.67    80.33    13.09 o
  2  4  0    88.03    93.55    21.24 o
  4  4  0   6831.82   6896.46   478.44 o
  6  4  0    68.49    75.53    12.27 o
 10  4  0   3211.59   3028.42   143.46 o
  3  5  0   8698.56   8470.50   776.77 o
  5  5  0    306.75    317.63    16.97 o
```

7	5	0	21445.84	21119.39	1537.29 o
9	5	0	979.42	996.40	87.78 o
11	5	0	2769.69	2427.77	192.67 o
4	6	0	1436.27	1416.54	158.46 o
6	6	0	279.74	316.13	41.68 o
8	6	0	1125.88	1053.08	66.79 o
10	6	0	2482.36	2326.53	255.07 o
5	7	0	1349.36	1151.01	85.27 o
7	7	0	1113.24	1170.99	152.67 o
9	7	0	446.65	405.77	42.42 o
10	8	0	724.63	753.64	74.90 o
-5	1	1	943.22	833.65	80.51 o
-3	1	1	4080.22	4146.33	278.82 o
-1	1	1	142.59	103.58	6.79 o
1	1	1	94.71	75.42	3.88 o
3	1	1	2794.44	3050.44	300.38 o
5	1	1	393.46	318.80	20.65 o
-8	2	1	3446.99	3011.16	380.37 o
-6	2	1	5242.01	4738.02	468.34 o
-4	2	1	10441.89	10408.81	601.58 o
-2	2	1	35924.14	34740.72	1961.60 o
0	2	1	66.15	83.21	4.88 o
2	2	1	23477.92	23153.94	422.46 o
4	2	1	4957.68	5010.24	124.29 o
6	2	1	8743.57	8309.12	220.79 o
-9	3	1	9145.26	8171.15	752.82 o
-7	3	1	498.10	469.38	40.03 o
-5	3	1	20115.82	18945.29	1309.00 o
-3	3	1	16992.39	17324.89	475.63 o
3	3	1	4996.86	5383.87	164.61 o
5	3	1	34526.37	32501.29	2698.38 o
-10	4	1	456.81	411.83	51.96 o
-6	4	1	30.63	47.98	11.13 o
-2	4	1	1354.15	1287.01	71.43 o
2	4	1	2312.35	2302.97	340.14 o
4	4	1	651.51	751.87	56.22 o
6	4	1	190.11	159.21	25.47 o
8	4	1	113.26	120.74	18.19 o
-9	5	1	211.10	191.16	14.35 o
-7	5	1	100.26	116.52	15.24 o
-5	5	1	123.19	131.60	11.29 o
-3	5	1	369.50	388.59	30.33 o
3	5	1	268.87	275.68	15.13 o
5	5	1	404.92	431.29	32.38 o
-10	6	1	349.79	258.04	16.66 o
-6	6	1	264.14	203.30	35.98 o
-4	6	1	761.88	856.16	64.48 o
4	6	1	178.12	174.34	26.27 o
8	6	1	217.09	202.14	15.89 o
10	6	1	299.78	219.18	41.81 o
-11	7	1	916.29	845.69	63.17 o
-9	7	1	2235.37	2179.24	276.56 o
-5	7	1	11650.83	12369.89	633.41 o
5	7	1	5064.91	4967.85	429.47 o

7	7	1	567.28	606.39	71.98 o
9	7	1	3882.25	3645.40	156.70 o
-10	8	1	453.28	373.66	29.03 o
-8	8	1	3149.29	2863.64	210.24 o
-6	8	1	1404.72	1459.97	158.47 o
6	8	1	5232.79	5047.42	388.29 o
8	8	1	890.09	807.25	117.89 o
-9	9	1	281.34	348.78	62.27 o
7	9	1	861.34	818.51	63.20 o
9	9	1	337.44	335.10	19.52 o
-4	0	2	23385.31	21881.32	1030.78 o
