

```
#
# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag
#
data_camp5
_shelx_title ' CaMnSi2O6 data collection in DAC by Xcaliber-I at VT'
_shelx_refl_list_code      4
_shelx_F_calc_maximum     201.52
_exptl_crystal_F_000      484.00
_reflns_d_resolution_high  0.7123
```

```
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  9.7895
_cell_length_b  8.9603
_cell_length_c  5.1886
_cell_angle_alpha 90.000
_cell_angle_beta  104.145
_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   1215.97   1188.68   32.09 o
  3  1  0  12611.07  12216.72  584.42 o
  5  1  0   1232.10   1141.18   221.82 o
  2  2  0   2595.29   2794.51   131.27 o
  4  2  0    28.09    74.23   10.30 o
  6  2  0    40.11    36.08    9.99 o
  1  3  0   110.34   108.91   24.68 o
  3  3  0   3559.06   3808.55   89.06 o
  5  3  0   1715.13   1722.69   63.59 o
  7  3  0    61.54    50.75    7.85 o
  2  4  0    90.00   125.09   14.54 o
  4  4  0   6975.63   6872.71   154.53 o
  6  4  0    34.59    56.64   12.91 o
  3  5  0   9725.18  10191.33  1167.04 o
  5  5  0    273.18   267.61   28.74 o
```

7	5	0	20168.88	19184.32	1099.89 o
9	5	0	1022.83	1012.50	92.71 o
4	6	0	908.59	929.27	100.57 o
6	6	0	291.96	289.88	16.69 o
8	6	0	836.11	869.56	63.48 o
10	6	0	1806.12	1818.77	208.08 o
5	7	0	818.63	758.37	71.45 o
7	7	0	1189.56	1189.23	132.98 o
9	7	0	172.05	123.94	30.28 o
11	7	0	29.86	42.58	13.36 o
6	8	0	252.82	282.66	36.88 o
10	8	0	863.14	906.14	166.06 o
7	9	0	956.86	938.10	81.58 o
-5	1	1	1021.38	932.33	165.38 o
-3	1	1	4087.29	4165.38	94.88 o
-1	1	1	152.90	112.17	6.00 o
1	1	1	40.27	28.58	3.89 o
3	1	1	2906.02	2441.97	561.81 o
-6	2	1	5560.76	5079.28	312.05 o
-4	2	1	10626.48	10841.56	526.19 o
-2	2	1	34365.77	34153.63	1284.50 o
0	2	1	14.98	26.21	2.76 o
2	2	1	25263.11	24839.92	431.86 o
4	2	1	4508.74	4334.06	320.90 o
6	2	1	8972.09	8059.37	773.97 o
-9	3	1	9311.94	8498.16	814.73 o
-7	3	1	553.14	547.24	38.53 o
-5	3	1	17614.90	17100.30	533.33 o
-3	3	1	16361.22	17754.21	322.79 o
3	3	1	4735.73	4637.72	241.42 o
5	3	1	33821.16	33729.57	979.79 o
-10	4	1	479.18	436.20	31.77 o
-6	4	1	37.69	23.64	10.87 o
-4	4	1	16.71	9.20	7.88 o
-2	4	1	1004.92	994.58	175.48 o
2	4	1	2490.34	2520.16	224.90 o
4	4	1	660.61	673.13	38.12 o
6	4	1	161.24	214.84	18.29 o
-9	5	1	384.91	380.88	16.77 o
-7	5	1	365.72	370.24	44.46 o
-5	5	1	239.87	220.30	9.98 o
-3	5	1	33.40	60.40	13.62 o
3	5	1	35.77	28.75	10.87 o
5	5	1	758.47	690.31	45.33 o
7	5	1	90.86	79.77	17.65 o
