

```
#
# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag
#
data_camp3
_shelx_title ' CaMnSi2O6 data collection in DAC by Xcaliber-I at VT'
_shelx_refl_list_code 4
_shelx_F_calc_maximum 202.79
_exptl_crystal_F_000 484.00
_reflns_d_resolution_high 0.7127
```

```
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 9.8337
_cell_length_b 9.0263
_cell_length_c 5.2169
_cell_angle_alpha 90.000
_cell_angle_beta 104.429
_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 1215.72 1227.64 54.10 o
3 1 0 12966.72 12800.96 407.90 o
5 1 0 1304.58 1248.44 49.47 o
2 2 0 2919.36 3171.61 72.02 o
3 3 0 3359.56 3740.79 144.11 o
5 3 0 1456.71 1415.89 51.68 o
7 3 0 64.37 84.57 15.32 o
9 3 0 821.09 706.84 52.88 o
2 4 0 99.96 131.98 18.58 o
4 4 0 6825.52 7262.58 385.60 o
6 4 0 39.49 39.66 15.19 o
10 4 0 3389.96 3316.23 287.96 o
3 5 0 9392.95 9606.84 1324.07 o
5 5 0 284.19 248.22 13.68 o
7 5 0 20709.29 19419.87 2327.21 o
```

9	5	0	1080.55	1096.42	158.35 o
11	5	0	2833.59	2907.93	135.69 o
4	6	0	998.24	1060.45	177.14 o
6	6	0	295.48	332.05	34.76 o
8	6	0	938.45	953.59	154.16 o
10	6	0	2013.79	2144.95	268.34 o
5	7	0	972.07	1113.99	279.43 o
7	7	0	1077.22	1159.49	90.35 o
9	7	0	247.78	247.68	51.27 o
6	8	0	173.09	161.99	30.44 o
8	8	0	89.60	74.66	34.25 o
10	8	0	804.10	951.92	206.13 o
-5	1	1	977.70	956.80	46.52 o
-3	1	1	4071.56	4309.34	170.61 o
-1	1	1	163.13	114.05	9.95 o
1	1	1	48.97	37.42	2.20 o
3	1	1	2872.38	3003.40	266.44 o
5	1	1	428.69	356.68	50.16 o
-8	2	1	3584.62	3293.83	195.12 o
-6	2	1	5415.96	4880.13	108.15 o
-4	2	1	10892.45	11087.88	310.50 o
-2	2	1	34759.11	33784.51	638.08 o
0	2	1	29.39	35.35	2.91 o
2	2	1	24769.96	24882.17	431.27 o
4	2	1	4726.82	4924.19	142.20 o
6	2	1	8935.94	8312.84	269.84 o
-9	3	1	9169.53	7794.06	696.81 o
-7	3	1	523.63	485.10	32.02 o
-5	3	1	18391.24	18080.48	346.14 o
-3	3	1	16587.89	18013.71	484.75 o
1	3	1	304.28	163.21	10.40 o
3	3	1	4814.66	5124.32	133.46 o
5	3	1	34420.00	34354.02	618.12 o
7	3	1	29.52	56.44	16.40 o
-10	4	1	493.37	519.48	81.24 o
2	4	1	2511.53	2260.94	358.12 o
4	4	1	732.99	702.10	39.78 o
6	4	1	158.05	199.76	25.17 o
8	4	1	125.16	160.43	23.29 o
-9	5	1	335.16	291.74	19.40 o
-7	5	1	286.08	296.09	14.32 o
-5	5	1	171.68	192.32	10.22 o
-3	5	1	115.30	126.05	26.68 o
3	5	1	92.17	98.09	15.36 o
5	5	1	640.58	565.01	35.41 o
9	5	1	189.66	193.88	13.04 o
-10	6	1	384.45	323.04	51.16 o
-6	6	1	441.33	382.24	39.13 o
-4	6	1	790.28	864.37	141.16 o
4	6	1	146.67	166.86	23.75 o
8	6	1	343.45	354.01	57.45 o
10	6	1	380.16	326.21	34.26 o
-11	7	1	1112.39	1061.58	206.49 o
-9	7	1	2124.21	1891.74	98.17 o