0	0	2	41778.95	43354.79	2074.54 o
2	0	2	16843.62	18457.66	1204.61 o
-7	1	2	14056.67	11952.07	1908.51 o
-5	1	2	64.44	70.19	11.01 o
-3	1	2	473.26	345.61	41.74 o
-1	1	2	1169.14	1207.79	41.59 o
1	1	2	8140.17	8400.16	318.73 o
3	1	2	2365.14	2014.55	320.03 o
5	1	2	579.85	556.21	49.20 o
-8	2	2	410.50	378.91	20.75 o
-6	2	2	2384.94	2160.99	79.54 o
-4	2	2	741.46	768.81	116.68 o
-2	2	2	48.76	40.39	9.90 o
2	2	2	1774.38	1820.38	69.35 o
4	2	2	1697.98	1506.70	63.07 o
6	2	2	843.52	865.45	49.90 o
-9	3	2	76.80	70.73	15.56 o
-7	3	2	677.96	658.45	67.45 o
-5	3	2	950.13	928.46	48.55 o
-3	3	2	158.30	200.06	38.96 o
1	3	2	1733.86	1910.48	170.26 o
3	3	2	140.54	122.19	7.84 o
5	3	2	677.48	740.58	63.59 o
7	3	2	541.29	452.83	89.57 o
-10	4	2	973.78	969.80	126.70 o
-8	4	2	273.06	293.83	31.72 o
-6	4	2	1161.90	1167.00	55.00 o
-4	4	2	619.74	651.84	47.31 o
2	4	2	423.52	452.45	28.64 o
4	4	2	2126.84	2037.05	84.34 o
6	4	2	463.92	439.95	24.89 o
-11	5	2	3039.51	2541.06	187.98 o
-9	5	2	1111.65	1020.88	83.68 o
-7	5	2	15241.07	14571.01	377.01 o
-5	5	2	1666.49	1651.91	87.64 o
-3	5	2	16232.21	17139.94	1307.59 o
1	5	2	11067.74	11832.36	380.70 o
3	5	2	19417.64	19287.51	1513.23 o
5	5	2	150.08	310.07	29.15 o
7	5	2	6933.59	6706.56	202.84 o
9	5	2	1465.74	1466.32	90.82 o
-12	6	2	112.67	133.43	14.91 o
-10	6	2	446.67	391.50	27.19 o

-8	6	2	290.04	296.19	17.04 o
-6	6	2	5100.38	5387.19	164.11 o
-4	6	2	848.90	976.54	70.01 o
2	6	2	185.39	198.18	49.71 o
4	6	2	1227.84	1083.10	303.12 o
6	6	2	8.45	18.25	13.72 o
8	6	2	838.90	823.07	44.98 o
10	6	2	1584.76	1556.11	224.78 o
-7	7	2	358.27	445.73	63.48 o
5	7	2	870.42	911.19	234.35 o
9	7	2	172.37	190.19	24.84 o
-10	8	2	351.17	374.14	87.68 o
-8	8	2	259.87	239.68	16.31 o
6	8	2	661.57	708.52	93.20 o
7	9	2	561.44	670.93	119.54 o
-7	1	3	1200.28	984.81	103.14 o
-5	1	3	1577.53	1496.44	61.90 o
-3	1	3	1955.06	1990.22	80.78 o
-1	1	3	8.74	32.60	8.06 o
1	1	3	90.10	79.30	11.39 o
3	1	3	385.67	467.99	28.19 o
-8	2	3	7393.76	7053.34	240.37 o
-6	2	3	1357.29	1252.77	128.70 o
-4	2	3	2374.28	2369.60	161.01 o
-2	2	3	26250.83	27299.52	794.91 o
0	2	3	900.16	968.53	65.51 o
2	2	3	8762.26	8868.41	194.57 o
4	2	3	612.66	637.59	40.67 o
6	2	3	7142.41	7120.02	203.37 o
-9	3	3	10440.69	9676.83	245.97 o
-5	3	3	9545.60	9595.94	888.04 o
