

```
#
# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag
#
data_camp6
_shelx_title ' CaMnSi2O6 data collection in DAC by Xcaliber-I at VT'
_shelx_refl_list_code      4
_shelx_F_calc_maximum     201.94
_exptl_crystal_F_000      484.00
_reflns_d_resolution_high  0.7112
```

```
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  9.7785
_cell_length_b  8.9430
_cell_length_c  5.1803
_cell_angle_alpha 90.000
_cell_angle_beta  104.084
_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   1216.03   1191.53   48.15 o
  3  1  0   12628.29   12163.75   753.01 o
  2  2  0   2580.37   2820.26   308.15 o
  1  3  0    118.56    130.25    36.32 o
  3  3  0   3620.60   3971.56   183.17 o
  5  3  0   1755.18   1761.62   101.28 o
  2  4  0    88.26    126.33    36.40 o
  4  4  0   6847.79   7029.79   141.57 o
  3  5  0   9838.27  10623.87   1334.37 o
  5  5  0    284.96    567.99    77.94 o
  7  5  0  20482.09  20500.07   503.45 o
  9  5  0   1086.21   1187.20   235.45 o
  4  6  0    891.42    972.10   105.14 o
  6  6  0    313.88    339.88    25.78 o
  8  6  0    862.66    909.73    60.83 o
```

10	6	0	1827.76	2077.23	333.18 o
5	7	0	791.90	764.77	183.03 o
7	7	0	1195.01	1264.74	78.22 o
9	7	0	165.71	160.22	36.52 o
11	7	0	33.08	34.62	38.88 o
6	8	0	294.07	358.95	52.61 o
8	8	0	172.57	171.08	39.77 o
10	8	0	898.43	931.11	48.48 o
7	9	0	1022.27	1262.79	526.55 o
-5	1	1	1005.24	911.76	45.77 o
-3	1	1	4069.01	4382.67	83.08 o
-1	1	1	158.23	110.85	6.12 o
3	1	1	2929.92	2985.49	323.93 o
-6	2	1	5574.65	5366.82	132.50 o
-4	2	1	10760.22	11358.82	199.76 o
-2	2	1	34316.41	35237.94	830.78 o
0	2	1	15.06	25.44	6.19 o
2	2	1	25432.72	23781.56	475.40 o
4	2	1	4558.80	4382.73	581.37 o
6	2	1	9065.65	8113.82	822.67 o
-7	3	1	539.90	509.85	29.14 o
-5	3	1	17563.80	17725.68	417.31 o
-3	3	1	16438.52	17964.31	1187.64 o
1	3	1	227.51	112.38	18.93 o
3	3	1	4797.73	4775.86	176.47 o
5	3	1	34212.73	33199.73	2012.23 o
-4	4	1	19.90	26.70	14.34 o
-2	4	1	977.03	1026.33	199.66 o
2	4	1	2568.39	2501.68	140.95 o
4	4	1	675.55	662.35	43.68 o
6	4	1	158.91	136.44	15.56 o
8	4	1	111.82	89.13	41.81 o
-9	5	1	415.57	392.67	42.07 o
-7	5	1	399.76	381.75	79.50 o
-5	5	1	240.40	245.77	31.10 o
3	5	1	30.13	46.31	19.34 o
5	5	1	806.83	759.63	164.36 o
7	5	1	95.59	102.46	26.51 o
-10	6	1	395.94	341.45	47.65 o
-8	6	1	1.02	29.10	25.66 o
-6	6	1	587.27	632.27	110.75 o
-4	6	1	815.53	965.00	180.38 o
4	6	1	152.70	269.11	56.39 o