-7	7	1	162.09	177.57	30.79 o
-5	7	1	12974.24	14051.36	2938.59 o
5	7	1	5201.92	5471.07	397.69 o
7	7	1	709.40	781.96	135.62 o
9	7	1	4257.76	4171.98	214.72 o
-10	8	1	359.81	317.94	45.59 o
-8	8	1	3084.94	3141.94	399.57 o
6	8	1	4884.56	5345.64	853.53 o
8	8	1	699.44	763.26	184.45 o
-9	9	1	196.93	308.64	33.85 o
-4	0	2	23752.91	20525.41	5770.27 o
0	0	2	41124.53	43300.30	1992.10 o
2	0	2	17795.76	18489.83	1861.16 o
-7	1	2	13679.55	12861.40	279.01 o
-5	1	2	165.80	164.38	15.90 o
-3	1	2	580.88	404.63	27.64 o
-1	1	2	1210.07	1288.55	56.03 o
1	1	2	7669.73	7600.07	564.20 o
3	1	2	2111.97	1878.71	70.95 o
-8	2	2	433.97	377.06	38.93 o
-6	2	2	1956.43	2016.19	68.28 o
-4	2	2	780.71	905.33	56.35 o
-2	2	2	48.08	35.63	7.89 o
0	2	2	1503.03	1924.03	53.48 o
2	2	2	1418.97	1392.18	65.79 o
4	2	2	1684.35	1490.87	112.94 o
6	2	2	827.88	849.68	100.76 o
-9	3	2	196.05	190.89	12.12 o
-7	3	2	710.52	692.98	108.66 o
-5	3	2	969.87	1009.86	45.93 o
-3	3	2	35.35	125.80	81.40 o
-1	3	2	3331.93	3555.82	177.05 o
1	3	2	1556.63	1741.78	71.20 o
3	3	2	79.38	57.93	11.89 o
5	3	2	1039.87	948.52	96.77 o
7	3	2	582.35	635.68	34.04 o
-10	4	2	1137.89	1142.36	75.13 o
-8	4	2	354.54	317.66	20.57 o
-6	4	2	1154.76	1085.39	67.17 o
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2	4	2	466.28	474.32	34.26 o
4	4	2	2638.59	2459.81	113.82 o
6	4	2	434.11	425.79	17.61 o
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-5	5	2	1719.17	1587.24	344.81 o
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3	5	2	18545.15	18904.26	1046.44 o
7	5	2	7195.56	6969.60	161.21 o
9	5	2	1436.90	1434.07	257.25 o
-12	6	2	153.77	190.05	26.55 o
-10	6	2	415.30	503.59	30.05 o

-8	6	2	158.71	164.74	11.99 o
-6	6	2	4515.87	5171.01	851.18 o
2	6	2	113.13	1267.44	329.30 o
4	6	2	1210.85	1231.52	177.89 o
8	6	2	724.72	600.23	47.45 o
10	6	2	1445.42	1502.54	97.96 o
-9	7	2	124.89	112.58	26.21 o
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7	7	2	136.15	164.70	22.04 o
9	7	2	115.98	100.53	14.89 o
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-8	8	2	469.44	489.08	59.51 o
6	8	2	884.89	860.04	84.35 o
7	9	2	556.12	630.42	43.94 o
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-1	1	3	7.03	20.86	9.85 o
1	1	3	64.34	36.47	11.10 o
3	1	3	370.27	459.44	25.85 o
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-6	2	3	1103.26	943.86	56.41 o
-4	2	3	2742.03	2751.54	175.85 o
-2	2	3	26182.15	26885.34	622.18 o
0	2	3	926.11	948.57	95.33 o
2	2	3	8983.62	9436.89	607.93 o
4	2	3	642.13	568.47	43.33 o
-9	3	3	9398.34	8988.10	256.31 o
-5	3	3	9336.47	9861.25	900.83 o
-3	3	3	2626.55	2819.70	250.15 o
-1	3	3	20222.06	21049.47	1332.43 o
1	3	3	2560.07	2610.01	74.21 o
3	3	3	264.26	316.91	12.98 o
5	3	3	11716.86	11813.90	653.92 o
7	3	3	769.85	763.39	61.00 o
-10	4	3	258.47	238.40	14.00 o
-8	4	3	681.76	806.55	98.02 o
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-4	4	3	355.46	364.74	57.40 o
0	4	3	1438.96	1556.32	61.67 o
2	4	3	269.25	239.80	34.41 o
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6	4	3	536.66	448.79	32.19 o
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-5	5	3	2423.30	2436.05	251.12 o
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3	5	3	173.15	177.56	22.97 o
9	5	3	714.36	730.14	85.47 o
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-8	6	3	177.76	89.37	27.70 o
-6	6	3	66.12	24.56	16.80 o
4	6	3	1158.69	1066.33	76.62 o
-11	7	3	895.05	773.66	66.16 o

