

```
#
# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag
#
data_camp7
_shelx_title ' CaMnSi2O6 data collection in DAC by Xcaliber-I at VT'
_shelx_refl_list_code      4
_shelx_F_calc_maximum     201.24
_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  9.7631
_cell_length_b  8.9173
_cell_length_c  5.1705
_cell_angle_alpha 90.000
_cell_angle_beta  103.996
_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  1201.14  1163.69  29.93 o
  3  1  0  12459.11  11359.27  1171.96 o
  5  1  0  1168.03  1096.51  47.27 o
  2  2  0  2417.19  2450.01  58.56 o
  3  3  0  3727.17  3907.86  83.00 o
  5  3  0  1959.73  1807.32  85.94 o
  7  3  0   69.20   96.31  17.31 o
  2  4  0   79.42   85.39  11.54 o
  4  4  0  7032.66  6626.77  330.22 o
  3  5  0  9954.24  10302.14  1108.78 o
  5  5  0   257.69  247.97  31.99 o
  7  5  0 20092.00  20072.89  464.19 o
  9  5  0  1080.36  1055.57  68.11 o
  4  6  0   865.14  767.44  99.04 o
  6  6  0   282.92  304.84  15.85 o
```

8	6	0	784.88	793.85	111.23 o
10	6	0	1759.63	1863.82	144.22 o
5	7	0	723.78	645.32	180.81 o
7	7	0	1229.09	1204.69	125.83 o
9	7	0	136.90	106.08	26.64 o
6	8	0	322.26	333.86	69.72 o
8	8	0	181.41	153.46	14.29 o
10	8	0	901.77	877.47	118.22 o
-5	1	1	1032.37	949.03	83.27 o
-3	1	1	4070.34	4149.06	462.96 o
-1	1	1	140.71	98.09	6.93 o
1	1	1	35.99	23.72	2.30 o
3	1	1	2919.29	2934.46	73.96 o
5	1	1	432.91	393.93	22.63 o
-6	2	1	5735.73	5100.09	437.20 o
-4	2	1	10593.14	10861.79	837.43 o
-2	2	1	34117.08	36102.36	1843.94 o
0	2	1	11.91	24.21	5.21 o
2	2	1	25541.32	24441.57	1719.48 o
4	2	1	4492.44	4502.38	213.78 o
6	2	1	9009.76	8129.76	236.09 o
-9	3	1	9343.60	8174.35	586.16 o
-7	3	1	565.66	591.97	35.23 o
-5	3	1	17434.33	17106.24	960.48 o
-3	3	1	16312.62	15275.33	2976.68 o
1	3	1	216.64	84.12	31.18 o
3	3	1	4616.68	4599.22	339.74 o
5	3	1	33842.60	29529.34	2022.58 o
7	3	1	34.41	47.70	17.46 o
-10	4	1	491.22	431.76	40.63 o
-6	4	1	41.41	49.50	13.65 o
-2	4	1	975.67	1041.38	110.55 o
2	4	1	2488.95	2503.61	425.24 o
4	4	1	609.73	675.01	40.13 o
6	4	1	142.29	108.92	31.50 o
-9	5	1	438.18	397.09	37.11 o
-7	5	1	439.43	437.48	20.34 o
-5	5	1	254.77	241.09	13.26 o
5	5	1	793.06	763.02	95.06 o
7	5	1	137.14	129.22	11.65 o
9	5	1	220.21	232.14	28.20 o
-10	6	1	367.50	329.92	18.63 o
-6	6	1	643.20	604.10	34.46 o
-4	6	1	766.29	837.45	71.02 o
4	6	1	156.53	168.68	25.83 o
8	6	1	453.10	401.89	21.02 o
10	6	1	485.94	376.46	69.61 o
-11	7	1	1095.58	1002.01	245.04 o
-9	7	1	2128.95	2013.87	114.08 o
-7	7	1	184.79	210.24	21.35 o
-5	7	1	13532.17	14519.53	2297.81 o
5	7	1	5330.09	5353.02	727.40 o
7	7	1	667.06	666.86	40.23 o
9	7	1	4629.42	4635.95	162.06 o