9	5	1	208.92	215.04	13.51 o
-10	6	1	374.42	291.93	60.76 o
-6	6	1	544.12	541.28	33.81 o
-4	6	1	791.27	865.27	268.57 o
4	6	1	158.59	151.84	12.57 o
8	6	1	394.54	374.42	26.46 o
10	6	1	417.91	338.50	20.53 o
-11	7	1	1059.47	1107.57	360.57 o
-9	7	1	2131.80	2160.48	124.59 o

-7	7	1	174.81	185.34	12.29 o
-5	7	1	13202.78	14412.36	2487.01 o
5	7	1	5218.79	4966.90	1073.72 o
7	7	1	678.43	736.96	59.87 o
9	7	1	4440.04	4294.88	160.40 o
-10	8	1	296.13	270.80	39.28 o
-8	8	1	2971.84	2908.53	289.47 o
-6	8	1	930.40	1126.62	253.65 o
6	8	1	4641.13	5048.13	442.60 o
8	8	1	673.05	675.69	39.29 o
-9	9	1	204.33	245.74	28.68 o
7	9	1	822.39	868.23	155.46 o
-4	0	2	24322.96	23708.41	730.79 o
-2	0	2	17.35	36.22	3.49 o
0	0	2	40609.66	41077.85	2549.88 o
2	0	2	17862.24	17843.65	347.12 o
-5	1	2	217.01	201.03	9.50 o
-3	1	2	629.97	425.94	40.26 o
-1	1	2	1198.60	1316.72	85.44 o
1	1	2	7568.31	8065.65	681.66 o
3	1	2	2027.56	1793.99	113.39 o
-8	2	2	418.24	421.49	35.26 o
-6	2	2	1722.59	1619.57	102.06 o
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-2	2	2	46.11	40.21	4.32 o
0	2	2	1363.70	1852.84	177.65 o
2	2	2	1280.48	1275.18	54.92 o
4	2	2	1716.49	1589.36	164.95 o
6	2	2	797.58	730.34	88.68 o
-9	3	2	296.85	257.50	35.06 o
-7	3	2	717.57	705.41	54.73 o
-5	3	2	972.19	995.08	59.43 o
-3	3	2	8.24	68.53	24.53 o
-1	3	2	3700.63	3799.14	83.21 o
1	3	2	1518.72	1727.99	122.23 o
5	3	2	1204.10	1073.32	60.66 o
7	3	2	588.87	554.52	29.20 o
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-8	4	2	393.84	383.16	42.96 o
-6	4	2	1083.58	1038.36	52.43 o
-4	4	2	553.15	538.16	36.20 o
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2	4	2	520.71	533.17	37.66 o
4	4	2	2826.02	2597.04	93.77 o
6	4	2	405.42	362.40	29.36 o
-11	5	2	3046.71	2622.48	122.95 o
-9	5	2	998.37	955.23	70.55 o
-7	5	2	14672.25	14413.02	332.18 o
-5	5	2	1653.29	1618.92	211.57 o
-3	5	2	15920.42	17434.18	3335.59 o
1	5	2	11433.14	11957.93	991.76 o
3	5	2	18006.14	18095.40	1182.36 o
5	5	2	183.24	187.85	12.85 o
7	5	2	7241.14	6748.24	176.63 o

9	5	2	1265.77	1207.47	81.32 o
-12	6	2	166.20	195.58	19.28 o
-10	6	2	410.01	455.24	30.11 o
-8	6	2	112.67	117.87	22.01 o
-6	6	2	4211.37	4561.93	142.59 o
-4	6	2	664.33	850.56	139.71 o
4	6	2	1192.76	1064.53	114.85 o
6	6	2	18.18	37.76	9.37 o
8	6	2	704.81	655.94	40.16 o
-9	7	2	109.77	92.68	23.52 o
-7	7	2	610.23	671.04	42.39 o
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3	7	2	764.53	743.48	119.67 o
5	7	2	535.43	497.80	27.60 o
7	7	2	180.49	209.47	14.55 o