8	6	1	440.49	411.59	47.82 o
10	6	1	444.96	408.10	70.80 o
-11	7	1	1178.69	933.81	172.63 o
-9	7	1	2182.86	2262.86	236.13 o
-7	7	1	167.17	196.37	37.42 o
-5	7	1	13474.12	14615.78	3525.05 o
5	7	1	5358.28	5372.26	750.90 o
7	7	1	715.17	738.42	39.20 o
9	7	1	4521.34	4579.20	226.21 o
-10	8	1	318.21	256.38	55.04 o
-8	8	1	3068.77	3073.32	373.83 o

-6	8	1	933.32	975.80	66.29 o
6	8	1	4749.21	5283.56	1256.50 o
8	8	1	677.82	663.40	137.62 o
-9	9	1	205.91	275.80	20.80 o
7	9	1	824.61	839.35	91.63 o
-4	0	2	24429.86	24781.53	385.72 o
-2	0	2	16.55	50.76	9.89 o
0	0	2	40778.95	39620.70	5232.36 o
2	0	2	18012.79	18165.53	2527.27 o
-5	1	2	204.81	198.85	12.40 o
-1	1	2	1198.11	1146.43	40.15 o
1	1	2	7573.50	7247.57	562.36 o
3	1	2	2033.52	1736.85	160.22 o
-8	2	2	416.82	378.02	60.77 o
-6	2	2	1720.86	1763.15	71.97 o
-4	2	2	794.14	933.84	54.99 o
-2	2	2	43.04	27.58	13.19 o
0	2	2	1359.35	1636.89	68.82 o
2	2	2	1256.95	1262.71	96.92 o
4	2	2	1717.11	1465.60	62.03 o
6	2	2	818.43	697.98	123.10 o
-9	3	2	310.87	290.61	15.93 o
-7	3	2	725.79	661.23	38.56 o
-5	3	2	1004.99	992.54	54.93 o
-3	3	2	4.44	89.67	41.30 o
-1	3	2	3761.35	3798.14	87.05 o
1	3	2	1515.47	1599.72	78.10 o
3	3	2	46.86	26.93	16.12 o
5	3	2	1271.67	1110.38	71.52 o
7	3	2	612.12	503.19	64.25 o
-10	4	2	1201.28	1238.51	68.71 o
-8	4	2	391.09	388.14	21.71 o
-6	4	2	1124.82	1106.24	106.84 o
-4	4	2	562.37	606.51	99.56 o
0	4	2	8769.02	8809.05	409.23 o
2	4	2	502.07	502.25	30.56 o
4	4	2	2857.89	2618.68	132.00 o
6	4	2	392.30	347.07	31.76 o
-11	5	2	3103.34	2718.44	402.30 o
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-7	5	2	15015.84	15179.90	368.68 o
-5	5	2	1695.41	1766.00	77.74 o
-3	5	2	15931.35	17431.50	3958.47 o
1	5	2	11652.19	11831.85	725.49 o
3	5	2	18146.75	17617.71	925.52 o
5	5	2	184.60	216.01	15.39 o
7	5	2	7458.14	6677.67	554.94 o
9	5	2	1365.37	1216.01	73.88 o
-10	6	2	424.73	445.51	131.03 o
-8	6	2	108.67	154.18	32.83 o
-6	6	2	4254.90	4535.46	400.24 o
-4	6	2	693.40	740.43	82.48 o
2	6	2	90.43	110.64	42.48 o
4	6	2	1221.08	1229.17	73.79 o

8	6	2	717.25	655.30	47.64 o
-9	7	2	108.30	96.80	16.49 o
-7	7	2	643.97	679.85	78.26 o
-5	7	2	426.94	408.54	77.12 o
3	7	2	761.15	685.11	38.34 o
5	7	2	526.18	469.00	49.30 o
7	7	2	199.46	214.09	17.46 o
9	7	2	76.65	52.88	25.62 o
-10	8	2	761.40	674.60	161.00 o
-8	8	2	654.25	711.88	89.66 o
4	8	2	1140.20	1162.18	259.90 o
6	8	2	1039.17	1072.58	192.38 o
8	8	2	162.44	134.13	39.04 o
7	9	2	600.49	745.36	89.43 o
-7	1	3	1365.91	1344.96	68.76 o