-10	8	1	286.79	294.05	53.87 o
-8	8	1	2934.75	2709.36	423.45 o
-6	8	1	894.44	968.30	102.51 o
6	8	1	4636.11	5239.88	1376.02 o
8	8	1	670.99	731.36	72.56 o
-9	9	1	174.42	252.53	18.92 o
-4	0	2	24519.18	24056.40	960.48 o
0	0	2	40497.85	40787.26	1314.52 o
2	0	2	17941.68	20005.91	2374.73 o
-5	1	2	258.85	235.40	20.83 o
-3	1	2	627.00	428.71	34.32 o
-1	1	2	1233.00	1315.87	41.25 o
1	1	2	7591.94	8109.90	133.21 o
3	1	2	1996.77	1643.24	387.78 o
5	1	2	496.01	455.74	36.17 o
-8	2	2	436.82	390.85	82.75 o
-6	2	2	1641.28	1680.96	103.18 o
-4	2	2	807.73	885.86	111.76 o
-2	2	2	37.99	42.35	9.18 o
0	2	2	1312.92	1584.04	96.55 o
2	2	2	1265.47	1293.01	82.37 o
4	2	2	1738.85	1567.16	92.10 o
6	2	2	755.43	747.12	72.25 o
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-7	3	2	716.57	750.48	47.81 o
-5	3	2	978.62	988.29	46.35 o
-3	3	2	0.78	243.76	42.22 o
-1	3	2	3931.02	4396.21	286.45 o
1	3	2	1503.41	1660.91	73.46 o
3	3	2	43.81	38.71	11.70 o
5	3	2	1316.12	1346.99	62.40 o
7	3	2	630.50	507.12	83.47 o
-10	4	2	1227.60	1225.39	81.42 o
-8	4	2	437.06	443.02	106.41 o
-6	4	2	1071.94	1019.33	53.94 o
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2	4	2	519.89	518.08	27.75 o
4	4	2	2823.17	2757.02	249.45 o
6	4	2	399.42	333.45	37.39 o
8	4	2	44.89	39.16	22.44 o
-11	5	2	3145.09	2591.85	242.33 o
-9	5	2	1017.31	930.58	58.35 o
-7	5	2	14643.70	14680.16	544.81 o
-5	5	2	1629.75	1623.54	67.51 o
-3	5	2	15971.14	17464.20	3081.79 o
3	5	2	17987.71	17708.09	1665.52 o
5	5	2	207.36	230.41	19.44 o
7	5	2	7251.79	6595.98	202.50 o
9	5	2	1262.31	1108.01	81.85 o
-12	6	2	185.52	208.49	37.48 o
-10	6	2	393.15	415.62	42.34 o
-6	6	2	4044.93	4455.17	476.03 o
-4	6	2	630.05	762.33	215.65 o
4	6	2	1142.31	1119.55	69.66 o

8	6	2	692.04	621.64	38.98 o
10	6	2	1285.52	1246.55	100.28 o
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-5	7	2	338.89	343.71	65.79 o
5	7	2	476.01	457.24	41.96 o
7	7	2	194.29	226.22	33.60 o
9	7	2	59.00	47.67	30.85 o
-10	8	2	755.83	717.85	47.97 o
-8	8	2	720.10	684.39	53.02 o
6	8	2	1127.06	1105.01	100.92 o
8	8	2	183.90	135.98	36.34 o
7	9	2	651.96	719.04	149.82 o
-7	1	3	1397.22	1321.92	109.22 o
-5	1	3	1682.40	1636.51	66.20 o
-3	1	3	2064.07	2204.61	69.38 o
1	1	3	39.45	34.45	10.10 o
3	1	3	353.76	447.80	59.72 o
-8	2	3	7974.59	7045.93	850.52 o
-6	2	3	1094.74	1071.89	62.17 o
-4	2	3	2933.67	2981.80	83.10 o
-2	2	3	25729.35	25018.48	562.48 o
0	2	3	911.00	979.61	46.49 o
2	2	3	9393.56	9447.62	163.73 o
4	2	3	626.77	674.47	56.61 o
6	2	3	7732.90	7827.31	192.74 o
-9	3	3	8913.44	8311.42	320.60 o
-5	3	3	9070.36	9274.62	489.76 o
-3	3	3	2145.86	2270.39	156.32 o
-1	3	3	20230.18	20575.54	408.76 o
1	3	3	2523.76	2630.26	83.44 o
3	3	3	254.75	296.05	22.26 o
5	3	3	11256.19	10578.80	461.86 o
7	3	3	745.38	774.52	55.15 o
-8	4	3	674.21	663.18	49.54 o
-6	4	3	711.59	703.58	69.00 o
-4	4	3	284.25	298.37	15.75 o
-2	4	3	3487.16	3704.91	490.41 o
0	4	3	1410.52	1424.55	124.10 o
2	4	3	210.62	209.36	22.88 o
4	4	3	523.19	482.13	30.09 o
6	4	3	586.91	506.45	20.69 o
-11	5	3	245.90	274.08	40.88 o
-9	5	3	12.83	16.85	10.84 o
-5	5	3	2700.17	2652.67	242.39 o
1	5	3	1710.67	1728.70	78.58 o
3	5	3	327.83	340.29	22.10 o
7	5	3	54.22	66.94	24.05 o
9	5	3	833.58	774.41	175.38 o
-10	6	3	455.44	454.36	23.53 o
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-6	6	3	102.19	90.20	22.33 o
2	6	3	122.00	182.24	35.71 o
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-9	7	3	4153.98	3936.58	735.95 o

