

```
#
# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag
#
data_camp2
_shelx_title ' CaMnSi2O6 data collection in DAC by Xcaliber-I at VT'
_shelx_refl_list_code 4
_shelx_F_calc_maximum 203.74
_exptl_crystal_F_000 484.00
_reflns_d_resolution_high 0.7103
```

```
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 9.8753
_cell_length_b 9.0814
_cell_length_c 5.2436
_cell_angle_alpha 90.000
_cell_angle_beta 104.725
_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 1253.57 1226.97 53.42 o
3 1 0 13062.82 12708.70 252.77 o
5 1 0 1314.13 1262.10 102.29 o
2 2 0 3183.31 3275.85 80.30 o
4 2 0 47.92 74.52 22.34 o
3 3 0 3211.25 3491.53 73.74 o
5 3 0 1255.14 1180.83 46.99 o
7 3 0 75.20 74.66 15.58 o
2 4 0 94.67 112.42 20.49 o
4 4 0 6979.64 6931.03 297.24 o
6 4 0 46.52 49.13 12.61 o
3 5 0 9210.88 9356.59 1417.11 o
5 5 0 300.71 285.19 13.66 o
7 5 0 21061.98 20804.81 457.26 o
9 5 0 1042.83 1005.81 99.07 o
```

4	6	0	1150.11	1201.41	309.96 o
6	6	0	271.49	305.59	58.85 o
8	6	0	1038.68	952.01	69.56 o
10	6	0	2228.96	2123.91	109.80 o
5	7	0	1177.55	984.01	129.32 o
7	7	0	1116.59	1140.31	137.57 o
9	7	0	323.00	310.79	16.26 o
10	8	0	770.32	667.62	123.07 o
-5	1	1	944.35	845.42	39.67 o
-3	1	1	4108.08	4195.31	135.63 o
-1	1	1	161.82	115.58	10.83 o
1	1	1	69.16	53.80	2.89 o
3	1	1	2802.71	3112.70	263.79 o
5	1	1	400.63	315.13	31.42 o
-6	2	1	5418.99	4855.85	125.54 o
-4	2	1	10726.81	10495.31	431.07 o
-2	2	1	35129.94	33587.37	589.85 o
0	2	1	39.55	52.63	3.01 o
2	2	1	24399.64	24575.73	1395.83 o
4	2	1	4781.69	4871.86	152.49 o
6	2	1	8931.97	7346.87	1698.24 o
-9	3	1	9129.94	8386.22	227.66 o
-7	3	1	518.78	516.64	35.21 o
-5	3	1	19282.63	17501.17	676.38 o
-3	3	1	16753.81	17566.58	611.34 o
1	3	1	396.83	241.00	45.79 o
3	3	1	4885.84	5136.00	277.13 o
5	3	1	34597.01	33864.29	593.84 o
-10	4	1	480.21	474.84	37.88 o
-2	4	1	1143.41	1232.37	236.22 o
2	4	1	2401.24	2269.36	361.74 o
4	4	1	689.19	718.78	42.83 o
6	4	1	176.67	144.92	8.90 o
-11	5	1	101.55	122.44	26.18 o
-9	5	1	282.50	270.90	16.69 o
-7	5	1	186.31	166.79	21.37 o
-5	5	1	145.64	142.64	9.07 o
-3	5	1	191.77	260.03	39.58 o
3	5	1	155.35	186.20	25.34 o
5	5	1	553.23	516.60	28.21 o
9	5	1	164.37	156.56	25.38 o
-10	6	1	371.34	301.59	19.11 o
-6	6	1	354.52	316.13	47.01 o
-4	6	1	803.26	866.46	156.56 o
4	6	1	164.89	177.89	10.05 o
8	6	1	284.37	263.35	16.36 o
10	6	1	335.17	265.10	16.97 o
-11	7	1	1018.00	949.91	237.13 o
-9	7	1	2230.83	2105.81	101.38 o
-7	7	1	158.73	175.51	25.38 o
-5	7	1	12500.14	12800.15	2373.84 o
5	7	1	5116.03	5277.50	710.99 o
7	7	1	649.97	666.98	54.91 o
9	7	1	4228.07	4046.63	196.72 o