-5	1	3	1665.33	1674.09	68.04 o
-3	1	3	2115.35	2042.13	177.68 o
-1	1	3	6.70	12.66	13.87 o
1	1	3	49.17	38.95	14.44 o
3	1	3	376.02	456.87	23.42 o
-8	2	3	8214.44	7164.85	917.34 o
-6	2	3	1083.03	1017.53	96.23 o
-4	2	3	2854.69	3015.77	85.05 o
-2	2	3	25974.09	25032.30	1875.78 o
0	2	3	936.37	975.44	110.98 o
2	2	3	9317.51	9061.99	769.99 o
4	2	3	642.70	696.18	92.11 o
-9	3	3	9207.05	8979.99	227.13 o
-5	3	3	9226.78	9522.63	333.40 o
-3	3	3	2239.92	2345.02	147.70 o
-1	3	3	20422.91	19261.69	1839.39 o
1	3	3	2554.40	2607.24	149.34 o
3	3	3	272.64	311.78	11.94 o
5	3	3	11520.05	10861.93	849.56 o
-10	4	3	223.32	210.79	41.27 o
-8	4	3	727.91	745.76	82.35 o
-6	4	3	686.55	612.58	48.19 o
-4	4	3	310.22	316.92	33.59 o
-2	4	3	3500.00	3584.05	775.05 o
0	4	3	1425.67	1365.80	72.97 o
2	4	3	239.66	174.62	32.97 o
4	4	3	540.57	499.53	60.88 o
6	4	3	583.24	511.49	24.95 o
-11	5	3	244.57	242.92	21.25 o
-5	5	3	2686.93	2857.64	235.47 o
-3	5	3	110.42	150.49	32.43 o
1	5	3	1661.57	1430.34	84.15 o
3	5	3	262.36	274.59	14.47 o
-10	6	3	416.27	371.24	24.37 o
-8	6	3	166.82	115.94	39.73 o
2	6	3	126.72	218.27	39.06 o
4	6	3	1343.97	1272.47	82.20 o
-11	7	3	1021.95	1114.52	140.61 o
-9	7	3	4183.91	4095.78	419.25 o

-7	7	3	130.03	111.61	31.42 o
3	7	3	869.27	890.30	59.37 o
5	7	3	5225.45	5027.50	300.52 o
7	7	3	187.73	190.55	22.35 o
-10	8	3	280.43	306.66	58.55 o
-8	8	3	2664.87	2706.84	503.72 o
6	8	3	3436.33	3376.87	333.19 o
-6	0	4	15394.08	15087.32	1189.91 o
-4	0	4	11028.44	10610.28	1379.12 o
-2	0	4	410.05	415.66	23.84 o
0	0	4	16537.78	16486.54	2417.79 o
2	0	4	2018.27	2232.62	259.00 o
-7	1	4	1904.74	1853.83	151.83 o
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-1	1	4	1163.72	1110.95	144.09 o
1	1	4	787.04	705.41	67.01 o
3	1	4	4737.74	4071.15	1326.18 o
-4	2	4	1030.58	1038.40	106.11 o
-2	2	4	118.00	128.43	10.86 o
0	2	4	1132.87	1024.75	175.65 o
2	2	4	2445.46	2337.73	254.89 o
-9	3	4	638.15	532.99	82.73 o
-5	3	4	1000.60	1071.16	64.60 o
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-1	3	4	217.14	205.10	16.53 o
1	3	4	205.67	194.67	45.80 o
3	3	4	750.88	762.91	50.30 o
5	3	4	273.71	335.26	35.14 o
-10	4	4	1828.47	1847.00	183.95 o
-6	4	4	538.64	531.15	28.79 o
-4	4	4	1541.01	1598.71	198.60 o
0	4	4	1576.94	1442.30	80.83 o
2	4	4	98.02	147.52	32.11 o
4	4	4	3054.27	2901.62	246.82 o
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-9	5	4	369.06	247.16	38.65 o
-7	5	4	11214.46	10152.79	1891.58 o
-5	5	4	1285.90	1313.88	181.56 o