9	7	2	78.11	67.87	14.71 o
-10	8	2	687.70	734.50	177.59 o
-8	8	2	624.55	593.38	117.56 o
4	8	2	1050.79	1057.11	78.92 o
6	8	2	989.06	958.54	102.05 o
8	8	2	143.71	124.79	24.98 o
7	9	2	614.89	751.50	118.91 o
-7	1	3	1342.24	1194.59	122.02 o
-5	1	3	1684.14	1572.02	68.51 o
-3	1	3	2086.33	2146.89	106.05 o
-1	1	3	7.52	16.92	5.08 o
1	1	3	49.52	36.54	8.92 o
3	1	3	352.99	433.31	17.88 o
-8	2	3	7987.39	7749.68	209.56 o
-6	2	3	1089.92	993.96	78.95 o
-4	2	3	2837.26	2763.40	182.45 o
-2	2	3	25676.49	26828.08	1114.69 o
0	2	3	921.32	919.09	80.89 o
2	2	3	9296.25	9588.23	366.49 o
4	2	3	608.53	671.22	41.21 o
-9	3	3	9049.30	8823.50	227.87 o
-5	3	3	9090.85	9275.43	192.26 o
-3	3	3	2230.18	2393.03	186.90 o
-1	3	3	20335.23	20212.93	585.90 o
1	3	3	2498.90	2655.00	96.42 o
3	3	3	261.73	296.97	12.65 o
5	3	3	11332.79	11358.76	940.95 o
-10	4	3	221.26	182.54	23.19 o
-8	4	3	694.38	710.66	34.04 o
-6	4	3	667.82	636.40	67.14 o
-4	4	3	304.82	289.33	80.16 o
0	4	3	1415.74	1525.39	82.63 o
2	4	3	244.81	221.91	32.78 o
4	4	3	555.30	516.49	33.24 o
6	4	3	573.04	497.73	37.70 o
-11	5	3	222.15	217.82	16.46 o
-5	5	3	2581.06	2570.67	317.04 o
1	5	3	1568.99	1673.39	88.18 o
3	5	3	247.94	241.61	23.18 o

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-10	6	3	406.03	371.61	35.48 o
-8	6	3	150.26	112.69	20.42 o
-6	6	3	81.81	40.68	24.21 o
2	6	3	137.21	187.93	15.06 o
4	6	3	1266.84	1171.48	78.40 o
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-9	7	3	3978.89	4236.34	194.79 o
-7	7	3	120.85	105.17	21.33 o
3	7	3	860.43	1012.99	64.07 o
5	7	3	5009.51	4920.27	542.12 o
7	7	3	166.47	186.07	67.27 o
-10	8	3	250.05	246.28	21.02 o
-8	8	3	2589.14	2854.74	530.14 o
6	8	3	3289.92	3297.30	239.61 o
-6	0	4	15084.43	14389.43	334.09 o
-4	0	4	10888.92	10890.06	249.24 o
-2	0	4	391.39	403.70	21.02 o
0	0	4	16316.90	17394.42	1292.04 o
2	0	4	1960.22	1912.02	132.83 o
-7	1	4	1901.56	1898.98	84.76 o
-5	1	4	49.08	70.24	10.25 o
-3	1	4	7539.13	7249.31	217.59 o
-1	1	4	1144.32	1013.16	66.24 o
1	1	4	767.01	752.85	82.88 o
3	1	4	4639.30	4489.57	132.68 o
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0	2	4	1138.63	1000.40	164.68 o
2	2	4	2417.14	2430.41	350.98 o
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-3	3	4	653.59	583.50	47.91 o
-1	3	4	197.17	285.60	56.98 o
1	3	4	188.96	196.77	10.54 o
3	3	4	734.51	743.77	48.39 o
5	3	4	262.54	351.25	26.94 o
-10	4	4	1808.33	1834.69	145.65 o
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0	4	4	1581.83	1480.27	80.61 o
2	4	4	103.55	141.87	10.80 o