-10	8	1	391.01	320.93	25.49 o
-8	8	1	3141.01	2668.80	633.50 o
-6	8	1	1203.22	1177.25	186.65 o
6	8	1	5119.46	5823.23	1183.34 o
8	8	1	781.52	743.88	114.23 o
-9	9	1	217.99	284.71	43.74 o
7	9	1	858.79	618.70	103.83 o
-4	0	2	23366.70	21900.98	428.05 o
-2	0	2	16.80	23.87	3.40 o
0	0	2	41508.29	42967.07	583.12 o
2	0	2	17303.46	19157.48	1148.53 o
-5	1	2	120.17	128.33	15.09 o
-3	1	2	520.95	343.80	34.22 o
-1	1	2	1168.45	1272.01	42.08 o
1	1	2	8026.11	8598.42	142.66 o
3	1	2	2186.16	2097.58	63.86 o
-8	2	2	434.76	390.04	34.94 o
-6	2	2	2127.67	2024.74	118.73 o
-4	2	2	758.11	750.93	42.56 o
-2	2	2	50.66	44.69	4.14 o
0	2	2	1591.05	1805.18	246.93 o
2	2	2	1579.05	1609.80	93.49 o
4	2	2	1689.61	1545.72	74.04 o
6	2	2	844.62	860.43	59.26 o
-9	3	2	139.06	128.53	23.00 o
-7	3	2	709.19	655.10	53.83 o
-5	3	2	969.79	994.51	44.92 o
-3	3	2	84.94	179.36	50.56 o
1	3	2	1659.92	1803.86	79.99 o
5	3	2	856.14	853.69	53.16 o
7	3	2	558.23	556.42	75.83 o
-10	4	2	1100.17	1029.65	87.47 o
-8	4	2	310.62	305.83	55.15 o
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0	4	2	8733.94	9312.82	1345.85 o
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4	4	2	2440.37	2347.17	79.10 o
6	4	2	455.98	394.10	38.01 o
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-7	5	2	15212.31	14670.93	730.50 o
-5	5	2	1673.28	1677.92	80.91 o
-3	5	2	16175.23	16488.88	2373.72 o
1	5	2	11490.99	12089.05	1002.00 o
3	5	2	18881.17	19447.43	1733.69 o
5	5	2	168.38	229.35	47.79 o
7	5	2	7138.38	6867.65	177.31 o
9	5	2	1433.17	1405.37	265.03 o
-12	6	2	151.55	158.01	33.29 o
-10	6	2	427.81	499.07	52.50 o
-8	6	2	219.92	225.34	14.35 o
-6	6	2	4781.10	5075.97	307.58 o
-4	6	2	715.88	885.16	196.67 o

2	6	2	142.05	165.69	11.57 o
4	6	2	1229.54	1253.50	123.82 o
8	6	2	788.75	774.50	82.83 o
10	6	2	1518.68	1323.19	150.40 o
-11	7	2	11.88	15.71	25.68 o
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9	7	2	138.67	108.82	53.00 o
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8	8	2	80.57	65.16	25.47 o
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-7	1	3	1235.04	1081.76	194.03 o
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1	1	3	68.63	53.87	9.24 o
3	1	3	356.12	383.80	28.57 o
-8	2	3	7737.40	6808.95	510.30 o
-6	2	3	1214.30	1116.68	99.16 o
-4	2	3	2646.38	2686.28	81.29 o
-2	2	3	26169.96	27741.00	1031.35 o
0	2	3	919.62	947.95	129.59 o
2	2	3	8960.08	9596.40	205.87 o
4	2	3	620.02	664.99	39.68 o
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-9	3	3	9835.35	9185.58	264.29 o
-5	3	3	9534.80	9634.81	201.39 o
-3	3	3	3011.96	2990.41	88.37 o
-1	3	3	20187.14	21179.45	702.88 o
1	3	3	2540.00	2725.55	260.82 o
3	3	3	287.84	326.13	55.71 o
5	3	3	12036.89	12526.85	267.39 o
7	3	3	749.94	688.99	96.83 o
-10	4	3	277.14	240.32	14.47 o
-8	4	3	654.82	714.96	67.64 o
-6	4	3	520.15	469.72	22.61 o
-4	4	3	410.63	436.13	47.92 o
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2	4	3	280.99	279.69	23.12 o
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6	4	3	568.66	475.55	69.40 o
-11	5	3	123.54	140.46	27.38 o
-7	5	3	5.99	42.48	17.99 o
-5	5	3	2138.67	2110.24	146.29 o
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3	5	3	116.20	128.52	20.44 o
5	5	3	23.06	15.44	20.81 o
-10	6	3	288.65	218.35	33.31 o
2	6	3	170.91	200.28	23.55 o
4	6	3	995.08	990.45	162.27 o