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-8	8	3	2493.66	2628.52	603.17 o
6	8	3	3155.38	3314.47	517.95 o
-6	0	4	14932.13	13944.88	1489.95 o
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-2	0	4	436.62	29252.48	37948.35 o
0	0	4	16341.14	16948.34	521.20 o
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-1	1	4	1184.26	1164.08	89.01 o
1	1	4	779.94	770.37	60.50 o
3	1	4	4674.35	4404.14	134.79 o
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-2	2	4	107.20	117.69	9.39 o
0	2	4	1176.53	1126.82	68.24 o
2	2	4	2366.54	2430.28	327.64 o
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-3	3	4	665.01	705.45	89.06 o
-1	3	4	243.74	278.80	32.96 o
1	3	4	208.99	212.29	13.25 o
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5	3	4	310.24	368.94	30.00 o
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0	4	4	1647.82	1706.02	88.16 o
2	4	4	97.63	101.55	23.70 o
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-9	5	4	399.47	327.72	97.46 o
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-5	5	4	1153.94	1182.08	203.47 o
1	5	4	5748.84	5851.71	162.36 o
3	5	4	6105.49	6376.10	188.55 o
5	5	4	1080.02	1135.50	83.63 o
7	5	4	5260.21	5029.73	353.61 o
-10	6	4	1466.05	1509.96	120.46 o
-8	6	4	680.20	710.37	56.19 o
-6	6	4	1720.90	2037.36	137.45 o
2	6	4	56.78	63.10	28.49 o
4	6	4	3935.07	3897.76	147.15 o
6	6	4	414.68	386.12	36.72 o
-9	7	4	170.41	140.06	27.78 o
-7	7	4	672.00	721.83	58.18 o
3	7	4	71.45	71.91	34.40 o
-7	1	5	999.65	953.12	109.15 o
-5	1	5	381.22	408.85	23.16 o
-3	1	5	617.89	700.26	54.40 o
1	1	5	166.48	193.66	23.81 o

3	1	5	12.75	19.97	21.02 o
-8	2	5	6478.48	6665.58	344.47 o
-6	2	5	1327.21	1244.90	74.26 o
-4	2	5	1227.72	1183.98	81.11 o
-2	2	5	5689.15	5751.74	183.69 o
0	2	5	1124.75	1160.84	103.43 o
2	2	5	7846.99	8339.98	830.95 o
-9	3	5	6124.45	6238.21	493.44 o
-7	3	5	807.84	766.27	57.71 o
-5	3	5	3874.66	4028.47	126.07 o
-1	3	5	11792.49	10967.47	1609.91 o
1	3	5	1856.06	1953.75	173.18 o
3	3	5	272.17	317.33	32.47 o
5	3	5	3487.58	3420.77	151.49 o
-10	4	5	523.93	482.72	26.67 o
-8	4	5	393.26	490.94	32.08 o
-4	4	5	120.44	151.10	13.73 o
0	4	5	183.09	192.29	15.08 o
2	4	5	1003.91	949.30	87.31 o
4	4	5	1324.22	1421.57	96.78 o
-9	5	5	296.51	315.58	18.53 o
-5	5	5	307.75	341.98	45.37 o
3	5	5	354.63	369.17	29.57 o
5	5	5	333.40	331.65	27.23 o
-6	6	5	667.16	714.50	163.99 o
4	6	5	275.81	293.34	21.91 o
-6	0	6	3291.97	3262.87	260.31 o
-4	0	6	8643.74	9516.96	232.47 o
-2	0	6	1946.18	2050.98	278.47 o
0	0	6	2772.71	3128.29	132.78 o
-7	1	6	1749.70	1762.52	112.98 o
-5	1	6	200.80	233.26	19.72 o
-3	1	6	2535.41	2490.89	187.33 o
1	1	6	397.48	420.27	24.36 o
-8	2	6	436.68	464.24	25.08 o
-2	2	6	278.21	334.22	29.87 o
2	2	6	185.68	260.38	34.22 o
-9	3	6	275.68	226.80	76.94 o
-7	3	6	429.17	465.11	24.92 o
-5	3	6	224.14	243.02	15.56 o
-1	3	6	950.91	1100.65	73.50 o
1	3	6	233.71	267.92	52.93 o
-6	4	6	987.41	1172.56	160.13 o
0	4	6	2043.43	1932.39	294.85 o
2	4	6	342.88	349.01	21.33 o
-7	5	6	2760.97	2768.32	306.22 o
-5	5	6	741.54	790.03	99.87 o
1	5	6	2206.33	2216.22	115.99 o
-5	1	7	109.82	110.43	16.49 o
-3	1	7	397.12	419.47	55.73 o
-6	2	7	679.43	672.97	40.29 o
-4	2	7	1164.38	1307.02	101.50 o
-2	2	7	1807.26	1728.24	121.23 o
-5	3	7	4753.84	5294.84	399.46 o