-3	3	3	3469.62	3442.03	108.39 o
-1	3	3	20020.55	20324.69	783.78 o
1	3	3	2678.40	2851.85	85.43 o
3	3	3	277.09	306.99	66.75 o
5	3	3	12523.04	12703.03	260.17 o
7	3	3	702.79	790.52	57.43 o
-10	4	3	292.67	246.05	20.44 o
-8	4	3	605.98	658.98	37.24 o
-6	4	3	363.56	316.10	15.02 o
-4	4	3	479.67	454.20	31.79 o
0	4	3	1369.24	1368.47	72.86 o
2	4	3	353.88	332.40	22.10 o
4	4	3	676.61	691.15	94.97 o
6	4	3	530.08	513.68	57.42 o
-9	5	3	14.03	36.86	15.37 o
-5	5	3	1826.87	1770.01	83.45 o
1	5	3	845.62	922.05	54.10 o
3	5	3	57.61	30.72	12.95 o
9	5	3	554.08	516.93	112.97 o
-12	6	3	95.32	158.61	25.75 o
-10	6	3	223.70	219.38	15.88 o
-8	6	3	164.86	111.33	11.40 o
2	6	3	155.40	156.38	18.87 o

4	6	3	826.73	881.74	59.51 o
6	6	3	54.24	62.11	18.80 o
-11	7	3	660.93	570.53	66.71 o
-9	7	3	3630.38	3633.93	188.98 o
-7	7	3	183.91	176.98	12.67 o
3	7	3	548.36	675.09	75.50 o
5	7	3	4641.19	4678.41	154.51 o
7	7	3	185.66	190.50	24.19 o
-10	8	3	637.05	564.51	29.76 o
-8	8	3	2888.44	2664.10	313.31 o
6	8	3	3660.23	3839.12	153.12 o
-6	0	4	16337.87	15408.49	317.26 o
-4	0	4	12330.16	12215.46	330.28 o
-2	0	4	47.45	104.15	19.37 o
0	0	4	17709.37	18530.34	359.40 o
2	0	4	2509.96	2723.05	361.17 o
-7	1	4	2327.70	2284.69	159.74 o
-3	1	4	8148.47	8062.31	176.45 o
-1	1	4	644.84	655.46	42.15 o
1	1	4	393.44	390.37	36.14 o
3	1	4	5259.12	5043.61	385.12 o
-8	2	4	33.75	62.79	18.13 o
-4	2	4	780.94	781.14	49.78 o
-2	2	4	435.54	466.66	22.90 o
0	2	4	1146.05	949.91	56.68 o
2	2	4	2233.58	2582.00	146.40 o
-9	3	4	613.33	548.68	74.96 o
-7	3	4	59.61	80.77	15.75 o
-5	3	4	496.88	468.18	37.78 o
-3	3	4	745.30	704.65	73.32 o
-1	3	4	101.12	112.71	9.57 o
1	3	4	41.13	68.53	12.89 o
3	3	4	614.31	678.64	71.09 o
5	3	4	216.87	282.86	13.87 o
-10	4	4	1936.92	1932.75	268.57 o
-6	4	4	162.97	170.65	27.68 o
-4	4	4	1717.65	1709.02	75.02 o
0	4	4	1214.06	1236.15	99.28 o
2	4	4	145.99	202.31	21.47 o
4	4	4	3001.34	3021.32	148.98 o
-11	5	4	2131.38	1770.03	111.58 o
-9	5	4	122.85	60.56	13.10 o
-7	5	4	12069.49	11805.99	243.88 o
-5	5	4	1751.50	1783.96	81.98 o
1	5	4	6024.59	6112.06	149.48 o
3	5	4	6678.66	7037.56	282.63 o
5	5	4	754.36	833.08	98.72 o
7	5	4	5255.47	5719.00	257.76 o
-10	6	4	1795.81	1722.20	172.78 o
-8	6	4	311.27	358.62	21.42 o
-6	6	4	1680.34	1747.85	96.54 o