-11	7	3	783.68	729.61	48.50 o
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-7	7	3	188.14	171.89	26.60 o
3	7	3	707.42	692.73	152.53 o
5	7	3	4904.23	4780.99	701.49 o
7	7	3	186.58	192.87	45.39 o
-10	8	3	492.10	416.13	42.55 o
-8	8	3	2765.59	2647.20	368.80 o
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-4	0	4	11515.36	11734.85	261.93 o
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1	1	4	559.33	493.48	31.76 o
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0	2	4	1136.78	1030.99	78.44 o
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5	3	4	231.10	277.71	19.89 o
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-6	4	4	289.98	303.58	14.21 o
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0	4	4	1364.09	1292.64	78.11 o
2	4	4	121.36	160.34	11.83 o
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-9	5	4	215.15	158.97	24.87 o
-7	5	4	11825.88	12062.03	1094.64 o
-5	5	4	1567.16	1552.69	78.39 o
1	5	4	6094.08	5810.23	582.11 o
3	5	4	6491.04	7140.24	197.35 o
5	5	4	908.03	1044.65	65.65 o
7	5	4	5218.32	5347.01	550.87 o
-10	6	4	1640.70	1582.75	101.08 o
-8	6	4	453.23	456.59	32.94 o
-6	6	4	1826.11	2054.52	101.42 o
4	6	4	4452.74	4461.98	146.21 o
6	6	4	338.59	347.12	21.11 o
-9	7	4	385.06	327.57	71.14 o
-7	7	4	712.54	754.68	66.10 o
5	7	4	151.14	182.96	63.01 o
-7	1	5	854.65	840.99	50.51 o
-5	1	5	481.09	529.17	32.19 o
-3	1	5	655.93	750.90	84.19 o

1	1	5	79.06	93.52	36.58 o
3	1	5	16.58	40.11	19.62 o
-8	2	5	6301.37	6186.60	184.33 o
-6	2	5	1309.55	1515.83	76.90 o
-4	2	5	1076.19	1046.27	64.89 o
-2	2	5	6135.00	6953.93	494.67 o
0	2	5	995.90	1162.74	128.95 o
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-9	3	5	6865.94	6644.11	733.49 o
-7	3	5	816.41	818.35	88.76 o
-5	3	5	3914.06	4079.93	256.60 o
-1	3	5	12303.08	13869.92	306.63 o
1	3	5	2130.72	2323.82	178.44 o
3	3	5	186.99	240.89	14.35 o
5	3	5	3736.02	3964.66	215.13 o
-10	4	5	405.37	407.55	31.31 o
-8	4	5	366.37	438.09	26.49 o
-6	4	5	50.30	63.37	23.77 o
-4	4	5	101.88	103.46	20.06 o
-2	4	5	154.83	157.99	24.79 o
0	4	5	304.75	341.49	16.87 o
2	4	5	1142.53	957.80	68.75 o
4	4	5	1208.49	1292.57	90.77 o
-9	5	5	146.30	153.33	30.70 o
-5	5	5	234.86	267.92	17.24 o
1	5	5	7.52	15.00	22.04 o
3	5	5	133.08	148.66	17.58 o
5	5	5	202.16	208.56	29.30 o
-10	6	5	187.85	147.58	17.24 o
-8	6	5	59.85	71.95	29.15 o
-6	6	5	400.84	407.52	105.93 o
2	6	5	16.59	54.28	22.83 o
4	6	5	185.30	160.08	29.94 o
-9	7	5	1579.85	1538.40	381.82 o
3	7	5	1019.79	1194.99	177.78 o
-6	0	6	2856.71	2832.21	227.05 o
-4	0	6	9164.94	9772.82	234.20 o
-2	0	6	1912.91	2074.65	103.97 o
0	0	6	2666.24	3153.85	132.58 o
-7	1	6	2014.45	2149.80	114.93 o
-5	1	6	93.20	141.25	17.96 o
-3	1	6	2350.45	2317.41	117.28 o
1	1	6	489.18	482.39	52.44 o
-8	2	6	304.69	294.92	24.63 o
-2	2	6	166.80	212.43	21.91 o
2	2	6	326.95	435.33	50.65 o
-7	3	6	337.35	330.62	78.33 o
-5	3	6	241.38	268.94	16.09 o
-1	3	6	629.31	711.84	89.28 o
1	3	6	240.67	282.23	18.71 o
-6	4	6	991.43	1123.22	85.75 o
0	4	6	2157.40	2192.91	120.26 o
2	4	6	305.32	337.08	45.53 o
-7	5	6	2718.22	2848.53	362.40 o

1	5	6	1767.92	1982.66	124.19 o
-7	1	7	357.27	274.31	40.77 o
-5	1	7	186.93	210.52	31.50 o
-3	1	7	325.42	374.89	36.09 o
-6	2	7	810.53	830.04	145.09 o
-4	2	7	868.82	892.31	97.93 o
-2	2	7	1869.62	1940.72	145.12 o
0	2	7	350.43	382.54	25.45 o
-5	3	7	4783.28	5121.01	476.55 o
-1	3	7	3063.35	3096.61	153.04 o