1	5	4	5845.17	5749.59	203.09 o
3	5	4	6335.06	6482.66	240.16 o
5	5	4	1108.23	1216.61	177.30 o
7	5	4	5249.21	4930.72	421.16 o
-10	6	4	1546.52	1656.29	106.78 o
-8	6	4	658.06	807.79	104.20 o
-6	6	4	1808.92	1975.28	266.69 o
4	6	4	4036.93	3974.85	343.83 o
6	6	4	400.05	393.99	38.16 o
-9	7	4	196.32	174.96	41.01 o
-7	7	4	673.18	808.42	109.51 o
5	7	4	68.53	95.83	54.40 o
-8	8	4	758.90	898.29	104.24 o
4	8	4	454.29	503.65	27.92 o
-7	1	5	947.99	940.01	53.36 o
-5	1	5	401.50	441.36	60.77 o

-3	1	5	653.21	648.36	58.57 o
-1	1	5	32.41	247.98	36.42 o
1	1	5	143.99	187.38	33.38 o
-8	2	5	6627.44	6822.50	198.99 o
-6	2	5	1356.30	1264.65	87.79 o
-4	2	5	1227.79	1240.26	192.32 o
-2	2	5	5705.06	5918.19	969.88 o
0	2	5	1165.11	1293.07	81.90 o
2	2	5	7920.70	7815.40	1011.66 o
-9	3	5	6311.94	6662.48	187.43 o
-7	3	5	873.06	826.68	107.83 o
-5	3	5	3927.17	4143.36	584.57 o
-3	3	5	7.23	41.93	28.67 o
-1	3	5	12096.17	10855.19	736.78 o
1	3	5	1882.02	1995.13	200.10 o
3	3	5	287.27	313.52	33.86 o
5	3	5	3609.14	3664.37	231.87 o
-10	4	5	518.17	516.05	129.94 o
-8	4	5	402.54	501.03	63.01 o
-6	4	5	37.28	84.12	60.16 o
-4	4	5	108.28	139.80	31.26 o
0	4	5	194.12	195.78	35.15 o
2	4	5	1067.88	910.03	143.19 o
4	4	5	1353.94	1469.70	92.86 o
-9	5	5	278.78	331.62	49.36 o
-5	5	5	305.07	317.44	21.53 o
-1	5	5	141.00	103.52	34.30 o
3	5	5	331.19	349.31	53.55 o
5	5	5	304.23	322.30	30.87 o
-8	6	5	66.83	99.15	41.46 o
-6	6	5	633.71	681.15	50.35 o
4	6	5	251.86	239.01	20.31 o
3	7	5	1064.58	983.47	82.38 o
-6	0	6	3289.88	3158.17	505.31 o
-4	0	6	8781.94	8851.98	1478.64 o
-2	0	6	2002.42	1865.73	105.28 o
0	0	6	2821.28	3072.89	724.57 o
-7	1	6	1783.40	1819.66	157.95 o
-5	1	6	187.62	233.78	16.71 o
-3	1	6	2604.36	2555.72	315.73 o
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-8	2	6	419.02	484.63	81.46 o
-2	2	6	251.16	271.12	39.16 o
2	2	6	215.98	282.25	61.08 o
-9	3	6	237.85	237.78	26.59 o
-7	3	6	421.40	447.23	23.05 o
-5	3	6	229.81	186.76	19.31 o
-3	3	6	0.32	85.54	34.22 o
-1	3	6	897.63	963.82	129.25 o
1	3	6	225.15	244.39	23.14 o
-6	4	6	981.19	1148.55	127.27 o
0	4	6	2036.60	2055.45	159.73 o
2	4	6	361.13	368.16	77.18 o
-7	5	6	2760.67	2903.70	268.64 o

-1	5	6	214.66	249.81	19.78 o
1	5	6	2217.88	2215.69	118.21 o
-5	1	7	132.45	156.71	18.99 o
-3	1	7	396.00	429.48	49.29 o
-6	2	7	723.53	706.77	124.84 o
-4	2	7	1183.65	1218.86	122.74 o
-2	2	7	1806.78	1967.51	406.58 o
-5	3	7	4907.87	5058.31	1387.33 o
-3	3	7	216.32	270.01	56.48 o