4	6	4	4678.38	4963.54	152.79 o
6	6	4	256.18	260.60	19.11 o
-9	7	4	527.97	491.81	26.93 o

-7	7	4	752.91	847.91	59.44 o
5	7	4	219.44	268.47	19.24 o
-7	1	5	818.23	737.62	51.44 o
-5	1	5	527.67	580.08	45.75 o
-3	1	5	650.66	684.08	44.11 o
1	1	5	36.96	39.10	17.35 o
3	1	5	26.08	70.65	18.82 o
-8	2	5	6058.12	5965.54	583.37 o
-6	2	5	1395.90	1380.86	74.90 o
-4	2	5	886.65	848.13	64.46 o
-2	2	5	6485.28	6477.13	697.54 o
0	2	5	870.92	1069.67	111.61 o
2	2	5	7335.31	7833.15	288.00 o
4	2	5	5.34	9.32	14.86 o
-9	3	5	7165.56	6631.19	192.19 o
-7	3	5	783.14	702.42	99.12 o
-5	3	5	4104.15	4209.84	144.85 o
-1	3	5	11965.74	13490.68	290.10 o
1	3	5	2461.54	2593.65	110.70 o
3	3	5	132.70	187.33	37.50 o
5	3	5	3897.27	4096.00	440.41 o
-10	4	5	351.36	296.69	21.04 o
-8	4	5	354.70	449.33	75.26 o
-6	4	5	36.86	45.53	17.08 o
-4	4	5	117.00	145.33	18.19 o
-2	4	5	241.45	226.45	14.00 o
0	4	5	383.59	448.94	20.64 o
2	4	5	1192.38	1093.28	175.11 o
4	4	5	1052.36	1037.49	82.47 o
6	4	5	57.26	30.96	24.10 o
-7	5	5	52.70	89.51	11.72 o
-5	5	5	223.37	233.19	15.75 o
3	5	5	62.79	61.81	22.20 o
5	5	5	153.73	176.06	25.19 o
-10	6	5	186.18	130.58	26.15 o
-8	6	5	47.54	89.09	26.65 o
-6	6	5	276.97	312.75	35.31 o
4	6	5	172.11	172.50	24.94 o
-9	7	5	1666.85	1474.14	195.53 o
3	7	5	899.91	1098.32	126.88 o
-6	0	6	2440.47	2375.92	111.33 o
-4	0	6	9434.62	9936.77	217.04 o
-2	0	6	1823.66	2038.99	323.87 o
0	0	6	2748.95	3096.91	123.71 o
-7	1	6	2156.33	2227.87	147.61 o
-3	1	6	2228.76	2086.74	129.78 o
-1	1	6	13.11	33.32	16.30 o
1	1	6	494.24	505.09	32.64 o
-8	2	6	227.46	184.73	16.78 o
-4	2	6	1.00	5.80	15.82 o
-2	2	6	131.58	162.14	31.51 o
2	2	6	408.54	463.27	109.41 o
-7	3	6	285.52	274.75	35.89 o
-5	3	6	261.24	282.69	17.88 o

-1	3	6	476.16	536.65	30.57 o
1	3	6	266.12	303.95	25.64 o
3	3	6	0.07	4.44	17.94 o
-6	4	6	921.67	957.83	66.55 o
0	4	6	2207.28	2269.18	113.12 o
2	4	6	280.67	300.49	32.92 o
-7	5	6	2758.79	2862.62	131.08 o
1	5	6	1426.90	1636.12	177.79 o
3	5	6	3839.74	4174.07	181.30 o
-7	1	7	375.67	386.51	48.83 o
-5	1	7	224.92	255.60	30.82 o
-3	1	7	285.45	337.36	23.87 o
-6	2	7	947.99	896.90	80.92 o
-4	2	7	683.15	792.86	54.89 o
-2	2	7	1954.60	2087.24	404.11 o
0	2	7	303.10	350.82	19.66 o
-5	3	7	4815.63	5299.26	491.35 o
-3	3	7	125.03	112.88	30.71 o
-1	3	7	2914.17	3246.33	343.25 o