4	4	4	2980.95	2994.96	327.73 o
-11	5	4	1757.66	1361.96	135.19 o
-9	5	4	351.06	327.54	38.43 o
-7	5	4	11038.88	11990.22	887.93 o
-5	5	4	1209.85	1211.25	71.35 o
1	5	4	5729.35	6002.25	154.78 o
3	5	4	6093.80	6459.72	630.62 o
5	5	4	1048.96	1038.18	90.46 o
7	5	4	5118.39	5320.39	183.20 o
-10	6	4	1526.03	1548.96	112.87 o
-8	6	4	653.76	722.93	53.96 o
-6	6	4	1757.22	1966.97	273.15 o

4	6	4	3992.11	4220.83	303.60 o
6	6	4	400.57	419.48	26.03 o
-9	7	4	200.29	167.75	15.03 o
-7	7	4	674.56	762.06	273.27 o
5	7	4	69.87	140.58	24.21 o
4	8	4	429.44	499.11	56.95 o
-7	1	5	945.52	915.01	55.15 o
-5	1	5	414.70	454.11	28.42 o
-3	1	5	625.61	655.39	39.07 o
1	1	5	142.55	179.53	15.41 o
-8	2	5	6414.86	6409.31	189.59 o
-6	2	5	1304.37	1161.06	115.29 o
-4	2	5	1198.45	1091.68	105.67 o
-2	2	5	5621.01	5943.14	251.51 o
0	2	5	1095.97	1264.44	180.92 o
2	2	5	7733.52	8159.33	611.21 o
-9	3	5	6101.58	6039.28	229.82 o
-7	3	5	823.55	784.22	62.00 o
-5	3	5	3880.18	4127.89	297.73 o
-1	3	5	11824.53	12145.33	628.66 o
1	3	5	1845.81	1990.33	179.86 o
3	3	5	269.03	319.30	20.10 o
-10	4	5	501.51	507.14	80.55 o
-8	4	5	399.19	417.83	34.84 o
-4	4	5	107.10	102.40	21.57 o
-2	4	5	91.15	68.62	11.76 o
0	4	5	199.94	215.54	23.76 o
2	4	5	1048.69	936.14	76.76 o
4	4	5	1298.57	1399.25	84.33 o
-9	5	5	256.69	235.65	67.32 o
-5	5	5	294.54	344.15	20.17 o
-1	5	5	128.96	96.20	17.93 o
3	5	5	307.68	317.47	44.98 o
5	5	5	281.34	287.25	20.45 o
-6	6	5	588.99	684.40	125.54 o
0	6	5	522.93	604.49	71.08 o
4	6	5	233.12	221.54	29.41 o
3	7	5	1046.75	1110.00	85.74 o
-6	0	6	3170.79	3243.83	266.55 o
-4	0	6	8502.68	8936.02	984.27 o
-2	0	6	1916.47	2079.43	157.23 o
0	0	6	2734.65	3166.77	233.11 o
-7	1	6	1764.14	1786.76	194.89 o
-5	1	6	189.06	206.77	29.91 o
-3	1	6	2533.37	2601.98	219.98 o
1	1	6	409.79	419.72	37.35 o
-8	2	6	402.52	430.99	22.52 o
-2	2	6	249.77	290.67	33.81 o
2	2	6	209.70	272.39	28.32 o
-9	3	6	221.71	199.92	22.45 o
-7	3	6	389.89	417.24	23.98 o
-5	3	6	215.75	231.77	17.13 o
-1	3	6	853.24	1031.09	74.64 o
1	3	6	207.71	221.15	58.80 o

-6	4	6	972.82	1033.84	69.65 o
0	4	6	2035.36	2146.45	123.61 o
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-7	5	6	2673.80	2640.96	317.05 o
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1	5	6	2131.06	1986.33	133.67 o
-5	1	7	129.95	156.42	20.26 o
-3	1	7	365.39	390.88	65.78 o
-6	2	7	671.24	654.63	99.39 o
-4	2	7	1125.71	1227.68	92.09 o
-2	2	7	1742.92	2095.86	185.43 o
-5	3	7	4716.19	5224.49	624.96 o
-3	3	7	217.38	233.48	29.82 o