-9	7	3	3937.50	3962.31	952.29 o
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3	7	3	770.85	905.63	86.05 o
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-8	8	3	2690.45	2865.96	518.26 o
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-6	0	4	15914.76	15276.10	393.46 o
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1	1	4	662.88	611.50	110.26 o
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2	2	4	2446.10	2565.90	85.94 o
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5	3	4	227.05	303.52	27.18 o
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0	4	4	1438.46	1467.83	70.65 o
2	4	4	98.72	122.33	59.41 o
4	4	4	2997.03	3023.78	186.25 o
6	4	4	1.79	18.43	11.41 o
-11	5	4	1841.07	1604.96	122.16 o
-9	5	4	276.17	246.88	33.67 o
-7	5	4	11396.27	11921.54	1409.41 o
-5	5	4	1453.48	1476.90	301.22 o
1	5	4	5877.89	5197.09	1112.94 o
3	5	4	6440.22	6738.25	470.84 o
5	5	4	996.26	1087.03	77.45 o
7	5	4	5078.20	5395.60	330.19 o
-10	6	4	1557.61	1438.98	102.91 o
-8	6	4	555.58	500.26	38.51 o
-6	6	4	1829.84	1812.00	301.47 o
4	6	4	4158.63	4279.09	162.90 o
6	6	4	361.98	326.33	21.02 o
-9	7	4	265.65	240.69	17.54 o
5	7	4	103.16	138.87	15.07 o
-7	1	5	887.98	957.98	62.58 o
-5	1	5	439.53	492.56	31.51 o

-3	1	5	639.31	680.87	99.18 o
1	1	5	102.43	130.90	13.44 o
3	1	5	12.74	27.95	22.17 o
-8	2	5	6401.48	6588.65	165.90 o
-6	2	5	1313.32	1405.93	81.55 o
-4	2	5	1118.52	999.49	64.83 o
-2	2	5	5866.57	6292.16	183.29 o
0	2	5	1092.58	1144.50	68.88 o
2	2	5	7617.59	8555.59	821.67 o
-9	3	5	6543.55	6667.86	208.72 o
-7	3	5	846.87	821.62	56.24 o
-5	3	5	3807.58	4142.94	446.22 o
-1	3	5	12125.68	12664.45	710.88 o
1	3	5	1993.77	2162.71	278.50 o
3	3	5	218.96	272.28	15.16 o
5	3	5	3631.58	3875.65	727.76 o
-10	4	5	449.02	443.97	113.21 o
-8	4	5	361.24	385.59	58.01 o
-2	4	5	109.36	126.28	21.45 o
0	4	5	252.21	240.04	17.57 o
2	4	5	1104.69	1103.43	71.98 o
4	4	5	1256.75	1204.26	84.14 o
6	4	5	74.34	42.31	13.36 o
-9	5	5	191.86	182.62	54.01 o
-7	5	5	32.34	39.10	24.78 o
-5	5	5	264.67	321.06	62.91 o
-1	5	5	104.53	110.21	23.52 o
3	5	5	221.92	223.98	14.66 o
5	5	5	245.38	262.17	17.35 o
-8	6	5	65.88	103.64	29.82 o
4	6	5	197.56	223.33	34.34 o
3	7	5	1006.15	1182.62	104.06 o
-6	0	6	3013.46	2960.25	136.35 o
-4	0	6	8996.29	9175.49	1158.56 o
-2	0	6	1898.82	1943.31	101.05 o
0	0	6	2647.48	3146.90	666.76 o
-7	1	6	1887.15	1989.14	130.57 o
-5	1	6	137.58	157.54	15.00 o
-3	1	6	2431.57	2497.56	194.07 o
-1	1	6	14.02	26.31	22.39 o
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-10	2	6	82.95	162.13	29.99 o
-8	2	6	355.10	348.04	49.18 o
-6	2	6	11.88	20.49	21.32 o
-2	2	6	213.38	248.19	26.65 o
2	2	6	257.68	332.02	47.87 o
-9	3	6	158.13	165.39	30.29 o
-7	3	6	374.60	377.35	54.93 o
-5	3	6	216.01	219.23	44.91 o
-1	3	6	745.90	848.20	49.11 o
1	3	6	220.69	250.64	17.55 o
-6	4	6	969.70	1066.79	181.22 o
0	4	6	2073.76	1867.61	245.81 o
2	4	6	339.89	328.34	24.36 o

-7	5	6	2620.98	2671.50	813.62 o
-1	5	6	207.69	256.68	20.29 o
1	5	6	1917.63	1932.86	183.83 o
-7	1	7	337.23	357.68	27.87 o
-5	1	7	158.19	159.11	15.45 o
-3	1	7	343.68	406.57	52.22 o
-6	2	7	757.77	764.18	69.01 o
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-2	2	7	1796.48	1936.12	279.11 o
0	2	7	351.23	393.64	21.98 o
-5	3	7	4748.63	5474.91	1239.18 o
-3	3	7	201.30	187.67	56.99 o
-1	3	7	3033.41	3228.23	270.91 o